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TESIS DOCTORAL
**DESARROLLO DE BASES DE DATOS DE
MASAS EXACTAS DE IONES PARA EL
CONTROL EXHAUSTIVO Y AUTOMATIZADO DE
CONTAMINANTES EN ALIMENTOS MEDIANTE
CROMATOGRAFÍA DE LÍQUIDOS-
ESPECTROMETRÍA DE MASAS DE ALTA
RESOLUCIÓN**

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Desarrollo de bases de datos de masas exactas de iones para el control exhaustivo y automatizado de contaminantes en alimentos mediante cromatografía de líquidos-espectrometría de masas de alta resolución.

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Tesis presentada para aspirar al grado de Doctor por la Universidad de Jaén
con Mención de Doctorado Internacional

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Jaén, 12 de febrero de 2015



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INFORMAN:

Que la Tesis Doctoral titulada “Desarrollo de bases de datos de masas exactas de iones para el control exhaustivo y automatizado de contaminantes en alimentos mediante cromatografía de líquidos-espectrometría de masas de alta resolución”, presentada por Dña. Patricia Pérez Ortega, ha sido desarrollada bajo nuestra dirección y autorizamos su presentación y defensa para optar al grado de Doctor por la Universidad de Jaén, con Mención de Doctorado Internacional.

En Jaén, a 12 de febrero de 2015

Dr. D. Juan Francisco García Reyes

Dr. D. Antonio Molina Díaz

Esta Tesis Doctoral ha sido realizada y, consecuentemente, será defendida con el propósito de optar al título de Doctor por la Universidad de Jaén con Mención de Doctorado Internacional.

Con anterioridad a su defensa, este trabajo ha sido evaluado por tres evaluadores extranjeros independientes Dr. László Abrankó (School of Food Science and Nutrition, University of Leeds, Reino Unido), Prof. Mihaly Dernovics (Faculty of Food Science, Corvinus University of Budapest, Hungría) y Prof. Joachim Franzke (Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V, Dortmund, Alemania).

A mi marido

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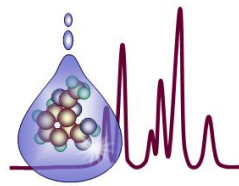
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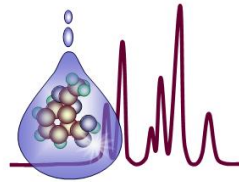
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Resumen

RESUMEN

Como el número total de pesticidas y otros contaminantes orgánicos susceptibles de ser encontrados en alimentos de origen vegetal y animal es cada vez mayor, los laboratorios oficiales de análisis necesitan usar métodos multiresiduo que permitan su determinación simultánea de forma eficaz. Actualmente los métodos que se emplean cubren una lista de entre 100 y 150 compuestos, generalmente los más utilizados o aquellos detectados con mayor frecuencia. Esto implica que existe una gran cantidad de contaminantes a los que no se presta suficiente atención ni control. La técnica habitual que se suele emplear es la cromatografía de líquidos con espectrometría de masas en tándem (LC-MS/MS) en modo de monitorización simultánea de transiciones MS/MS (MRM), que dependiendo de la instrumentación que se utilice permiten la inclusión de entre 100 y 300 compuestos en un método, en base al tiempo dedicado a cada transición y el número de coeluciones. La principal desventaja de esta metodología es que sólo se centra en los compuestos incluidos en el método, para los cuales se conoce el tiempo de retención y las condiciones instrumentales (MS/MS) óptimas, quedando excluidos del análisis compuestos desconocidos o no incluidos inicialmente en el método además de otras especies derivadas de interés como posibles productos de degradación o metabolitos. Esto pone de manifiesto la necesidad de desarrollar métodos de *screening* que incluyan un mayor número de analitos y que proporcionen flexibilidad para el análisis de forma retrospectiva de compuestos no incluidos en el método desarrollado.

Por ello, como alternativa al empleo de LC-MS/MS, en los últimos años se está examinando e introduciendo el uso de cromatografía de líquidos/espectrometría de masas de alta resolución (LC-HRMS). El uso de espectrómetros de masas de alta resolución, como el analizador de tiempo de vuelo (TOF), proporcionan elevada exactitud de masas y gran poder de

resolución en modo *full scan*, permitiendo el seguimiento de, en teoría, un número ilimitado de contaminantes orgánicos. Esta metodología es apropiada para el desarrollo de bases de datos de masa exacta, que son muy específicas y a la vez universales, de forma que pueden ser transferidas fácilmente de unos laboratorios a otros.

Esta Tesis Doctoral se centra en el empleo de la cromatografía de líquidos-espectrometría de masas de alta resolución para el desarrollo de bases de datos de masas exactas, que permitan el control exhaustivo y automatizado de contaminantes orgánicos de distintas categorías en muestras reales de alimentos. El trabajo se puede dividir en dos bloques fundamentales:

- 1.- Desarrollo de una base de datos de masa exacta empleando valores de tiempo de retención y masa exacta para más de 600 contaminantes orgánicos susceptibles de ser detectados en muestras de alimentos.
- 2.- Aplicación de la base de datos para el desarrollo de métodos de *screening* y posterior aplicación en muestras de alimentos.

La memoria está organizada en cuatro apartados principales (**III.1 al III.4**) que se corresponden con artículos científicos de investigación, que están publicados o pendientes de publicación.

En el primer trabajo (**sección III.1**) se ha desarrollado un estudio sobre la viabilidad de este tipo de métodos, examinando en detalle las principales fortalezas y limitaciones que presentan. Para ello, se ha puesto a punto una base de datos que incluyen datos de más de 625 contaminantes orgánicos (426 pesticidas, 117 productos veterinarios, 42 residuos de envases alimentarios, 21 micotoxinas, 10 compuestos perfluorados, 9 nitrosaminas y 5 edulcorantes). Los aspectos más relevantes que se han estudiado han sido

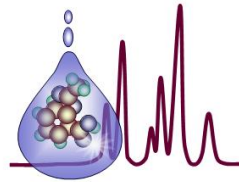
la separación cromatográfica y la necesidad de la misma, la selectividad global del método y aspectos relacionados con análisis cualitativo y cuantitativo empleando la base de datos, incluyendo la capacidad de confirmación que proporciona la espectrometría de masas de alta resolución, los parámetros de búsqueda automática de los compuestos, los modos de adquisición más apropiados para el tipo de aplicación teniendo en cuenta la fragmentación y aspectos prácticos como efectos de supresión de señal (efectos matriz) entre analitos.

En el segundo trabajo (**sección III.2**) se ha desarrollado un método de *screening* empleando cromatografía de líquidos de ultra-elevada resolución (UHPLC) y espectrometría de masas de alta resolución para la detección de más de 625 contaminantes orgánicos de distintas familias en alimentos empleando UHPLC acoplada a espectrometría de masas con analizador de tiempo-de-vuelo (UHPLC-(Q)TOFMS). La separación de los analitos se llevó a cabo empleando un sistema UHPLC con una columna C₁₈ (2.1 x 50 mm, 1.8 µm de tamaño de partícula). Se ensayaron diferentes gradientes de elución empleando agua con 0.1 % de ácido fórmico y acetonitrilo con 0.1 % de ácido fórmico como fases móviles. El método final seleccionado (gradiente de 10 minutos) permitía una separación adecuada de los analitos en un tiempo corto. La identificación de los compuestos se llevó a cabo mediante medidas de masas exactas de los iones característicos de cada analito (principalmente molécula (de)protonada, e información de tiempo de retención junto con la fragmentación característica para cada especie, todo ello llevado a cabo de forma automatizada a través de un programa específico. El método propuesto permite la detección de la mayoría de los compuestos estudiados a niveles de concentración muy bajos, del orden de 1 a 10 µg Kg⁻¹. Para una caracterización completa del rendimiento del método, se llevó a cabo el estudio de los límites de cuantificación de los compuestos estudiados, y para

el caso particular de los pesticidas, se estudiaron tres matrices representativas (tomate, naranja y productos infantiles combinando verduras y carne).

En el tercer trabajo (**sección III.3**) se detalla el desarrollo de un tratamiento de muestra genérico para la determinación simultánea de 60 pesticidas y 9 micotoxinas en vino mediante cromatografía de líquidos-espectrometría de masas con analizador de tiempo de vuelo. La extracción en fase sólida (SPE) fue la técnica de preparación de muestra empleada para la realización de este estudio. Se emplearon inicialmente dos cartuchos de tipo polimérico, Oasis HLB® y Plexa®, y en base al menor efecto matriz se seleccionó el primero de los cartuchos mencionados. Los estudios de recuperación realizados a dos niveles de concentración (2.5 y 25 $\mu\text{g L}^{-1}$) concluyeron que para el 90% de los compuestos el valor de porcentaje de recuperación era entre un 70 y un 120%. Finalmente, el método fue aplicado a 24 muestras nacionales de vino, detectándose metalaxyl (pesticida) y aflatoxina B₂ (micotoxina) en el 50 y 75% de ellas, respectivamente.

En el cuarto trabajo (**sección III.4**) se desarrolló un método para la determinación de 355 pesticidas en mermeladas mediante UHPLC-TOFMS. Se construyó una base de datos con valores de tiempo de retención y masa exacta, incluyéndolos en un archivo compatible con el software empleado para la búsqueda de los compuestos en las muestras a analizar. Las muestras fueron sometidas a un tratamiento de muestra genérico (QuEChERS). La base de datos y el método desarrollado fueron aplicados a 54 muestras de mermelada obtenidas a base de fruta. Los resultados obtenidos mostraron que en todas las muestras el contenido de los pesticidas detectados era inferior a sus MRLs excepto en una de ellas.



Summary

SUMMARY

The determination of residues from pesticides and other organic contaminants in foods is of great interest for the protection of human health, and is thoroughly controlled worldwide with a plethora of regulations. Nowadays, for the examination of pesticides and other organic contaminants in food, official laboratories rely on targeting a list of priority substances, typically those more often detected or more widely used. A list of around 100-150 of LC and GC-amenable compounds is usually examined. The more common approach used is liquid chromatography-tandem mass spectrometry (LC-MS/MS) operated in the multiple reaction monitoring (MRM) mode, which offers excellent quantitative performance for typically from 100 to 300 compounds (depending on the instrument scan speed/dwell-time) using a carefully optimized acquisition method. However, one of the main weaknesses of this approach is the previous knowledge of both retention time and optimized MS/MS transition conditions of each analyte sought, required to set-up the acquisition method. MS/MS MRM methods lack the flexibility of full-scan acquisition methods for instance in terms of analyte scope modification. Consequently, LC-MS/MS multi-residue methods are blind to compounds not defined in the MRM method (*non-targeted* analysis), so that none or scarce information on possible non-target or unknown pesticides or their degradation products are available when using these techniques.

Liquid chromatography high-resolution mass spectrometry (LC-HRMS) instruments enable the development of databases of accurate masses of ions, which are universal and reproducible (regardless the high resolution instrument used) unlike the fragmentation libraries attempted with MS/MS instruments (not reproducible within instruments from different manufacturers). This PhD Thesis deals with the evaluation of LC- HRMS using

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time-of-flight instrumentation for the development of a universal methodology for the screening of multiple classes of organic contaminants that must be controlled in foods of plant origin (fruits and vegetables), animal origin (milk, eggs, honey, etc.) or derivative products (for instance drinks (juices, wine, beer, soft drinks, etc)).

The aims of the PhD Thesis are as follows:

1. To develop a database of accurate masses of ions from organic contaminants for the comprehensive screening of over 600 compounds relevant in the field of food safety.
2. To evaluate and to demonstrate the usefulness of the proposed automated screening method for the control of organic contaminants in real market-purchased food samples.

The PhD Thesis comprises 4 research articles:

In article 1 (section III.1), the feasibility of LC-HRMS accurate-mass screening methods has been examined using as case study the determination of over 625 multiclass food contaminants. Compelling aspects such as chromatographic separation and the selectivity and confirmation capability provided by HRMS with different acquisition modes (full-scan or full-scan combined with collision induced dissociation (CID) with no precursor ion isolation), along with caveats such as sensitivity or automated data processing are examined and discussed. In-source CID fragmentation was evaluated in depth, although in terms of fragmentation information were not as thorough as those obtained using CID MS/MS experiments without precursor ion isolation (*all ion mode*). This acquisition mode is definitely the best suited for this type of large-scale screening method instead of classic

SUMMARY

product ion scan, as provides excellent fragmentation information for confirmatory purposes for an unlimited number of compounds.

Article 2 (section III.2), addresses the development of an accurate-mass multi-residue screening method using liquid chromatography high-resolution mass spectrometry for the determination of over 625 multiclass food contaminants in different matrices using Ultrahigh performance Liquid Chromatography-(Quadrupole) Time-of-Flight Mass Spectrometry (UHPLC-(Q)TOFMS). The compounds included in the study were 426 pesticides, 117 veterinary drugs, 42 food packaging contaminants, 21 mycotoxins, 10 perfluorinated compounds, 9 nitrosamines and 5 sweeteners. The separation of the targeted compounds was carried out by liquid chromatography using a C₁₈ column (50 mm x 2.1 mm and 1.8 µm particle size). The performance of the screening method was examined in terms of linearity, matrix effect and limits of quantification (LOQs) for three representative food matrixes (tomato, orange and baby food) using a generic sample treatment (QuEChERS). Most of compounds showed limits of quantification from 1 to 10 µg Kg⁻¹. The overall method performance was satisfactory with limits of quantification lower than 10 µg Kg⁻¹ for the 44% of studied compounds. Matrix effects occurring were also examined. Orange was the matrix which produced limits of quantification > 100 µg Kg⁻¹ more frequently. Signal suppression was the most common effect produced. In general, orange was the matrix which produced the highest matrix effect, and baby food, the lowest.

Article 3 (section III.3) describes a generic sample treatment method for simultaneous determination of multiclass pesticides and mycotoxins in liquid food matrices such as wines. The proposed method is based on solid-phase extraction (SPE) using polymeric-type SPE cartridges. A LC-TOFMS method including 60 representative pesticides and 9 mycotoxins was used to

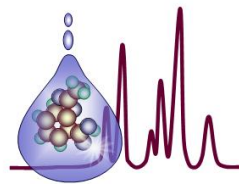
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evaluate the proposed sample treatment. Two different polymeric sorbents were evaluated, being hydrophilic-lipophilic-balanced (HLB) polymer cartridges selected (OasisTM HLB) as the most suitable for the present study. Limits of detection were below $1 \mu\text{g L}^{-1}$ for the 87% of the studied compounds. With the selected 4:1 preconcentration factor, 70% of the target compounds showed relatively low matrix effects, corresponding to signal suppressions lower than 30%. Recovery studies ($n = 10$) were carried out at two concentration levels, $2.5 \mu\text{g L}^{-1}$ and $25 \mu\text{g L}^{-1}$, obtaining mean recovery rates between 70 and 120% for the 90% of studied analytes. The relative standard deviation (RSD%) values of the entire procedure were below 15% in most cases (97% of the studied analytes). The proposed method was successfully applied to different red wine samples produced in different regions of Spain.

Finally, in article 4 (section III.4), an ultra-high performance liquid chromatography-time-of-flight mass spectrometry (UHPLC-TOFMS) multi-residue method was developed and applied to the determination of over 350 multiclass pesticides in jams in different market samples. Prior to analysis, a simple sample extraction step based on liquid partitioning with acetonitrile and a cleanup step with dispersive solid-phase extraction (QuEChERS) was implemented. The identification and confirmation of the compounds was based on retention time and the accurate mass measurements of the protonated molecules ($[\text{M}+\text{H}]^+$). Screening method limits of detection were below $10 \mu\text{g Kg}^{-1}$ for 90% of the studied compounds. The proposed method was successfully applied to 54 market-purchased jams samples. The concentration levels of the target compounds found in the studied samples were in compliance with the current regulations with the exception of a sample (M23). The relatively low concentration levels detected suggest that part of the pesticide residues in the actual fruits used to prepare the

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derivative product eventually have been partially abated during processing stages.



Introducción y Antecedentes

I. INTRODUCCIÓN Y ANTECEDENTES

I.1. Seguridad alimentaria

En la sociedad actual, la calidad y seguridad de los alimentos es un tema de amplio interés para consumidores, productores, autoridades sanitarias y gubernamentales. Hoy en día es fácil adquirir productos e ingredientes de cualquier parte del mundo, lo cual aumenta las fuentes de contaminación que puedan afectar a la calidad de los alimentos a lo largo de la cadena alimentaria. Este hecho, junto con los casos publicados de incidentes ocurridos a nivel mundial como la presencia de melamina en leche en polvo, vertidos de petróleo en agua o la presencia de pesticidas en bebidas, entre otros, hacen que el estudio de la presencia de contaminantes en alimentos sea cada vez más necesario [1].

La *seguridad alimentaria* puede definirse como la *garantía de que todas las personas, en todo momento, tengan acceso físico, social y económico a alimentos suficientes, seguros y nutritivos para cubrir sus necesidades nutricionales y las preferencias culturales para una vida sana y activa*. En esta definición, el término *seguro* se refiere a la *inocuidad de los alimentos* y a la *garantía de su salubridad para el consumidor* [2]. Para garantizar la inocuidad de los alimentos es necesario conocer la presencia o ausencia de sustancias ajenas al alimento que puedan haber sido incorporadas a él por diversos motivos y que conlleven un riesgo para la salud del consumidor. A estas sustancias contaminantes se le presta especial atención. La palabra *contaminante*, por tanto, hace referencia a *cualquier sustancia que no haya sido agregada intencionadamente al alimento en cuestión, pero que, sin embargo, se encuentra en el mismo como residuo de la producción, fabricación, transformación, preparación, tratamiento, acondicionamiento, empaquetado, transporte o almacenamiento de dicho alimento o como*

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consecuencia de la contaminación medioambiental [3]. Es evidente que el uso de sustancias químicas en el sector alimentario es común hoy en día. Cabe destacar la mejora en los rendimientos de las cosechas y de la producción ganadera conseguida gracias al uso de *productos fitosanitarios y medicamentos de uso veterinario*. Además, se utilizan materiales, como *plásticos, papel o cartón* para mantener en condiciones higiénicas los alimentos y permitir su distribución, así como para mejorar su presentación. Todas estas prácticas hacen posible la presencia en el propio alimento de las sustancias empleadas. El origen de estas sustancias químicas en los alimentos puede ser debido a la contaminación ambiental (aire, suelo o agua) al tratamiento térmico empleado para su preparación (frituras, barbacoa, etc) o a su crecimiento de forma natural en el propio alimento (caso de las micotoxinas) [4]. Existe otro tipo de sustancias que sí que son adicionadas intencionadamente a los alimentos con un interés tecnológico y que forman parte de él como ingredientes: los aditivos alimentarios. Por tanto, este tipo de compuestos al ser adicionados intencionadamente, no se incluyen dentro de la propia definición de contaminante; aún no siendo contaminantes, sí que pueden comportarse como compuestos tóxicos si la cantidad empleada es superior a la permitida. El motivo de interés por la no presencia de este tipo de sustancias en los alimentos o de que, al menos, se encuentren en valores por debajo de los máximos permitidos por las legislaciones vigentes, se debe a que estas sustancias, una vez ingresadas en el organismo del consumidor, *pueden alterar componentes bioquímicos fundamentales para la vida*. De acuerdo con el *Reglamento 315/93/CEE* [5] queda prohibida la comercialización de productos alimenticios en los que se haya comprobado la presencia de un contaminante en proporciones inaceptables desde el punto de vista toxicológico. Los contaminantes deben mantenerse al mínimo nivel posible. No sólo una dosis alta de estos agentes tóxicos en alimentos implica riesgos en la salud del consumidor, sino que

I. INTRODUCCIÓN Y ANTECEDENTES

dosis bajas pueden producir problemas a corto y medio plazo debido a su acumulación en el organismo.

En la actualidad, el número de compuestos tóxicos que deben ser controlados en los alimentos es muy amplio y variado. En la figura 1 se detalla la clasificación de los compuestos tóxicos en función de su origen [6,7]:

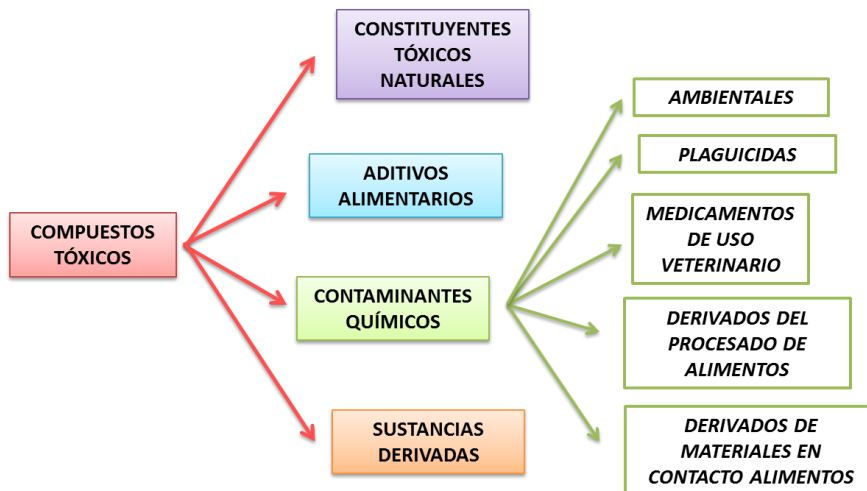


Figura 1. Clasificación de los compuestos tóxicos en función de su origen.

A continuación se indican los aspectos más característicos y algunos ejemplos de los compuestos tóxicos detallados en la figura 1.

✿ Constituyentes tóxicos naturales:

Son productos originados en el metabolismo de animales y plantas empleados como alimentos. Como ejemplos se pueden citar los siguientes: glucósidos cianogénicos en melocotón o albaricoque, inhibidores de la colinesterasa en patata o tomate, aminas vasoactivas en plátanos o cebada, cafeína, teofilina y teobromina en café y té, ácido erúxico en aceite de semilla de mostaza y algunas variedades de aceite de colza.

Aditivos alimentarios:

Se definen como sustancias que se añaden a los alimentos para mejorar su textura, color, sabor o simplemente para mantener su conservación durante un periodo de tiempo más prolongado [8]. *Colorantes, edulcorantes, antioxidantes o estabilizantes* son algunos ejemplos de aditivos empleados en el sector alimentario.

Contaminantes químicos:

Llegan al alimento durante las fases de producción, procesado, distribución y manipulación. En los últimos años su uso se ha visto aumentado debido principalmente al incremento de la productividad agrícola y al desarrollo industrial. Como se indica en la figura 1, dentro de este grupo se encuentran diferentes tipos de contaminantes, que serán tratados a continuación.

Contaminantes ambientales:

Son fabricados para uso industrial, estables y difícilmente degradables. Pertenecen a este grupo metales pesados como el mercurio (usado en fungicidas, pinturas, etc), cadmio (se encuentra formando parte de otros compuestos en pinturas, pigmentos, etc), o arsénico (usado en medicamentos, plaguicidas, cerámica, etc), que pueden absorberse en el agua y el suelo de forma natural acumulándose en los alimentos, y compuestos orgánicos persistentes como dioxinas (empleadas en la industria del papel, combustión de la gasolina con plomo, etc) o bifenilos policlorados (PCBs, empleados en sistemas hidráulicos de barcos, entre otros).

Residuos de plaguicidas:

La presencia de residuos de plaguicidas en alimentos a concentraciones superiores al *límite de residuos máximo* (MRL) legalmente establecido es común a día de hoy. La causa más frecuente de este incumplimiento suele encontrarse en una mala práctica agrícola, como la aplicación de dosis superiores a las recomendadas o el incumplimiento de los plazos de seguridad entre la aplicación del plaguicida y recogida del producto. También cabe la posibilidad de encontrar residuos de plaguicidas no autorizados, lo cual constituye un fraude que, en ocasiones, es fruto de un error al haber usado un plaguicida no registrado para un cierto cultivo, aunque pueda estar autorizado para muchos otros. Plaguicidas (herbicidas, insecticidas, acaricidas, fungicidas, etc) o fertilizantes con nitrógeno (nitratos y nitritos), son algunos ejemplos de este tipo de contaminantes químicos.

Residuos de medicamentos de uso veterinario:

Durante su vida, los animales pueden ser tratados con medicamentos para la prevención o cura de enfermedades, con lo cual, cabe la posibilidad de encontrar dichos medicamentos en alimentos de origen animal. El clenbuterol es un ejemplo de anabolizante empleado de forma fraudulenta para el engorde del ganado, existiendo la posibilidad de encontrarlo en productos derivados de dicho ganado.

Residuos tóxicos derivados del procesado de alimentos:

Nitrosaminas, ácidos grasos trans producidos en la transformación de aceite líquido en sólido para la obtención de margarinas, furanos formados en el tratamiento térmico de alimentos como café o sopa, hidrocarburos aromáticos policíclicos (PAHs) producidos en procesos

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térmicos de preparación de alimentos, acrilamida formada en alimentos fritos ricos en carbohidratos, son algunos ejemplos de este tipo de residuos.

Residuos tóxicos derivados de materiales en contacto con alimentos:

Plastificantes (ftalatos, bisfenol A, etc) o tintes de impresión empleados en la fabricación de envases para alimentos y bebidas, pueden ser transferidos al propio alimento, con el consiguiente riesgo para la salud del consumidor.

Sustancias derivadas:

Aparecen como consecuencia de reacciones de degradación de los alimentos. Los propios componentes de los alimentos pueden reaccionar debido a la acción de agentes físicos como el calor o la luz, produciendo sustancias cancerígenas. Peróxidos y radicales libres procedentes de la oxidación de lípidos o micotoxinas originadas por procesos metabólicos de mohos son algunos ejemplos de este tipo de contaminantes.

Debido al riesgo que suponen para la salud del consumidor, es *necesario controlar la presencia de estos agentes tóxicos en los alimentos*. La legislación alimentaria actualmente está encaminada a asegurar un nivel elevado de protección de la vida y la salud de las personas, teniendo en cuenta el bienestar de los animales, los aspectos fitosanitarios y medio ambiente. Dicha legislación establece, tanto a escala nacional como comunitaria, el derecho de los consumidores a la seguridad de los alimentos y a disponer de una información precisa y veraz.

En España, la Agencia Española de Consumo, Seguridad Alimentaria y Nutrición (AECOSAN) es un organismo autónomo adscrito al Ministerio de

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Sanidad, Política Social e Igualdad, que se creó en 2001 con la misión de garantizar el más alto grado de seguridad alimentaria, como aspecto fundamental de la salud pública, promover la salud de los ciudadanos y que éstos tengan confianza plena en los alimentos que consumen y dispongan de información para tener capacidad de elección.

A *escala comunitaria*, la legislación alimentaria tiene por objeto armonizar requisitos nacionales a fin de garantizar la libre circulación de alimentos y piensos en la Unión Europea (UE). La *Comisión Europea* (EC) plasmó sus prioridades estratégicas en el *Libro Blanco de la Seguridad Alimentaria* [9]. Hasta el momento de su creación sólo existían disposiciones comunitarias específicas para algunos contaminantes, pero a escala nacional se aplicaban múltiples medidas. El hecho de las disparidades en la protección de la salud de los consumidores llevó al planteamiento de nuevas normas a nivel comunitario, aplicables a contaminantes a lo largo de toda la cadena alimentaria. En este libro queda reflejado que una de las prioridades de la Comisión de las Comunidades Europeas es velar por los más elevados niveles de seguridad alimentaria en la UE y por ello se plantea la necesidad de crear un conjunto de normas comunes para la Unión Europea en materia de seguridad alimentaria.

El planteamiento de la seguridad alimentaria es ahora más integrado: se sigue cuidadosamente la pista de los alimentos y los piensos a través de toda la cadena alimentaria, desde la misma explotación hasta la mesa del consumidor (trazabilidad). Las autoridades de la UE evalúan meticulosamente el riesgo y consultan a los mejores expertos científicos antes de prohibir o permitir la inclusión de cualquier producto, ingrediente, aditivo u organismo genéticamente modificado, en cualquier pienso o alimento, venga de dentro o de fuera de la UE. Por ello, para evitar infracciones en el ámbito de la seguridad alimentaria, así como para

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garantizar la inocuidad de los alimentos de consumo humano, entre otros aspectos, *hay que desarrollar nuevas técnicas y metodologías analíticas avanzadas para la detección de sustancias químicas y métodos de producción de alimentos prohibidos o no conformes con las buenas prácticas que permitan la identificación y cuantificación de este tipo de sustancias en una amplia gama de alimentos y productos derivados.* Aunque en los últimos años se han producido grandes avances en los métodos de control de contaminantes en alimentos, son evidentes las limitaciones que presentan las metodologías que se usan actualmente en la mayoría de laboratorios acreditados de control de residuos. Por tanto, es muy importante que se investigue en el desarrollo y mejora de los métodos actuales de control de sustancias químicas en alimentos así como la incorporación de nuevas técnicas de detección que proporcionen mayor información de alta calidad de forma rápida y efectiva.

Cabe destacar la importancia del *acoplamiento de cromatografía y espectrometría de masas* en el ámbito de investigaciones analíticas en el área ambiental y de seguridad alimentaria, de manera que la cromatografía permite la separación de los componentes de la muestra para realizar su detección, identificación y cuantificación y la espectrometría de masas aporta información sobre la estructura del compuesto detectado, fundamental para llevar a cabo una correcta identificación.

Para que este control sobre la presencia de residuos de contaminantes en alimentos sea efectivo, se establecen *límites máximos de residuos tolerados* (MRLs) de acuerdo con el procedimiento del *Comité permanente de la Cadena Alimentaria y Sanidad Animal* y previa consulta a la *Autoridad Europea de Seguridad Alimentaria (European Food Safety Authority, EFSA)* [10].

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Además, se define lo que se conoce como *Ingesta Diaria Admisible (IDA)* como un *índice toxicológico* establecido por las autoridades competentes, tanto a nivel nacional como internacional, que indica la *cantidad de un compuesto químico (incluidos los plaguicidas), expresada en relación con el peso corporal, que puede ser ingerida a diario durante toda la vida de una persona sin que llegue a representar un riesgo apreciable para la salud.* Teniendo en cuenta la IDA y las buenas prácticas agrícolas, se establece el *límites máximo de residuos*. Este límite es definido como el *máximo nivel de residuos que se puede aceptar en un determinado alimento para que un humano que lo consume en forma normal y abundante no supere el IDA para el residuo en cuestión.*

I.2. Residuos de contaminantes en alimentos

Se pueden definir como residuos de contaminantes en alimentos pequeñas cantidades de estos compuestos o de sus productos de degradación que permanecen y se acumulan en los alimentos, de forma que al ser ingeridos en grandes cantidades por el ser humano puede afectar a su salud. En la sección I.1. de esta introducción se hace especial hincapié en la amplia variedad de contaminantes susceptibles de ser detectados en muestras de alimentos. Con los avances en instrumentación y metodologías analíticas se pretende garantizar la inocuidad de los alimentos, confirmando la inexistencia de contaminantes o su presencia pero en cantidades inferiores a las consideradas como perjudiciales para la salud del consumidor. En esta Tesis el estudio se centrará básicamente en los compuestos indicados en la tabla 1.

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Tabla 1. Tipos de compuestos tóxicos tratados en la presente Tesis, procedencia y ejemplos.

Compuesto tóxico	Tipo	Origen	Ejemplos
Plaguicidas	Químico	Productos fitosanitarios	Organoclorados, organofosforados, simazina, diuron, imazalil, tiabendazol
Micotoxinas	Sustancia derivada	Producción natural por mohos y hongos	Aflatoxinas, fumonisinas, ochratoxina A, patulina
Medicamentos de uso veterinario	Químico	Prevención de enfermedades. Se emplean en productos de origen animal o en acuicultura	Tranquilizantes, antihelmínticos, antiinflamatorios, esteroides, beta-agonistas
Plastificantes	Químico	Procesado, envasado y almacenamiento de alimentos	Ftalatos, Bisphenol A, 2-isopropiltioxantona
Edulcorantes	Aditivo	Aditivo alimentario	Sacarina, aspartamo, ciclamato
Nitrosaminas	Químico	Procesado de alimentos	N-nitrosodietilamina
Compuestos perfluorados	Químico	Tintes, barnices, envasado en general	Ácido perfluorooctanoico, sulfonato de perfluorooctano

I.2.1. Residuos de plaguicidas

La producción primaria (vegetal y animal) tiene una importancia considerable en la alimentación, pero el rendimiento de dicha producción se ve constantemente afectado por organismos y plantas dañinos. Con el objetivo de proteger plantas, productos derivados y ganado, así como evitar la reducción de la producción y aumentar la productividad agrícola, se emplean los *plaguicidas*. Sin embargo, el uso de estos compuestos tiene efectos secundarios peligrosos en la salud de consumidores de vegetales y animales.

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Los pesticidas pueden ser incorporados al medio ambiente de varias formas. Además de contaminar el agua, suelo y aire por su aplicación, pueden ser acumulados en los cultivos y, como consecuencia, pasar a los alimentos. En la figura 2 se detalla el ciclo de circulación de los pesticidas en la naturaleza.

La cantidad de plaguicida aplicado debe ser lo más baja posible y el intervalo de tiempo entre la aplicación y el consumo del producto debe ser lo más amplio que se pueda, de forma que el residuo se reduzca al mínimo. Generalmente, los plaguicidas aparecen en los alimentos a muy bajas concentraciones, del orden de partes por millón (mgkg^{-1}) o menos [11].

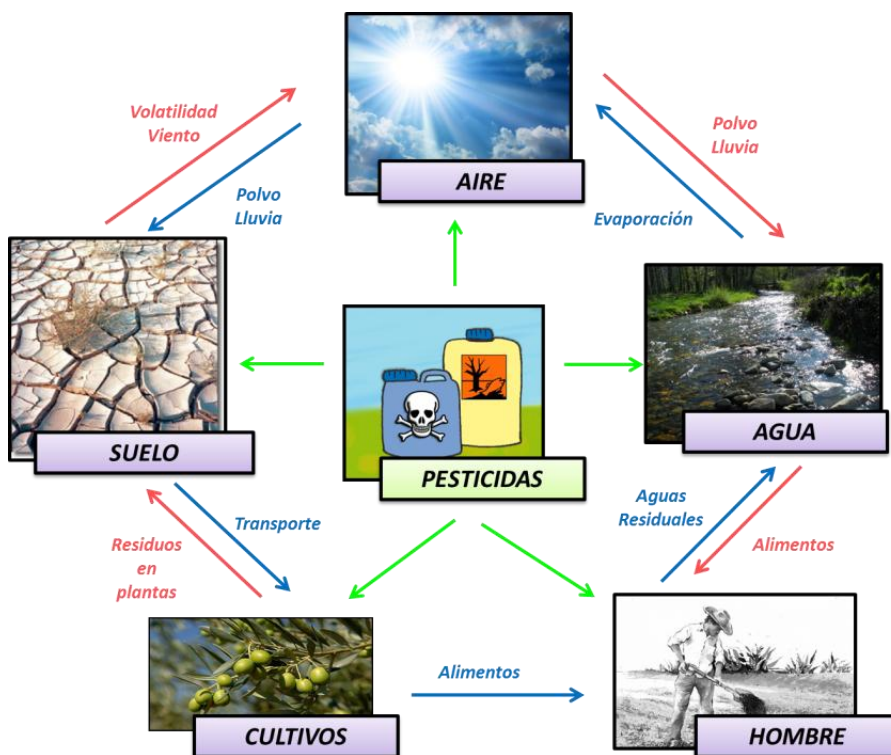


Figura 2. Ciclo de circulación de los pesticidas en la naturaleza.

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1.2.1.1. Clasificación de los plaguicidas:

Se pueden realizar distintas clasificaciones de los plaguicidas, atendiendo a diversos criterios:

a) Según su toxicidad aguda: [12]

Esta clasificación se hace de acuerdo a los valores de DL_{50} (dosis letal media por vía oral o dérmica con la que muere el 50% de la población de las ratas estudiadas) y CL_{50} (concentración letal media por vía respiratoria con la que muere el 50% de la población de ratas estudiadas). La clasificación se muestra detalladamente en la tabla 2.

Tabla 2. Clasificación de los plaguicidas según su toxicidad aguda.

Entrada al organismo	Estado del plaguicida (unidad)	Grado de toxicidad		
		Muy tóxicos	Tóxicos	Nocivos
Vía oral	Sólido ($mgkg^{-1} PC^*$)	$DL_{50} \leq 5$	$5 < DL_{50} \leq 50$	$50 < DL_{50} \leq 500$
	Líquido ($mgkg^{-1} PC$)	$DL_{50} \leq 25$	$25 < DL_{50} \leq 200$	$200 < DL_{50} \leq 2000$
Vía respiratoria	Gaseosos/Fumigantes /Aerosoles ($mgL^{-1} aire$)	$CL_{50} \leq 0.5$ (4h)	$0.5 < CL_{50} \leq 2$ (4h)	$2 < CL_{50} \leq 20$ (4h)
Vía dérmica	Sólido ($mgkg^{-1} PC$)	$DL_{50} \leq 10$	$10 < DL_{50} \leq 100$	$100 < DL_{50} \leq 1000$
	Líquido ($mgkg^{-1} PC$)	$DL_{50} \leq 50$	$50 < DL_{50} \leq 400$	$400 < DL_{50} \leq 4000$

*PC. Peso corporal.

b) Según su acción específica:

Cuatro clases de pesticidas pueden diferenciarse en función de este criterio. Pueden emplearse para control de invertebrados, vertebrados, de plantas y microorganismos. A su vez, estas clases presentan diferentes

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subgrupos en función de su composición química [13]. Esta clasificación se detalla en la figura 3.

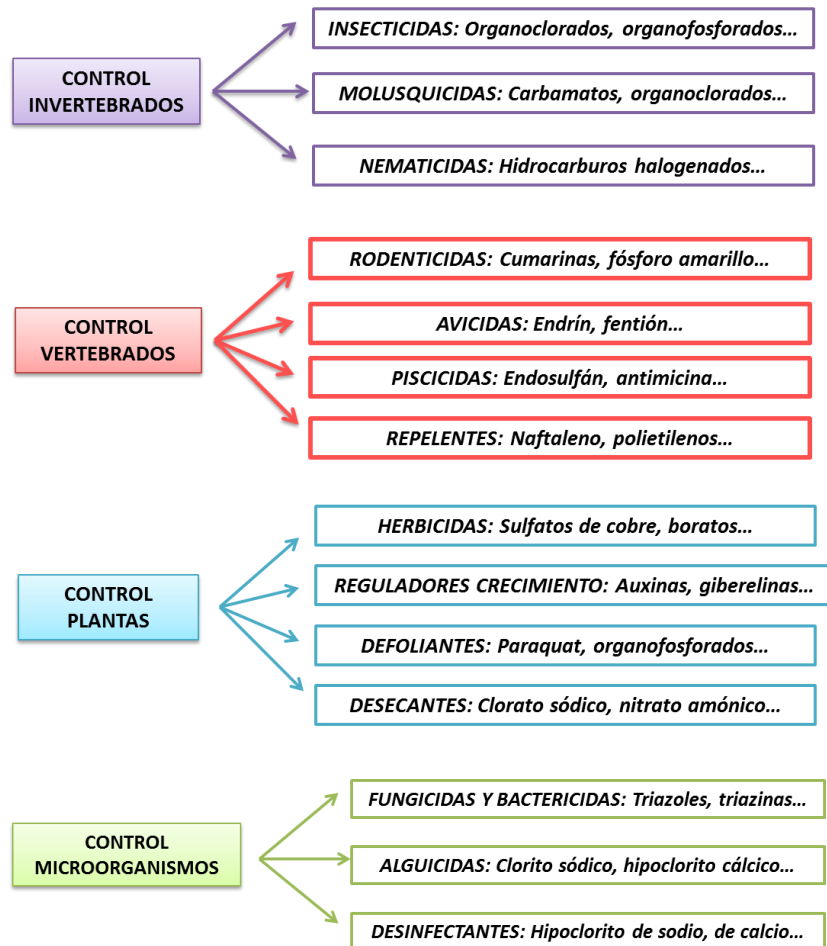


Figura 3. Clasificación de los plaguicidas en función de su acción específica.

1.2.2. Residuos de micotoxinas

Las *micotoxinas*, término derivado de las palabras griegas *mikes* y *toxina*, que significan *hongo* y *veneno* respectivamente, también conocidas como toxinas fúngicas, son *metabolitos secundarios de bajo peso molecular, producidos por varios centenares de especies de mohos que pueden crecer sobre los*

I. INTRODUCCIÓN Y ANTECEDENTES

alimentos en determinadas condiciones. El efecto perjudicial para la salud se conoce desde antiguo y entre las prescripciones de la medicina clásica está la recomendación de evitar los alimentos enmohecidos [14].

Éstas pueden contaminar alimentos, piensos o materias primas para su elaboración, originando un grupo de enfermedades y trastornos, tanto en humanos como en animales, denominados *micotoxicosis*. La presencia de estas micotoxinas en los alimentos puede ser individual o simultánea con otras, lo que puede provocar efectos sinérgicos en su acción sobre el organismo, aumentando su toxicidad. La ingesta de alimentos con este tipo de contaminantes, si éstos se encuentran en dosis bajas, no induce síntomas clínicos, pero con el tiempo puede traer graves consecuencias sobre la calidad y durabilidad de la vida. Sólo en las últimas décadas se ha dado importancia a su estudio. Elevados niveles de micotoxinas en la dieta pueden causar efectos adversos agudos o crónicos sobre la salud del hombre y gran variedad de especies animales. Los efectos adversos pueden afectar a diferentes órganos, aparatos o sistemas, especialmente al hígado, riñón, sistema nervioso, endocrino e inmunitario. En términos generales, el riesgo de intoxicación aguda por micotoxinas en el hombre es bajo o moderado en comparación con intoxicaciones de origen microbiológico o por contaminantes químicos. Según algunos autores [15], las micotoxinas presentan mayor riesgo tóxico que los aditivos alimentarios y plaguicidas. En la tabla 3 se muestra una clasificación de las micotoxinas en cuanto a la toxicidad crónica, de acuerdo con la *Agencia Internacional de Investigación sobre el Cáncer (International Agency for Research on Cancer, IARC)* [16].

Las micotoxinas más importantes son las producidas por mohos de los géneros *Aspergillus*, *Fusarium* y *Penicillium*.

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Factores como la resistencia genética del cultivo, las condiciones climatológicas caracterizadas por temperaturas y humedades relativas altas, condiciones de transporte y almacenamiento inadecuado y un secado deficiente pueden influir en la contaminación por hongos productores de micotoxinas. Por tanto, la contaminación del producto puede ocurrir en cualquier punto de la cadena alimenticia, desde la cosecha, pasando por la recolección, almacenaje, transporte, elaboración y conservación.

Tabla 3. Clasificación de las micotoxinas en función de su toxicidad crónica.

Micotoxinas	Grupo
Aflatoxina M ₁	2B(*)
Citrinina	3(**)
Esterigmastocistina, Fumonisina B ₂ , Ochratoxina A	2B(*)
Patulina, Toxina T-2	3(**)
Zearalenona, Deoxinivalenol, Nivalenol	3(**)

(*)Grupo 2B: agente *posiblemente carcinogénico*; la evidencia en humanos es limitada y tampoco hay suficiente evidencia con animales de experimentación. (**)Grupo 3: agente *no clasificable como carcinógeno* para humanos.

1.2.2.1. Clasificación de las micotoxinas:

De acuerdo con uno de los criterios de clasificación de las micotoxinas, en la figura 4 se muestra su clasificación en función del hongo por el que están producidas [17]:

a) Aflatoxinas

Producidas por mohos del género *Aspergillus*. El interés en ellas se despertó con motivo de la aparición, en 1961 de una epidemia entre la población de pavos de las granjas de Gran Bretaña, que ocasionó la muerte a más de

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100.000 ejemplares. La investigación reveló que la causa era la harina de cacahuets, contaminada con *Aspergillus flavus*, importada de Brasil.

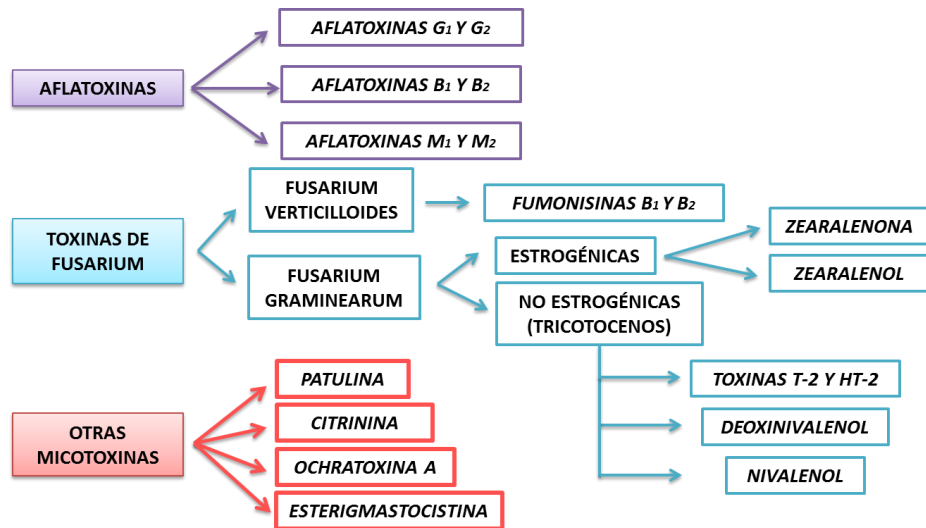


Figura 4. Clasificación de las micotoxinas según el tipo de hongo que las producen.

Este tipo de micotoxinas puede proliferar en muchos alimentos, causando problemas en cacahuets, maíz, semillas de algodón, todo tipo de frutos secos y cereales. Su producción tiene lugar entre los 12º y 27ºC.

Destacan las *aflatoxinas B₁* (AFB₁), *B₂* (AFB₂), *G₁* (AFG₁) y *G₂* (AFG₂). La letra indica el tipo de fluorescencia frente a la luz ultravioleta: azul (las de letra B) y verde (las de letra G). Entre las AFB₁ y AFB₂ difieren en la presencia o ausencia de un doble enlace en su estructura, al igual que ocurre con las AFG₁ y AFG₂. Las aflatoxinas B difieren de las aflatoxinas G porque el anillo de furano de las primeras se convierte en un anillo de lactona en las segundas. La *aflatoxina M₁* (AFM₁) procede de la AFB₁ y la *aflatoxina M₂* (AFM₂), de la AFB₂.

Las aflatoxinas, en general, son tóxicos hepáticos y su grado de toxicidad y carcinogenicidad sigue el orden B₁ > G₁ > B₂ > G₂.

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En humanos, las aflatoxinas son probablemente responsables de múltiples episodios de intoxicaciones masivas en distintas zonas de la India, Sudeste Asiático y África tropical y ecuatorial, y un factor de agravamiento de enfermedades producidas por la malnutrición. También son responsables muy probablemente, combinadas con otros factores, de la elevada tasa de cáncer hepático observado en algunas de esas zonas. Desde 1988, la *Organización Mundial de la Salud (World Health Organization, WHO)* considera a la aflatoxina B₁ como un carcinógeno para el hombre.

Las aflatoxinas resisten los tratamientos habituales de los alimentos. En el caso de determinados productos, como los cacahuetes, los frutos de cáscara, los frutos secos y el maíz, está demostrado que los métodos de selección u otros tratamientos físicos permiten reducir el contenido de aflatoxinas. Con el fin de minimizar las repercusiones en el comercio, conviene admitir contenidos de aflatoxinas más elevados en los productos en cuestión cuando no se destinen al consumo humano directo o a su utilización como ingredientes de productos alimenticios. Si éste fuese el caso, deberán etiquetarse de forma que se demuestre claramente su destino, incluida la indicación *“producto destinado a ser sometido obligatoriamente a un tratamiento de selección u otros métodos físicos con objeto de reducir el nivel de contaminación de aflatoxinas”*.

El *Comité Científico de la Alimentación Humana (CCAH)* afirmó en su dictamen de 23 de septiembre de 1994 que las *aflatoxinas son cancerígenos genotóxicos*. Con arreglo a este Dictamen, se consideró conveniente limitar el contenido total de aflatoxinas en los alimentos (la suma de las aflatoxinas B₁, B₂, G₁ y G₂), así como el contenido de AFB₁ en particular, ya que la AFB₁ es un componente mucho más tóxico que los demás [18]. Por otro lado, debe estudiarse la posible reducción del actual contenido máximo para la AFM₁ en

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los alimentos para lactantes y niños de corta edad, en función de la evolución de los procedimientos analíticos.

b) Toxinas de Fusarium

Son micotoxinas producidas por hongos del género *Fusarium*. En este subgrupo de micotoxinas se pueden diferenciar diferentes toxinas de *Fusarium* en función del moho que las produce:

Fusarium verticilloides:

Produce las micotoxinas conocidas como fumonisinas.

Fusarium graminearum:

Produce toxinas estrogénicas (zearalenona (ZEN) y zearalenol) y no estrogénicas o tricotecenos (deoxinivalenol (DON), nivalenol (NIV), toxina T-2 (T-2), toxina HT-2 (HT-2) y diacetoxiscirpenol).

Son toxinas mucho más comunes en animales domésticos, aunque se conocen algunos casos de intoxicaciones en humanos. Destaca su presencia en maíz, diversos cereales y en la malta empleada para la producción de cerveza.

En lo que respecta a las fumonisinas, los resultados del control de las cosechas han indicado que el maíz y los productos a base de maíz pueden estar muy contaminados y por tanto es conveniente tomar medidas para evitar su incorporación en la cadena alimentaria. Se conocen al menos 15 tipos de fumonisinas, de las cuales la más importante es la fumonisin B₁ (FB₁). Estas toxinas están relacionadas con la aparición de cáncer de esófago e hígado, defectos neuronales e intoxicación aguda.

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Estudios han revelado que la presencia de toxinas T-2 y HT-2 puede ser preocupante para la salud pública. Por lo tanto, se ha considerado necesario investigar más los factores que influyen en la aparición de toxinas T-2 y HT-2 en los cereales y los productos a base de cereales, en particular en la avena y los productos a base de avena.

En cuanto a otros tricotecenos examinados hasta el momento, entre ellos el diacetoxicispernol, la limitada información disponible indica que no están muy extendidos y los niveles descubiertos suelen ser reducidos.

Las condiciones climáticas durante el crecimiento de la planta tienen una gran influencia en el contenido de toxinas de fusarium. Sin embargo, las buenas prácticas agrícolas pueden prevenir la contaminación por este tipo de toxinas.

c) Otras micotoxinas

✿ *Ochratoxina A:*

La ocratoxinas son micotoxinas producidas por determinados hongos, entre ellos *Aspergillus ochraceus* y *Penicillium verrucosum*, entre las que se encuentran la ochratoxina A, B y C. La ocratoxina más importante es la *ocratoxina A (OTA)*, debido a su toxicidad e incidencia en los alimentos.

Estructuralmente, tiene la particularidad de contener un átomo de cloro. Se encuentra presente de manera natural en numerosos productos vegetales de todo el mundo, como los cereales, los granos de café, el cacao y los frutos secos. Se ha detectado, asimismo, en productos tales como los elaborados a base de cereales, el café, el vino, la cerveza y el zumo de uva, pero también en productos de origen animal, como los riñones de cerdo.

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Presenta propiedades carcinógenas, nefrotóxicas, teratógenas, inmunotóxicas y, posiblemente, neurotóxicas. Se la ha asociado también a la nefropatía en los seres humanos.

Se han establecido contenidos máximos para cereales, productos a base de cereales, uvas pasas, café tostado, vino, zumo de uva, especias y alimentos para lactantes y niños de corta edad, todos ellos productos que contribuyen significativamente a la exposición humana general a la OTA o a la exposición de grupos vulnerables de consumidores, como por ejemplo los niños.

✘ *Patulina:*

La patulina es una micotoxina producida por diversas especies de *Penicillium*, *Aspergillus* y *Byssochyلامys*. Se encuentra con frecuencia en productos derivados de la manzana, especialmente en zumos de manzana y en sidra, uva y pera, aunque también se ha detectado en vegetales y granos de cereales. Las condiciones que promuevan al pudrimiento de la fruta aumentan la probabilidad de formación de esta micotoxina.

Esta micotoxina posee características de antibiótico y se ha probado para tratar el resfriado común. Sin embargo, nunca se ha demostrado su efectividad y no se ha insistido en su uso médico porque es un irritante estomacal y produce náuseas y vómitos. Entre otros síntomas de intoxicación por patulina se sabe que produce hemorragia del tracto digestivo en ganado.

✘ *Citrinina:*

Es una micotoxina nefrotóxica producida por varias especies de los géneros *Aspergillus*, *Penicillium* y *Monascus*. Fue aislada por primera vez en 1931. Aunque se caracterizó como antibiótico, demostrando su capacidad antifúngica y bacteriostática, posteriormente se la hizo responsable de

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neuropatía porcina en varios países de Europa. Se forma principalmente tras la recogida de la cosecha y aparece principalmente cuando los granos de cereales son almacenados, pero además se produce en frutas, zumos de fruta y verdura y productos en mal estado [19]. También ha sido aislada en bellotas, nueces, zanahoria, tomate y carne [20,21].

Esta micotoxina tiene efectos nefrotóxicos y mutagénicos. Su ingestión provoca diarrea y pérdida de peso por degeneración renal. Es importante el efecto sinérgico observado cuando se presenta de forma combinada con la OTA [20, 22].

✖ Esterigmastocistina:

La esterigmastocistina (STE) es precursora de las aflatoxinas G₁ (AFG₁), G₂ (AFG₂) y B₁(AFB₁). Esta micotoxina está relacionada con carcinomas gástricos, hepáticos y esofágicos. Su presencia ha sido detectada en cereales, café, jamón, pimienta y queso entre otros alimentos [23].

1.2.3. Residuos de medicamentos de uso veterinario

Las técnicas ganaderas de explotación intensiva se caracterizan por la convivencia de un gran número de animales confinados en un espacio reducido, favoreciéndose el contagio rápido de enfermedades, lo que ha dado lugar a la *utilización de medicamentos veterinarios con el fin de prevenir y tratar estas enfermedades. Por medicamento veterinario se entiende cualquier sustancia aplicada o administrada a cualquier animal destinado a la producción de alimentos, como los que producen carne o leche, las aves de corral, peces o abejas, tanto con fines terapéuticos o de diagnóstico, o para modificar sus funciones fisiológicas o el comportamiento.*

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Otras sustancias que se emplean para tratar a los animales son los *aditivos para la alimentación animal*. En la *Directiva del Consejo 70/524/EEC* [24] se definen los *aditivos para alimentación animal* como *sustancias que mejoran tanto los piensos en los que se incorporan como la producción ganadera*. Deben cumplir como prerequisite que no afecten a la salud animal o humana ni al medio. Incluyen antibióticos, promotores del crecimiento, muchos coccidiostáticos, agentes de unión y enzimas. Como consecuencia del uso de los medicamentos veterinarios en la producción animal, en los animales pueden quedar residuos de estos medicamentos que pueden pasar a la cadena alimentaria. Se define como *residuos de medicamentos veterinarios* a los *productos originales y sus metabolitos en cualquier porción comestible del producto animal, así como los residuos de impurezas relacionadas con el medicamento veterinario correspondiente* [25]. Con el fin de proteger la salud de los consumidores, la Unión Europea ha determinado los *límites máximos de residuos (MRLs)* para varios fármacos relativos en leche, carne y otros alimentos, por medio del *Reglamento del Consejo 2377/90/CEE* [26].

Los grupos de medicamentos más utilizados en el sector ganadero se indican en la figura 5 [27]:

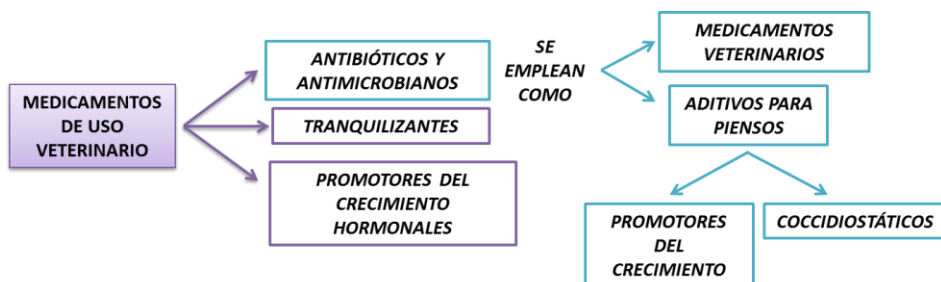


Figura 5. Grupos de medicamentos más empleados en el sector ganadero.

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A continuación se describe cada grupo indicado en la figura 5 con más detalle.

1.2.3.1. Antibióticos y antimicrobianos

Su utilización en animales puede ser con fines terapéuticos como medicamentos veterinarios o en forma de aditivos para piensos.

Utilización como medicamentos veterinarios

Se llevan utilizando con el fin de tratar y prevenir las enfermedades en ganado y aves de corral desde hace más de 50 años. Su uso con fines terapéuticos o profilácticos se encuentra autorizado bajo prescripción veterinaria. Tras su utilización es necesario respetar los tiempos indicados entre la suspensión de la administración del compuesto a los animales y su faena u ordeño antes de utilizar los productos alimenticios obtenidos a partir de ellos, para que no queden residuos o éstos se encuentren por debajo de sus límites máximos fijados. Aunque los problemas de toxicidad aguda debido a la aparición de residuos de estas sustancias en tejidos comestibles, leche o huevos son poco probables, sí pueden tener otros efectos nocivos para la salud de los consumidores incluyendo alteraciones de la flora intestinal o inducción de alergias, así como en la industria alimentaria por la inhibición de microorganismos de interés tecnológico, como los cultivos iniciadores utilizados en la elaboración de productos cárnicos o productos lácteos [28].

Utilización como aditivos para piensos

Promotores del crecimiento:

El uso de antibióticos en dosis subterapéuticas en animales sanos provoca un aumento en la velocidad de crecimiento. La utilización de

antibióticos como promotores del crecimiento se debe a que se usan en dosis significativamente inferiores a las dosis terapéuticas y se refiere sólo a aquellos antibióticos que no se usan en medicina humana. La *Comisión Europea* ha prohibido el uso de algunos de estos antibióticos con fines zootécnicos, restringiéndolo a aquellos que no se absorben y/o se metabolizan rápidamente y cuyo uso no se ha generalizado en terapia humana, de acuerdo con el *Reglamento 2821/98* [29].

Coccidiostáticos:

Son compuestos muy usados para prevenir y tratar las coccidiosis, que son infecciones producidas por amebas que afectan al ganado, particularmente a las aves de corral. Estos compuestos están autorizados para su utilización como aditivos de piensos durante un intervalo de tiempo determinado para broilers y polluelos, pero no para gallinas ponedoras. No se han establecido MRLs, pero se han asignado tiempos de retirada antes del sacrificio.

1.2.3.2. Tranquilizantes

El estrés en los animales de abasto es un factor que causa elevada mortalidad, principalmente durante el transporte de los animales de la explotación ganadera al matadero. Además, en el caso de los cerdos principalmente, la carne que se obtiene de los animales estresados se denomina “pálida, suave y exudativa”, y presenta unas cualidades tecnológicas no adecuadas, no siendo apta para la elaboración de determinados productos cárnicos. Existen varias sustancias que se utilizan regularmente para tranquilizar a los animales, algunas de las cuales están prohibidas, como los derivados de las fenotiazinas, y para otras se han establecido MRLs como es el caso de la azaperona y el carazolol [30].

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Existen tranquilizantes que se usan como promotores del crecimiento como las benzodiazepinas, que tienen un efecto ansiolítico y sedativo, contribuyendo a eliminar los temblores que se producen por el uso de algunas hormonas esteroideas y además provocan una estimulación de la ingesta en animales débiles o enfermizos.

1.2.3.3. Promotores del crecimiento hormonales

A pesar de que el uso de sustancias hormonales promotoras del crecimiento se encuentra prohibido en la Unión Europea desde 1988, en otros países está autorizado el uso de algunas de ellas (en Estados Unidos y Canadá por ejemplo está permitido el uso de progesterona, testosterona, zeranol, acetato de trembolona, acetato de melengestrol y 17- β -estradiol) lo que hace que sea necesario realizar controles muy estrictos en las carnes que se importan de estos países. Por otra parte, en Europa existe un uso ilegal de estos compuestos y de otro tipo de sustancias desconocidas cuyo control es muy difícil debido a que algunas de estas drogas se metabolizan en compuestos desconocidos o para los que no existen patrones [31].

1.2.4. Residuos de materiales en contacto con los alimentos

Compuestos que forman parte del material de envasado, almacenamiento y transporte de los alimentos pueden ser transferidos al propio alimento, con los consiguientes riesgos que ello conlleva para la salud del consumidor. En la figura 6 se indican los residuos de materiales en contacto con alimentos que se tratarán a continuación:

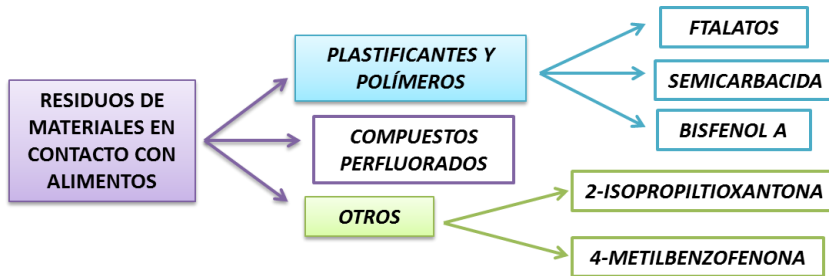


Figura 6. Residuos de materiales en contacto con alimentos tratados en la presente Tesis.

1.2.4.1. Plastificantes y polímeros

Se encuentran dentro de este grupo los materiales y objetos destinados a entrar en contacto con los alimentos a lo largo de la cadena alimentaria (procesado, envasado, almacenamiento y consumo) tales como envases y contenedores, utensilios de cocina, cubiertos y platos [32]. Para estos materiales y objetos plásticos se define lo que se conoce como *límite de migración específica (LME)* de acuerdo con en el *Reglamento 10/2011* [33]: *cantidad máxima de los constituyentes de materiales y objetos plásticos que pueden ser cedidos a los alimentos con los que se encuentran en contacto, expresado en $mgkg^{-1}$* . En caso de que la sustancia de interés no se encuentre contemplada de manera específica en el Reglamento citado, se emplea lo que se conoce como *límite de migración global (LMG)*, según el cual los materiales y objetos plásticos no cederán al alimento con que se encuentran en contacto una cantidad de sus constituyentes superior a 10mg por decímetro cuadrado de superficie de contacto.

Los *plásticos* están hechos a partir de monómeros y otras sustancias de partida que, mediante una reacción química, dan lugar a una estructura macromolecular, el *polímero*, que forma el principal componente estructural de los plásticos.

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Al polímero se le añaden aditivos para obtener determinados efectos tecnológicos. Como tal, el polímero es una estructura inerte de alto peso molecular. Dado que las sustancias con un peso molecular superior a 1000 Dalton normalmente no pueden ser absorbidas por el cuerpo, el riesgo potencial para la salud que supone el propio polímero es mínimo. El riesgo puede derivarse de monómeros u otras sustancias de partida que no hayan reaccionado o lo hayan hecho de forma incompleta, o bien de aditivos de bajo peso molecular que son cedidos a los alimentos por migración a partir del material plástico en contacto con estos. Por lo tanto, los *monómeros, las otras sustancias de partida y los aditivos* deben ser sometidos a una evaluación de riesgos, y su uso en la fabricación de materiales y objetos plásticos debe estar sujeto a autorización. De acuerdo con la *Directiva 2002/72/CE* [34] se establece una lista de monómeros y otra de aditivos autorizados para la obtención de polímeros. Entre monómeros autorizados se encuentran acetaldehído, acetato de vinilo, trietilenglicol, nitrocelulosa o ácido palmítico. En la lista de aditivos autorizados se citan monoglicéridos y diglicéridos de ácidos grasos, 2-aminobenzamida, azodicarbamida, benzaldehído o tetraborato de bario.

✳ *Ftalatos:*

Cabe destacar el uso de *ftalatos* en la industria del plástico. Se adicionan a los polímeros para mejorar la estabilidad y elasticidad del producto fabricado. El principal material en el que los ftalatos son empleados es el PVC. Los ftalatos mayormente usados con este fin son di (2-etilhexil) ftalato (DEHP) y di (iso-nonil) ftalato (DINP). Es posible la contaminación de alimentos por migración de polímeros que contengan ftalatos desde el material que sirve para su envasado y almacenamiento. Además, la contaminación de piensos y alimentos puede ser debida a la presencia de ftalatos en el medio ambiente, por ejemplo, adsorbidos por el suelo y

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sedimentos, pudiendo ser transferidos a estos productos a lo largo de la cadena alimentaria. Este tipo de compuestos se emplea para la fabricación de tubos de PVC usados diariamente en el proceso de obtención y transporte de la leche en granjas. La migración de estos compuestos a la leche ha sido estudiada desde los años 70 [35, 36]. Debido al riesgo que implica la presencia de ftalatos en leche y productos derivados, varios países han prohibido el uso de DEHP en la fabricación de estos tubos destinados a la industria de la leche, siendo sustituido dicho plastificante por otros. Entre estos países destacan Reino Unido, Dinamarca y Noruega [37,38]. Sin embargo, países como Canadá aún permiten el uso de DEHP para la fabricación de tubos de PVC usados con el fin anteriormente detallado [39]. Estudios recientes también han demostrado el uso de ftalatos para la fabricación de tapones de envases que se encuentran en contacto con alimentos, con el consiguiente riesgo de migración de estos desde dichos envases al alimento [40].

✘ *Semicarbacida:*

Es una sustancia carcinogénica débil y no genotóxica que ha sido encontrada en una gran variedad de alimentos y cuya presencia puede tener diferentes orígenes. Este compuesto es un metabolito del medicamento veterinario nitrofurazona, no autorizado en la UE, por lo que en principio no es previsible que se detecte a partir de esta fuente. Puede estar presente en alimentos como resultado de la migración del material plástico utilizado en las juntas de cierre de las tapas metálicas de los envases de vidrio. El origen del mismo es la degradación térmica del azodicarbonamida [41], descrito en la lista de aditivos autorizados detallada en la *Directiva 2002/72/CE* [34].

✘ *Bisfenol A:*

Es una sustancia química que se utiliza principalmente en combinación con otros productos químicos para la fabricación de plásticos y resinas. Forma parte del policarbonato plástico utilizado en la fabricación de envases de alimentos, como botellas retornables de bebidas, alimentación infantil, botellas, vajilla (platos y tazas) y recipientes de almacenamiento. El bisfenol A está autorizado en la UE como material de contacto con alimentos y puede migrar en pequeñas cantidades a los alimentos y bebidas con los que se encuentra en contacto. El riesgo que implica su uso está relacionado con su potencial de interactuar con el sistema hormonal (disruptor endocrino) que podría afectar a la fertilidad y la reproducción [42].

Otro tipo de materiales que pueden encontrarse en contacto con alimentos y cuyas sustancias son susceptibles de migrar a ellos son los conocidos como *materiales activos e inteligentes*. Estos materiales y objetos están destinados a prolongar la vida útil o a mantener y mejorar el estado del alimento envasado. Para ello, incorporan intencionadamente componentes que liberan o que absorben sustancias del alimento o su entorno, que pueden estar en un recipiente aparte, por ejemplo en una bolsita de papel, o estar directamente incorporadas en el material de envase, por ejemplo en el plástico de una botella hecha de ese material [43].

1.2.4.2. Compuestos perfluorados.

Los *compuestos perfluorados* pertenecen al grupo de sustancias perfluoroalquiladas (PFAS) entre los que destacan el *sulfonato de perfluorooctano* (PFOS) y el *ácido perfluorooctanoico* (PFOA). Estas sustancias son altamente persistentes. Estos compuestos son absorbidos por el organismo y se acumulan principalmente en el hígado y la sangre, siendo

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lentamente excretados por los riñones. Al ser sustancias que pueden disolverse tanto en agua como en aceite, son ampliamente usadas en productos domésticos e industriales, incluyendo material de envasado de alimentos, tintas, adhesivos, barnices, etc. Tanto PFOA como PFOS han sido detectados en muestras de marisco, carne, pescado, bebidas, aceite para cocinar y tejido adiposo de cerdo [44]. Debido a la amplia gama de aplicaciones que presentan, estos compuestos se encuentran distribuidos en el medio ambiente.

La Autoridad Europea de Seguridad Alimentaria (EFSA) emitió una opinión científica en febrero de 2008 sobre la importancia de los alimentos en la exposición humana a estas sustancias [45].

Según el Panel de Contaminantes (CONTAM) de la EFSA, los alimentos, en particular el pescado y los productos de la pesca, parecen ser una fuente importante de la exposición humana a estos contaminantes. Para el ácido PFOA, otras fuentes de exposición no alimentarias, como la contaminación del aire, también contribuyen a la exposición total. El Panel CONTAM reconoció que faltaban muchos datos sobre la contribución de los diferentes alimentos a la exposición humana y que era necesario recopilar más datos. Basándose en los datos existentes, el Panel estableció *Ingestas Diarias Admisibles (IDAs)* tanto para el PFOS como para el PFOA, y concluyó que es improbable que la población media en Europa pueda sufrir efectos negativos para la salud derivados de la exposición en la dieta a estos contaminantes. Para PFOS y PFOA la Autoridad Europea de Seguridad Alimentaria estableció como valor indicativo relativo a la exposición del ser humano a estos compuestos 60 ngkg^{-1} y 2 ngkg^{-1} , respectivamente, referidos ambos valores a kg de peso corporal.

1.2.4.3. Residuos de otros materiales en contacto con alimentos.

Otros compuestos que pueden ser cedidos al alimento por parte del envase son, entre otros, 2-isopropiltioxantona y 4-metilbenzofenona, perteneciendo estas sustancias a envases TetraPak y cartón, respectivamente:

2-isopropiltioxantona:

Es un componente de la tinta que se emplea en la preparación del material de embalaje del sistema de envasado TetraPak. En 2005 fue detectada en muestras de leche líquida para bebés distribuida en este tipo de envases [46].

4-metilbenzofenona:

Se emplea en la obtención de tintas y lacas usadas en la impresión de los envases que contienen alimentos, principalmente en los de cartón. Debido a su volatilidad, puede migrar al envase y contaminar productos alimenticios. En 2009 fue certificada por parte de autoridades alemanas y belgas la presencia de este contaminante en productos de cereales, siendo su posible procedencia el material de envasado en el que se encontraban [47].

1.2.5. Aditivos

Los aditivos son sustancias que se añaden intencionadamente a los alimentos con un propósito tecnológico y tiene como resultado que, tanto el propio aditivo como sus subproductos, se van a convertir en un componente de éstos. No se consumen como alimentos ni se usan como ingredientes característicos en la alimentación, independientemente de que tengan o no valor nutritivo.

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Al convertirse en componentes de los alimentos son, por tanto, ingredientes y, por ello deben figurar en el etiquetado de los alimentos. Se denominan con la letra E seguida de un número de tres o cuatro dígitos. De esta manera, el etiquetado proporciona información al consumidor que le va a permitir elegir o evitar consumir alimentos que contengan determinados aditivos. El hecho de que un aditivo tenga un número E asignado da garantías de que el aditivo ha pasado controles de seguridad y que ha sido aprobado para su uso en la Unión Europea [48]. La detección y cuantificación de estos compuestos es de gran interés por diversos motivos. En primer lugar, pueden identificarse posibles usos fraudulentos, por ejemplo, cuando se adicionan colorantes para enmascarar los signos de deterioro de un producto o cuando se utilizan aditivos en alimentos no autorizados o en concentraciones superiores a las permitidas. También se han observado reacciones alérgicas por su ingestión en personas hipersensibles, especialmente, en el caso de algunos colorantes.

En muchos productos alimenticios más de un aditivo es empleado, especialmente en bebidas bajas en calorías que contienen conservantes, edulcorantes artificiales y cafeína [49]. El número de aditivos existente imposibilita el análisis de todos ellos para presentar un listado detallado. Estas sustancias pueden encontrarse en la base de datos del Comité de Expertos en Aditivos Alimentarios FAO/OMS. En la figura 7 se indican los aditivos más conocidos en el ámbito de la alimentación. Algunos de ellos se describen posteriormente:



Figura 7. Aditivos más conocidos en el ámbito de la alimentación.

✿ Conservantes:

Pueden actuar como agentes antimicrobianos y antioxidantes. Algunos, como la tartracina (E-102), se han asociado a reacciones alérgicas en personas asmáticas o sensibles a la aspirina. Otros, el amaranto (E-123) y el verde ácido brillante BS (E-142), han sufrido importantes restricciones debido a su potencial tóxico en espera de nuevas evidencias científicas que lo confirmen. Y otros se han retirado recientemente de las listas. De hecho, en diciembre del año 2003 se prohibió la utilización de la cantaxantina (E-161G), un colorante de piensos animales (salmón, trucha, mariscos de piscifactoría), al demostrarse su capacidad para dañar la retina humana [50].

✿ Edulcorantes:

Los grupos en los que se pueden dividir los edulcorantes así como los compuestos incluidos en cada grupo quedan detallados en la figura 8.

Los más comúnmente empleados son sacarina, ciclamato, sucralosa y aspartamo. Se caracterizan por su elevado poder endulzante, siendo muy pequeñas las cantidades necesarias para conseguir dar sabor dulce a alimentos y bebidas. Por este motivo se consideran no calóricos o bajos en calorías.

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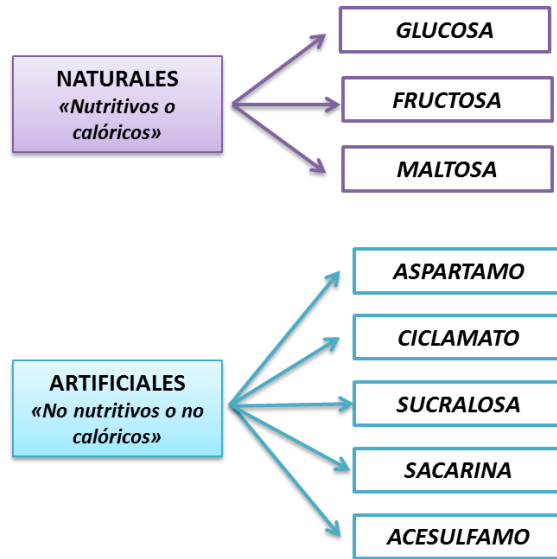


Figura 8. Clasificación de los principales edulcorantes.

La diabetes y la obesidad son dos enfermedades muy comunes en la sociedad actual. Debido a que el principal problema para personas que padecen este tipo de enfermedades es el consumo de azúcar, hoy en día se emplean numerosas alternativas a su uso. Numerosos alimentos y bebidas bajos en calorías se encuentran disponibles actualmente en el mercado: chicles, dulces, yogures, refrescos, helados, etc. Algunos estudios ponen de manifiesto que el uso moderado de estos edulcorantes puede ayudar a reducir peso y mejorar la salud de personas que ingieren grandes cantidades de azúcar o que tienen problemas para metabolizarla. Sin embargo, algunos edulcorantes artificiales están relacionados con la aparición de ciertos tumores en animales, así como vinculados a la aparición de enfermedades de corazón y riñón. Por eso se aconseja el consumo moderado principalmente de bebidas endulzadas a base de edulcorantes no nutritivos [51]. Debido al importante aumento en el consumo de estos productos y el riesgo que para la salud puede provocar su consumo, se ha desarrollado una legislación que limita el contenido de estos aditivos en alimentos de consumo humano. Así,

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la *Directiva 94/35/CE* [52], conocida como la *Directiva de los edulcorantes*, restringe los niveles a los que determinados edulcorantes pueden estar presentes en ciertos alimentos. Se define como *máxima dosis de uso* la *cantidad máxima de edulcorante que puede ser añadida a un producto alimenticio*. En caso de que no se especifique un valor máximo, se emplea el término *quantum satis*, que significa *cantidad adecuada*. Algunos edulcorantes para los que se indica el valor de máxima dosis empleada en esta Directiva son: acesulfamo K (E-950), aspartamo (E-951), ácido ciclámico y sus sales de Ca y Na (E-952), sacarina y sales de sodio y potasio (E-954) y taunatina (E-957). Para edulcorantes como sorbitol (E-420), manitol (E-421) o xilitol (E-967) se indica como dosis máxima de empleo el término *quantum satis*.

Teniendo en cuenta el interés que actualmente presenta el uso correcto de estos aditivos en alimentación, se han desarrollado diferentes metodologías para su análisis principalmente en bebidas refrescantes, con el principal objetivo de conocer si su contenido cumple con la legislación vigente [53].

1.2.6. Residuos tóxicos derivados del procesado de los alimentos

1.2.6.1. Nitrosaminas

A lo largo de la cadena alimentaria pueden incorporarse sustancias al alimento que reaccionen con otros de sus compuestos, dando lugar a productos tóxicos para la salud del consumidor. Es el caso de las *nitrosaminas*.

Son compuestos tóxicos que derivan de la *reacción de aminas secundarias con nitritos*, obtenidos estos últimos a partir de nitratos. Los *nitratos* en sí no son tóxicos, lo son su producto de transformación, los *nitritos*. El proceso por el cual se forman las nitrosaminas queda detallado en la figura 9.

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El nitrato puede transformarse en nitrito por reducción bacteriana tanto en los alimentos (durante el procesado y el almacenamiento), como en el propio organismo (en la saliva y el tracto gastrointestinal). Esto implica que el principal riesgo de formación de nitrosaminas proviene de la presencia de nitratos en los alimentos. Las diferentes vías de exposición humana a nitratos se indican en la figura 10. Como se indica en la figura, los nitratos pueden incorporarse a la cadena alimentaria por medios naturales, por su uso como fertilizantes o como aditivos para la conservación de la carne y embutidos.

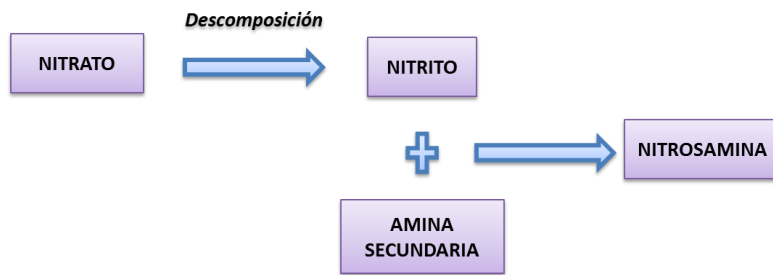


Figura 9. Formación de nitrosaminas.

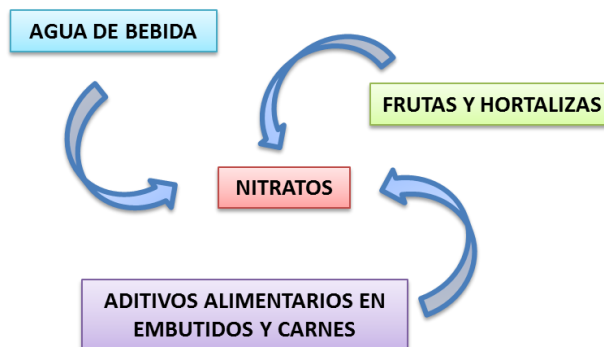


Figura 10. Vías de exposición humana a nitratos.

Los nitratos están presentes en el medio ambiente de forma natural como consecuencia del ciclo de nitrógeno. Se encuentran ampliamente distribuidos en los alimentos, siendo la principal fuente de exposición humana a nitratos el consumo de verduras y hortalizas, y en menor medida, el agua de bebida y

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otros alimentos. Algunas especies de vegetales acumulan los nitratos en sus partes verdes. Por tanto, los cultivos de hoja como las lechugas y espinacas generalmente presentan mayores concentraciones de estos compuestos. La clave para explicar esta situación reside en las condiciones climáticas, en concreto la luz como factor fundamental en el cultivo de estas hortalizas.

Una elevada intensidad lumínica favorece el metabolismo de la planta fijando el nitrógeno en compuestos orgánicos nitrogenados, como aminoácidos, proteínas, clorofila, etc., lo que reduce el contenido de nitratos, de modo que cualquier factor que reduzca la intensidad luminosa o la velocidad de la fotosíntesis favorece la acumulación de los mismos en la planta. Por eso, los cultivos de invierno presentan concentraciones de nitratos superiores a los de verano y por la misma razón, los cultivos en los países del norte de Europa presentan niveles superiores a los que tienen lugar en la zona sur. Por la misma razón, los cultivos al aire libre tienen menor contenido en nitratos que los de invernadero.

Además, los nitratos son empleados como fertilizantes o como aditivos alimentarios. Cabe destacar este último uso de nitratos en la cadena alimentaria. Los nitratos han sido empleados para la conservación de la carne y productos derivados durante décadas y actualmente se siguen empleando. Su adición inhibe el crecimiento de *Clostridium botulinum*, con la consiguiente disminución del riesgo de aparición de botulismo, una enfermedad causada por esta bacteria. Aunque el uso como conservante de nitratos inhibe el crecimiento de esta bacteria, existe el riesgo de transformación de nitratos a nitritos y posteriormente a nitrosaminas.

Numerosos estudios concluyen que hay una relación entre la ingesta de carne, por su tratamiento con nitratos como conservantes, y el riesgo de aparición de cáncer, principalmente cáncer de estómago [54-55]. Se conoce

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la presencia de aproximadamente 20 nitrosaminas diferentes en alimentos procesados procedentes de carne. De todas ellas, la que presenta mayor poder carcinogénico es N-nitrosodietilamina [56].

A nivel internacional, la EFSA ha evaluado el riesgo del consumo de nitratos para la salud humana, estableciendo un valor de referencia toxicológico: Ingesta Diaria Admisible (IDA) 3.65mgkg^{-1} de peso corporal. El Panel de Contaminantes en la Cadena Alimentaria (CONTAM) de la EFSA en 2008 evaluó los riesgos y los beneficios del consumo de productos vegetales debido a su contenido en nitratos [57] y concluyó que los efectos beneficiosos del consumo de estos alimentos supera el riesgo potencial para la salud humana derivado de la exposición a los nitratos a través de estos vegetales para la población general. Dado que la población más vulnerable al efecto toxicológico de los nitratos es la infantil, EFSA complementó la citada opinión en 2010 con un dictamen sobre los posibles efectos agudos de nitratos en bebés y niños pequeños que consumen espinacas y lechuga [58]. En este dictamen, el Panel concluyó que los niveles de nitratos en estos vegetales no son un problema de salud para la mayoría de los niños. Sin embargo, los bebés y niños pequeños de 1-3 años que consumen altas cantidades de espinacas con altos niveles de nitratos podrían, a veces, llegar a un nivel de consumo para los cuales el riesgo de metahemoglobinemia no se puede excluir. Otra de las conclusiones fue que el almacenamiento inadecuado de hortalizas de hoja cocidas (por ejemplo, verduras almacenadas a temperatura ambiente durante largos períodos de tiempo) puede resultar en la conversión de nitrato a nitrito, conversión que puede verse acelerada cuando estas hortalizas están en forma de puré. Partiendo de esta última conclusión, y teniendo en cuenta que las concentraciones de nitratos en vegetales pueden verse influenciadas no solo por diversos factores de tipo medioambiental o agronómico, sino también por las técnicas de procesado o cocinado utilizadas para preparar dichos vegetales, EFSA

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publicó en 2013 un Estudio sobre la influencia del procesado en los niveles de nitratos en las hortalizas [59]. Según este estudio, basándose en los resultados de los contenidos de nitratos medidos en vegetales antes y después de ser procesados, se puede concluir que el lavado, y el lavado en combinación con la ebullición, disminuyen los contenidos de nitratos independientemente del tipo de verdura [60].

I.3. Legislación aplicable a residuos de contaminantes en alimentos de origen animal, vegetal y productos derivados

I.3.1. Normativa sobre residuos de plaguicidas

I.3.1.1. Legislación Europea

La legislación europea aplicable a residuos de plaguicidas queda resumida en la tabla 4.

Tabla 4. Legislación europea aplicable a residuos de plaguicidas en alimentos.

Normativa	Descripción
<i>Directiva 91/414/CEE del Consejo</i> [61]	Relativa a la comercialización de productos fitosanitarios
<i>Directiva 2002/63/CE de la Comisión</i> [62]	Se establecen los métodos comunitarios de muestreo para el control oficial de residuos de plaguicidas en los productos de origen vegetal y animal y se deroga la <i>Directiva 79/700/CEE</i>
<i>Reglamento (CE) 396/2005 del Parlamento Europeo y del Consejo</i> [63]	Relativo a los límites máximos de residuos de plaguicidas en alimentos y piensos de origen vegetal y animal y que modifica la <i>Directiva 91/414/CEE del Consejo</i> [61]
<i>Reglamento (CE) 1213/2008 de la Comisión</i> [64]	Relativo a un programa comunitario plurianual coordinado de control para 2009, 2010 y 2011 destinado a garantizar el respeto de los límites máximos de residuos de plaguicidas

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<i>Reglamento (CE) 1107/2009 del Parlamento Europeo y el Consejo [65, 66]</i>	Relativo a la comercialización de productos fitosanitarios, por el que se derogan las Directivas 79/117/CEE y 91/414/CEE del Consejo
<i>Directiva 2009/128/CE del Parlamento Europeo y del Consejo [67]</i>	Se establece el marco de la actuación comunitaria para conseguir un uso sostenible de los plaguicidas
<i>Reglamento (CE) 901/2009 de la Comisión [68]</i>	Relativo a un programa comunitario plurianual coordinado de control para 2010, 2011 y 2012 destinado a garantizar el respeto de los límites máximos de residuos de plaguicidas
<i>Reglamento (UE) 915/2010 de la Comisión [69]</i>	Relativo a un programa plurianual coordinado de control de la Unión para 2011, 2012 y 2013 destinado a garantizar el respeto de los límites máximos de residuos de plaguicidas
<i>Reglamento en Ejecución (UE) 1274/2011 de la Comisión [70]</i>	Relativo a un programa plurianual coordinado de control de la Unión para 2012, 2013 y 2014 destinado a garantizar el respeto de los límites máximos de residuos de plaguicidas
<i>Reglamento en Ejecución (UE) 788/2012 de la Comisión [71]</i>	Relativo a un programa plurianual coordinado de control de la Unión para 2013, 2014 y 2015 destinado a garantizar el respeto de los límites máximos de residuos de plaguicidas
<i>Reglamento de ejecución (UE) 400/2014 de la Comisión [72]</i>	Relativo a un programa plurianual coordinado de control de la Unión para 2015, 2016 y 2017 destinado a garantizar el respeto de los límites máximos de residuos de plaguicidas. El procedimiento de muestreo seguido debe ser conforme con las disposiciones de la <i>Directiva 2002/63/CE</i> [62]

1.3.1.2. Legislación española.

La legislación española aplicable a residuos de plaguicidas en alimentos queda resumida en la tabla 5.

I. INTRODUCCIÓN Y ANTECEDENTES

Tabla 5. Legislación española aplicable a residuos de plaguicidas en alimentos.

Normativa	Descripción
<i>Ley 43/2002 [73]</i>	Se establece la base jurídica en materias de comercialización y utilización de productos fitosanitarios, así como en las relativas a la racionalización y sostenibilidad de su uso, que no tuvieron desarrollo normativo en previsión de divergencias con la normativa comunitaria pendiente de surgir en la aplicación de la estrategia sobre el uso sostenible de plaguicidas
<i>Real Decreto 1201/2002 [74]</i>	Se regula la producción integrada de productos agrícolas para el control y la lucha contra las plagas
<i>Real Decreto 290/2003 [75]</i>	Se establecen los métodos de muestreo para el control de residuos de plaguicidas en los productos de origen vegetal y animal
<i>Real Decreto 1702/2011 [76]</i>	Sobre inspecciones periódicas de los equipos de aplicación de productos fitosanitarios
<i>Real Decreto 1311/2012 [77]</i>	Se establece el marco de actuación para conseguir un uso sostenible de los productos fitosanitarios y el fomento de la gestión integrada de plagas y de planteamientos o técnicas alternativos

1.3.2. Normativa sobre residuos de micotoxinas

1.3.2.1. Legislación española

✳ *Real Decreto 475/1988 [13]*, de 13 de Mayo de 1988, por el que se establecen los límites máximos permitidos de las aflatoxinas B₁, B₂, G₁ y G₂ en alimentos para consumo humano.

1.3.2.2. Legislación europea

La tabla 6 muestra de forma resumida la legislación europea aplicable a micotoxinas.

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Tabla 6. Legislación europea aplicable a micotoxinas.

Normativa	Descripción		
<i>Directiva 93/5/CEE [89]</i>	Se han establecido contenidos máximos para la patulina en determinados productos alimenticios		
<i>Recomendación 2003/598 [86]</i>	Relativa a la prevención y la reducción de la contaminación por patulina del zumo de manzana y los ingredientes de zumo de manzana en otras bebidas		
<i>Recomendación 2006/583/CE de la Comisión [87]</i>	Contiene principios generales para la prevención y la reducción de la contaminación con toxinas de <i>Fusarium</i> (zearalenona, fumonisinas y tricotecenos) en los cereales		
<i>Reglamento 1881/2006 [78]</i>	Se fija el contenido máximo de determinados contaminantes en los productos alimenticios.	Aflatoxinas	Frutos secos, cereales, leche y alimentos infantiles
		Ochratoxina A	Cereales, uvas pasas, café, vino, zumo de uva, alimentos a base de cereales, alimentos dietéticos, alimentos para lactantes y niños de corta edad
		Patulina	Zumos de frutas, bebidas elaboradas con manzana, alimentos infantiles y productos sólidos elaborados con manzana
		Deoxinivalenol	Cereales, pasta, pan y alimentos infantiles a base de cereales
		Zearalenona	Cereales, aperitivos y alimentos infantiles a base de cereales
		Fumonisinias	Cereales y alimentos elaborados a base de maíz

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<i>Reglamento 1881/2006 [78]</i>	Modificado por: Reglamento (UE) 1126/2007 de la Comisión [79], Reglamento (UE) 165/2010 de la Comisión [80], Reglamento (UE) 105/2010 de la Comisión [81], Reglamento (UE) 1058/2012 de la Comisión [82], Reglamento (UE) 594/2012 de la Comisión [83]
<i>Reglamento (CE) 401/2006 de la Comisión [84]</i>	Se establecen los métodos de muestreo y de análisis para el control oficial del contenido de micotoxinas en los productos alimenticios
<i>Reglamento 178/2010 de la Comisión [85]</i>	En lo que respecta a los cacahuets y otras semillas oleaginosas, a los frutos de cáscara arbóreos, a los huesos de albaricoque, al regaliz y al aceite vegetal
<i>Recomendación 2013/165/UE [88]</i>	Sobre la presencia de las toxinas T-2 y HT-2 en los cereales y los productos a base de cereales

1.3.3. Normativa sobre residuos de medicamentos de uso veterinario

1.3.3.1. Legislación europea

La legislación europea más destacada y que es aplicable a este tipo de residuos se indica en la tabla 7.

Tabla 7. Legislación europea aplicable a residuos de medicamentos de uso veterinario.

Normativa	Descripción
<i>Reglamento (CEE) 2377/90 del Consejo [26]</i>	Por el que se establece un procedimiento comunitario de fijación de los límites máximos de residuos de medicamentos veterinarios en los alimentos de origen animal. Se detalla un listado de sustancias farmacológicamente activas cuya utilización en animales productores de alimentos está prohibida
<i>Reglamento (CEE) 2377/90 del Consejo [26]</i>	Modificado por: Reglamento (CE) Nº 324/2004 de la Comisión [92], Reglamento (CE) 124/2009 de la Comisión [93], este último modificado a su vez por Reglamento (UE) 610/2012 de la Comisión [94]
<i>Reglamento 2821/98 del Consejo [90]</i>	Sobre los aditivos en la alimentación animal, en lo que respecta a la revocación de la utilización de determinados antibióticos

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<i>Reglamento (CE) 470/2009 del Parlamento Europeo y del Consejo [95]</i>	Se establecen procedimientos comunitarios para la fijación de los límites de residuos (MRLs) de las sustancias farmacológicamente activas en los alimentos de origen animal, se deroga el Reglamento (CEE) 2377/90 del Consejo [26] y se modifican la Directiva 2001/82/CE [96] y el Reglamento (CE) 726/2004 [97]
Reglamento (UE) 37/2010 de la Comisión [98]	Relativo a las sustancias farmacológicamente activas y su clasificación por lo que se refiere a los límites máximos de residuos en los productos alimenticios de origen animal. En él se recogen los límites máximos de residuos (MRLs) de sustancias farmacológicamente activas en los alimentos de origen animal contemplados en los anexos del Reglamento 2377/90 [26]

1.3.3.2. Legislación española

En la tabla 8 se indica la normativa española aplicable a residuos de medicamentos de uso veterinario más destacada.

Tabla 8. Legislación española aplicable a residuos de medicamentos de uso veterinario en alimentos.

Normativa	Descripción
<i>Real Decreto 1749/1998 [99]</i>	Se establecen las medidas de control aplicables a determinadas sustancias y sus residuos en los animales vivos y sus productos. Incorpora la <i>Directiva 96/23/CEE del Consejo</i> [100]. Se desarrolla la creación y organización de planes de vigilancia de residuos en los productos de origen animal, estableciéndose medidas de seguimiento ante resultados no conformes
<i>Real Decreto 2178/2004 [101]</i>	Se prohíbe utilizar determinadas sustancias de efecto hormonal y tireostático beta-agonistas de uso en la cría de ganado

1.3.4. Normativa sobre residuos de materiales en contacto con alimentos

1.3.4.1. Plásticos y polímeros

1.3.4.1.1. Legislación europea

La legislación europea más destacada aplicable a residuos de plásticos y polímeros en alimentos se indica en la tabla 9.

Tabla 9. Legislación europea aplicable a residuos de plásticos y polímeros en alimentos.

Normativa	Descripción
<i>Reglamento (CE) 282/2008 de la Comisión [102]</i>	Sobre materiales y objetos de plástico reciclado destinados a entrar en contacto con alimentos y por el que se modifica el Reglamento (CE) 2023/2006 [103] sobre buenas prácticas de fabricación de materiales y objetos destinados a entrar en contacto con alimentos
<i>Reglamento (UE) 10/2011 de la Comisión [33]</i>	Sobre materiales y objetos plásticos destinados a entrar en contacto con alimentos

1.3.4.1.2. Legislación española

La legislación española aplicable a residuos de plásticos y polímeros en alimentos se indica en la tabla 10.

Tabla 10. Legislación española aplicable a residuos de plásticos y polímeros en alimentos.

Normativa	Descripción
<i>Directiva 85/572/CEE del Consejo [108]</i>	Se determina la lista de los simulantes que se deben utilizar para controlar la migración de los componentes de los materiales y objetos de material plástico destinados a entrar en contacto con los productos alimenticios

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<i>Directiva 2002/72/CE de la Comisión [34]</i>	Relativa a los materiales y objetos plásticos destinados a entrar en contacto con productos alimenticios
<i>Real Decreto 866/2008 [104]</i>	Aprueba la lista de sustancias permitidas para la fabricación de materiales y objetos plásticos destinados a entrar en contacto con los alimentos Modificado por: Real Decreto 103/2009 [105], Reglamento (CE) 975/2009 de la Comisión [106], Orden PRE/628/2011 de 22 de marzo [107]
<i>Real Decreto 846/2011 [109]</i>	Se establecen las condiciones que deben cumplir las materias primas a base de materiales poliméricos reciclados para su utilización en materiales y objetos destinados a entrar en contacto con alimentos. Modificado por: Real Decreto 517/2013 [110]

1.3.4.2. Compuestos perfluorados

La normativa europea aplicable a residuos de compuestos perfluorados en alimentos se indica en la tabla 11.

Tabla 11. Legislación europea aplicable a residuos de compuestos perfluorados en alimentos.

Normativa	Descripción
<i>Dictamen científico de la EFSA [45]</i>	Sobre sulfonatos de perfluorooctano (PFOS), el ácido perfluorooctanoico (PFOA) y sus sales. Se estima poco probable que estas sustancias estén teniendo efectos nocivos en la población general, pero se manifiestan ciertas dudas respecto a las repercusiones en el desarrollo de organismos vivos

1.3.5. Normativa sobre aditivos

1.3.5.1. Legislación europea

La legislación europea aplicable a aditivos en alimentos se detalla en la tabla 12.

Tabla 12. Legislación europea aplicable a la presencia de aditivos en alimentos.

Normativa	Descripción
<i>Reglamento 1331/2008 del Parlamento Europeo y del Consejo [111]</i>	Se establece un procedimiento de autorización común para los aditivos, las enzimas y los aromas alimentarios. En el anexo II de este Reglamento se recogen los aditivos que se pueden utilizar en el territorio de la Unión y se indican las dosis máximas y los alimentos en los que se pueden adicionar
<i>Reglamento (UE) 231/2012 de la Comisión [112]</i>	Se establecen especificaciones para los aditivos alimentarios que figuran en los anexos II y III del Reglamento (CE) 1333/2008

1.3.5.2. Legislación española

En la tabla 13 se indica la normativa española aplicable a aditivos en alimentos.

Tabla 13. Legislación española aplicable a la presencia de aditivos en alimentos.

Normativa	Descripción
<i>Directiva 94/35/CE [116]</i>	Relativa a los edulcorantes utilizados en los productos alimenticios
<i>Real Decreto 2001/1995 [113]</i>	Se aprueba la lista positiva de colorantes autorizados para su uso en la elaboración de productos alimenticios así como sus condiciones de utilización

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<i>Real Decreto</i> <i>2002/1995 [114]</i>	Se aprueba la lista positiva de aditivos edulcorantes autorizados para su uso en la elaboración de productos alimenticios, así como sus condiciones de utilización
Real Decreto 142/2002 [115]	Se aprueba la lista positiva de aditivos distintos de colorantes y edulcorantes para su uso en la elaboración de productos alimenticios, así como sus condiciones de utilización

1.3.6. Normativas sobre el uso de nitratos, precursores de nitrosaminas

En la tabla 14 se indica la legislación europea más destacada y aplicable al uso de residuos de nitratos en alimentos.

Tabla 14. Legislación europea aplicable al uso de nitratos en alimentos.

Normativa	Descripción
<i>Reglamento (CE)</i> <i>1881/2006 de la</i> <i>Comisión [78]</i>	Se establecen límites máximos en lechugas, espinacas y alimentos infantiles. En él se afirma que la principal fuente de ingesta humana de nitratos son las hortalizas, como afirmó el Comité Científico de la alimentación humana (CCAH). Modificado por: Reglamento (UE) 1258/2011 [117]

I.4. Estrategias para el análisis de residuos de plaguicidas, micotoxinas, medicamentos de uso veterinario, plastificantes, edulcorantes, nitrosaminas y compuestos perfluorados en frutas, vegetales y productos derivados. Aspectos generales

Dada la *gran cantidad de contaminantes orgánicos* objeto de estudio en la amplia variedad de muestras de alimentos sólidos, semisólidos y líquidos disponibles, es importante el desarrollo de *métodos analíticos precisos, selectivos, sensibles y automáticos* que permitan la extracción, separación, identificación y cuantificación de estos compuestos. El procedimiento que se

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sigue para la determinación de estos compuestos en muestras de alimentos es el que se muestra en el esquema de la figura 11:



Figura 11. Procedimiento seguido para la determinación de contaminantes.

La muestra es sometida a un *tratamiento* en el que se obtiene un extracto con los analitos de interés, aislados del resto de la matriz e interferencias en una etapa de *clean up* o purificación del extracto. Tras esto, el extracto es sometido a técnicas adecuadas de separación, identificación y cuantificación de los analitos. Las técnicas analíticas que se vienen empleado en los últimos años para el análisis multi-residuo de contaminantes orgánicos están basadas en el acoplamiento cromatografía/espectrometría de masas.

A continuación se exponen los tratamientos de preparación de muestra que se emplean con mayor frecuencia para el análisis multi-residuo en frutas, verduras y productos procesados, así como las técnicas más comunes empleadas para la separación, detección e identificación.

1.5. Tratamientos de muestra empleados en fruta, verdura y productos procesados para análisis multiresiduo. Antecedentes

El procedimiento de preparación de la muestra consiste en una serie de pasos encaminados a la obtención de un extracto con los analitos de interés.

La *muestra* de fruta, verdura o producto procesado es *homogeneizada* normalmente con un disolvente orgánico (o con disolvente orgánico y agua) para facilitar la extracción de los analitos. Para muestras sólidas y semisólidas se requiere un paso previo de trituración. Una vez se produce la *extracción*, en el extracto quedarán interferencias, pudiendo ser eliminadas mediante una *etapa de purificación*. El extracto resultante deberá encontrarse en un

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disolvente apropiado, compatible con la técnica de separación y determinación de los analitos que posteriormente se empleará.

Los tratamientos de muestra que con mayor frecuencia se emplean para el análisis multiresiduo en muestras de fruta, verdura y productos procesados son los que se indican en la figura 12.

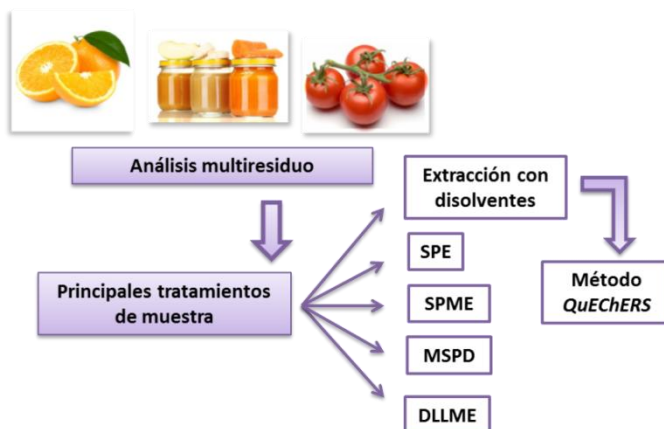


Figura 12. Principales tratamientos de muestra empleados para el análisis multiresiduo en muestras de verdura, fruta y productos procesados.

En los siguientes apartados se indicarán aspectos generales y antecedentes en análisis multiresiduo en muestras de fruta, verdura y productos procesados de cada uno de ellos. Los más destacados son la extracción con disolventes (SLE y LLE), dentro de la cual puede incluirse el conocido como *método QuEChERS* y la extracción en fase sólida (SPE). Debido a la creciente tendencia a la disminución de las cantidades de disolvente empleado en la extracción y a la miniaturización de los procesos de tratamiento de muestra, están siendo cada vez más común el empleo de técnicas miniaturizadas como la microextracción en fase sólida (MSPE), la dispersión de matriz en fase sólida (MSPD) y la extracción líquido-líquido dispersiva (DLLME), motivo por el cual serán incluidos en este apartado. Cabe destacar que algunos de los tratamientos de muestra descritos pueden ser empleados como etapa de

clean up o purificación del extracto obtenido con otro tratamiento previamente empleado. Así, se puede realizar una SPE, MSPD ó dSPE (segunda etapa del método *QuEChERS*) tras una extracción con disolventes.

1.5.1. Extracción con disolventes

La extracción con disolventes, que puede ser posteriormente seguida por una etapa de *clean up* o purificación del extracto obtenido, es una técnica de preparación de muestra fácil de emplear y con un amplio rango de aplicabilidad. El procedimiento varía ligeramente en función de si la muestra es sólida o líquida.

Uno de los aspectos importantes a tener en cuenta es la *elección del disolvente de extracción*, que permita la solubilidad y extracción de compuestos con un amplio rango de polaridad, así como su compatibilidad con la técnica de separación e identificación que posteriormente se emplee.

Para la extracción de pesticidas en muestras de fruta y verdura inicialmente se empleaba acetona seguida de diclorometano y éter de petróleo (método Luke) [118] y acetato de etilo. Con el tiempo, diferentes aspectos de estos métodos se han modificado, como la sustitución de disolventes organoclorados como diclorometano por otros que causan menor impacto ambiental [119]. Los disolventes de extracción que con mayor frecuencia se han empleado hasta el momento en métodos de análisis de contaminantes orgánicos en muestras de fruta y verdura son *acetona* [118,120,150], *acetato de etilo* [121,122] y *acetonitrilo* [123-126].

Una posterior *etapa de limpieza* de los extractos suele ser requerida debido a que con ella se mejoran los límites de detección de los analitos y se eliminan interferencias de la matriz. Esta suele llevarse a cabo mediante SPE [124, 127-129], cromatografía de permeación en gel (*CPG, gel permeation*

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chromatography) [130,131] o extracción en fase sólida dispersiva (dSPE, *dispersive solid-phase extraction*) [125,126].

Algunas de las desventajas de esta técnica son la gran cantidad de disolvente empleado y la posibilidad de formación de emulsiones en la interfase de ambos disolventes.

Dentro de esta categoría se puede incluir el *método QuEChERS* (acrónimo de las palabras inglesas “*Quick, Easy, Cheap, Effective, Rugged and Safe*”). Esta metodología consta de dos etapas, como queda reflejado en la siguiente figura:

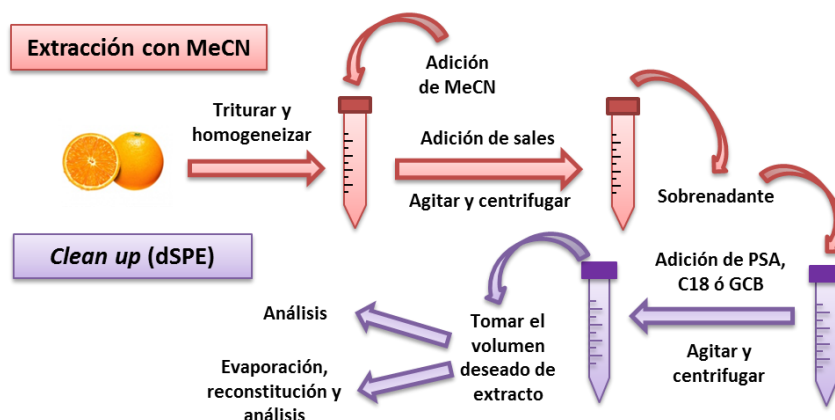


Figura 13. Procedimiento seguido para la realización del método QuEChERS.

Una vez la muestra es triturada y homogeneizada es sometida a las dos etapas de este método:

1.-*Extracción con acetonitrilo:* en esta etapa se puede adicionar un tampón formado por el par acetato sódico/ácido acético, además de $MgSO_4$ anhidro que ayuda a mejorar las recuperaciones así como a favorecer el reparto de los analitos en la fase orgánica. La muestra se agita y centrifuga.

2.-*Clean up*: esta etapa de purificación está basada en una extracción en fase sólida dispersiva (dSPE). Para ello, se toma un volumen determinado de sobrenadante generado en la etapa anterior y se adicionan MgSO_4 anhidro para la eliminación del agua que pueda quedar en la fase orgánica y un sorbente (generalmente amina primaria secundaria (PSA), C_{18} o carbono grafitizado (GCB)), que proporciona una elevada capacidad de limpieza de los componentes de la matriz (azúcares, ácidos grasos, ácidos orgánicos, pigmentos, etc). El sorbente empleado dependerá de los analitos de interés. Así, para mejorar la extracción en frutas y vegetales de algunos plaguicidas sensibles al pH, se desarrolló un protocolo en el que el tampón ácido acético/acetato aseguraba la extracción a pH ácido [132]; para la extracción de plaguicidas en alimentos con bajo contenido graso se utilizó C_{18} además de PSA en la etapa de purificación del extracto [133]; finalmente, para alimentos con alto contenido graso se incorporó el carbón grafitizado [134]. Tras este proceso se lleva a cabo una centrifugación y el extracto podrá ser analizado posteriormente o bien evaporado y reconstituido en otro disolvente para su posterior análisis.

Este método de extracción fue desarrollado en 2003 [135] y posteriormente validado [136,137] para la recuperación de más de 200 pesticidas en frutas y verduras. En bibliografía, se han publicado más de 700 artículos que emplean como tratamiento de muestra el descrito anteriormente. Muchos de ellos están dedicados al análisis multiresiduo de pesticidas [138,141], micotoxinas [142], pesticidas y micotoxinas [143] y drogas veterinarias [144-145] en muestras de fruta, verdura o productos procesados.

1.5.2. Extracción en fase sólida (SPE)

En la extracción en fase sólida, empleada principalmente para muestras líquidas, la muestra se pasa a través de un cartucho que contiene un

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sorbente sólido, donde los analitos son retenidos y posteriormente eluidos con un disolvente apropiado. Volúmenes entre 2 y 100 mL de muestra son empleados.

Existe gran variedad de sorbentes para SPE permiten la determinación de analitos con amplio rango de polaridad y propiedades físico-químicas. Así, pueden encontrarse sorbentes como las sílices enlazadas químicamente con cadenas alquílicas (C-18, C-8), grupos polares (-CN, -NH₂), grupos como el ácido carboxílico o grupos amino, polímeros porosos (estireno-divinilbenceno), Florisil (silicato de magnesio activado) y GCB. Recientemente, el empleo de adsorbentes de balance hidrofílico-lipofílico, como el Oasis® HLB (Waters) [146] está teniendo una gran aplicación.

El procedimiento seguido para llevar a cabo la SPE consta de 4 etapas. Un esquema de los pasos seguidos se detalla en la figura 14.

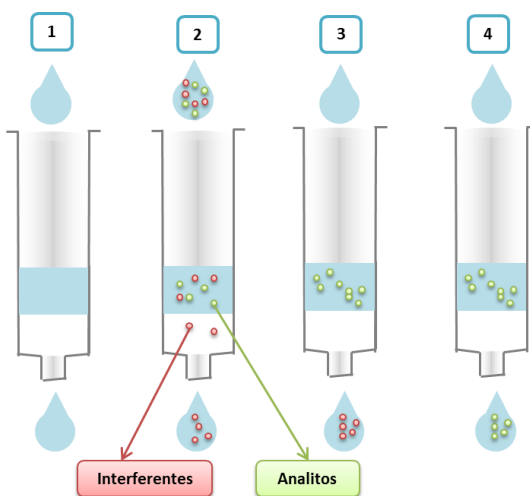


Figura 14. Procedimiento de extracción en fase sólida.

1. *Acondicionamiento*: el sorbente es acondicionado con un disolvente de propiedades similares a la muestra.

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2. *Carga de la muestra*: la muestra que contiene los analitos se pasa a través del sorbente. En esta etapa los analitos y otros interferentes quedarán retenidos en el cartucho.
3. *Lavado*: se emplea un disolvente o mezcla de disolventes que, al pasar a través del cartucho, elimina interferencias pero no eluye los analitos.
4. *Elución*: a través del sorbente previamente lavado en el que se encuentran retenidos los analitos, se pasa un disolvente apropiado para eluirlos.

El extracto obtenido puede ser evaporado y reconstituido en otro disolvente que sea más apropiado y afín con la técnica que posteriormente se emplee para la separación, identificación y cuantificación de los analitos [142].

Esta técnica ha sido muy utilizada en el análisis de contaminantes en alimentos [147,148]. Se ha empleado para el tratamiento previo de la muestra en análisis de residuos de plaguicidas en vinos [142,149], frutas y vegetales [150,151] o miel [152]. También ha sido utilizada como técnica de clean up o purificación del extracto obtenido mediante otra técnica de preparación de muestra, como extracción con disolventes [150] o MSPD [153,154].

1.5.3. Dispersión de matriz en fase sólida (MSPD)

El procedimiento seguido para la MSPD queda esquematizado en la figura 15. Una pequeña cantidad de muestra (entre 0.5 y 1 g) se mezcla en un mortero con una cantidad similar (2 g) de un sorbente adecuado (C_{18} , alúmina, sílice enlazada con aminopropil, etc) hasta conseguir una mezcla homogénea [155]. Esta mezcla se coloca en un cartucho de extracción y los analitos son eluidos con un disolvente. El volumen de disolvente extractante suele estar comprendido entre 2 y 10 mL.

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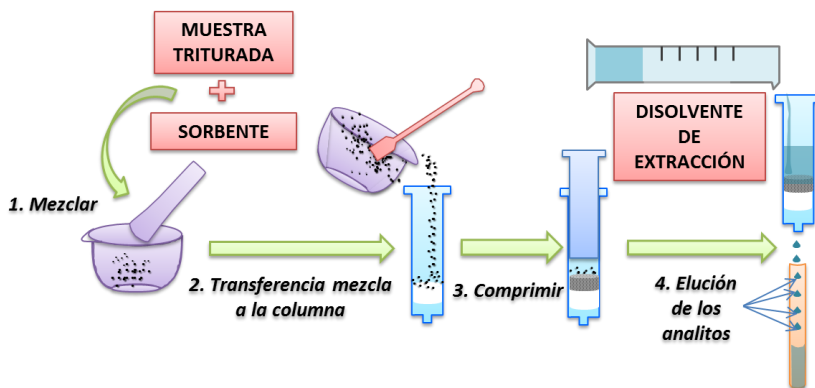


Figura 15. Procedimiento seguido para la MSPD.

La elección del sorbente empleado depende de la polaridad de los analitos y de sus propiedades fisicoquímicas. Los sorbentes empleados con mayor frecuencia son sílice enlazada- C_{18} y fluorisil, aunque también pueden utilizarse tierra de diatomeas, alúmina y C_8 .

Este tratamiento de muestra ha sido empleado en la determinación de pesticidas [156, 157] y micotoxinas [158-160] en alimentos.

En general, presenta como ventaja el empleo de pequeños volúmenes de disolvente extractante y de poca cantidad de muestra.

1.5.4. Microextracción en fase sólida (SPME)

Este tratamiento de muestra se basa en el uso de una fibra de sílice fundida recubierta con una película delgada de un polímero adecuado, que actúa de fase estacionaria [161]. Esta fibra está unida a una varilla de acero inoxidable y se encuentra en el interior de un tubo hueco, de modo que puede retraerse y sacarse de su interior, quedando expuesta a la muestra. Entre las ventajas de esta técnica se puede destacar que se emplean pequeños volúmenes de disolvente y muestra; permite la extracción de contaminantes polares, semipolares y no polares en matrices sólidas, líquidas y gaseosas; es compatible con cromatografía de líquidos y gases y posibilidad de

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automatización; permite realizar extracción y preconcentración de los analitos al mismo tiempo; no implica el uso de disolventes tóxicos.

En este proceso están implicadas *dos etapas*:

1. *Etapas de extracción*: en ella los analitos son retenidos en la fase estacionaria por medio de un proceso de adsorción. Para ello, la fibra se sumerge directamente en una disolución, proceso conocido como SPME de inmersión directa (*DI-SPME – direct inmersión SPME*) o se mantiene en el espacio en cabeza que está en equilibrio con la disolución, proceso conocido como SPME de espacio de cabeza (*HS-SPME – headspace-SPME*).
2. *Etapas de desorción*: se puede hacer térmicamente (en el inyector de un cromatógrafo de gases), o utilizando un disolvente orgánico (de forma manual, o acoplado con un cromatógrafo de líquidos).

Los factores que hay que optimizar para llevar a cabo la SPME son: fuerza iónica, PH, disolvente de desorción, temperatura de adsorción y desorción, velocidad de agitación de la muestra (para homogeneizarla durante el calentamiento), volumen de muestra y tiempo de extracción. Éste último va a depender del espesor de la fibra, siendo este tiempo mayor cuanto más gruesa es. Una ventaja del empleo de fibras de mayor espesor de adsorbente es que la cantidad de analitos extraídos es mayor, aunque el riesgo de que se retengan también compuestos de la matriz aumenta.

El recubrimiento de la fibra empleada en este proceso dependerá de las propiedades fisicoquímicas de los analitos. Existen en el mercado fibras con recubrimiento homogéneo y heterogéneo. La fibra que más comúnmente se emplea para la extracción de pesticidas en muestras de fruta y verdura es PDMS (polidimetilsiloxano) [162-165]. Otras fibras que se han empleado con el mismo fin son PDMS/DVB (polidimetilsiloxano/divinilbenceno) [166],

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CW/PDMS (carbowax/PDMS) [167], CW/TPR (CW/resina) [168] y AC/PVC (carbón activo/cloruro de polivinilo) [169].

1.5.5. Microextracción Líquido-Líquido Dispersiva (DLLME)

Esta técnica miniaturizada de preparación de muestra permite la realización de una extracción y preconcentración al mismo tiempo. Ha sido empleada satisfactoriamente para la extracción de compuestos orgánicos e inorgánicos a nivel de trazas [170,171]. Comparada con la extracción de disolventes convencional, la recuperación de los analitos puede ser menor, pero la concentración que queda en la fase orgánica final es claramente incrementada. El procedimiento de extracción se detalla en la siguiente figura:

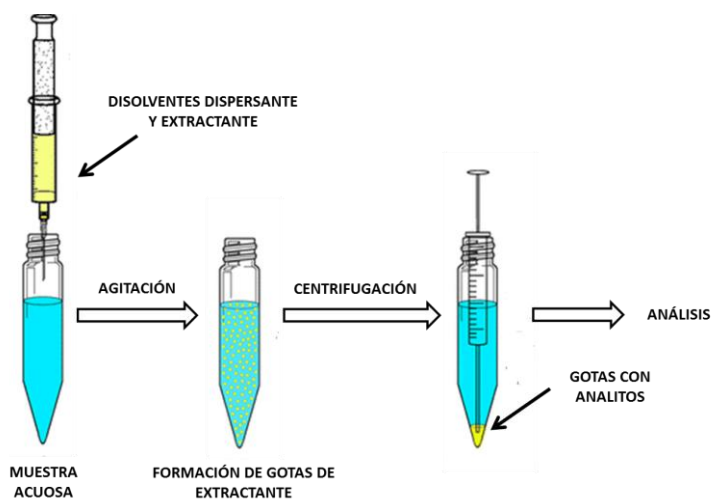


Figura 16. Procedimiento seguido para la DLLME.

La DLLME se basa en el empleo de un sistema ternario formado por un disolvente no polar e inmiscible con agua (disolvente extractante), un disolvente polar y miscible con agua (disolvente dispersante) y la muestra en fase acuosa.

El procedimiento consiste en preparar una mezcla con los disolventes extractante y dispersante de modo que el volumen de disolvente extractante suponga entre un 1 y un 3% del volumen total de la mezcla. Esa mezcla se añade rápidamente mediante inserción con jeringa al tubo de centrifuga que contiene la muestra acuosa que contiene los analitos de interés. Esta rápida inyección produce una gran turbulencia, originándose la formación de finas gotas de extractante que se dispersan a través de la muestra acuosa. Tras la centrifugación, las gotas se depositan en el fondo de un tubo cónico, siendo posible el análisis de esta fase para la determinación de los analitos de interés.

Factores que afectan a este proceso son la elección del disolvente extractante y agente dispersante y los volúmenes empleados de cada uno de ellos. Por lo general, los agentes dispersantes que con mayor frecuencia se emplean son acetona, metanol y acetonitrilo, mientras que como disolventes extractantes se emplean disolventes clorados (clorobenceno, tetracloruro de carbono, tetracloroetileno) y no clorados (undecanol, 1-dodecanol, 2-dodecanol y n-hexadecano).

Esta técnica de preparación de muestra ha sido aplicada mayormente al análisis de pesticidas y fármacos en muestras de agua, con interés medioambiental. También ha sido aplicada a muestras de fruta y verdura para la determinación de pesticidas [172-174].

I.6. Determinación de pesticidas y otros contaminantes en alimentos mediante el acoplamiento cromatografía-espectrometría de masas.

Antecedentes

La determinación de pesticidas y otros contaminantes en alimentos ha evolucionado considerablemente. En los años 70, los análisis de residuos de pesticidas se llevaban a cabo mediante cromatografía de gases (GC)

combinada con detector de captura de electrones (ECD), detector fósforo-nitrógeno (NPD) y detector fotométrico de llama (FPD) y se requería otro tipo de detector para realizar la confirmación de los resultados. Mucho menos frecuente era el uso de la cromatografía de líquidos (LC), debido a que los detectores de ultravioleta (UV) y de fluorescencia con los que se empleaba eran poco sensibles y poco selectivos comparados con los detectores empleados en aquel momento para GC [175].

Actualmente, la *espectrometría de masas* (MS) es la técnica de detección de contaminantes en alimentos más empleada. Para introducir la muestra en un espectrómetro de masas éste debe ser acoplado a una técnica separativa: cromatografía gaseosa (GC-MS) o cromatografía líquida (LC-MS).

Así, en lo que concierne al acoplamiento GC-MS y LC-MS, una de las mejoras que la espectrometría de masas introduce en GC con respecto al uso de detectores ECD, FPD y NPD es que permite la determinación y confirmación en un único análisis y acoplada a LC proporciona una mayor sensibilidad en comparación con los detectores de fluorescencia y UV que se empleaban antiguamente [175]. Estas y otras ventajas, junto con los requerimientos de la DG Sanco 12571/2013 [176] y de la Directiva 2002/567/CE [177] para la identificación de los analitos y la confirmación de resultados, hacen que la cromatografía tanto de gases como de líquidos acoplada a espectrometría de masas sea una de las técnicas de detección más importantes empleadas en el análisis de residuos de pesticidas y otros contaminantes a día de hoy [175].

Hasta la fecha se conoce un *gran número de pesticidas y otros compuestos* que pueden ser empleados a lo largo de la cadena alimentaria y que son susceptibles de ser detectados en muestras de alimentos. Además de ese amplio número hay que destacar la *variabilidad de propiedades fisicoquímicas* que presentan. Así, el intervalo de polaridad de los compuestos objeto de análisis en alimentos es bastante amplio. Las

metodologías analíticas empleadas para el análisis multiresiduo que se han empleado usando GC-MS han sido aplicadas a *compuestos apolares, térmicamente estables y volátiles* [178]. El análisis de *compuestos polares, térmicamente inestables y/o con baja volatilidad* requiere una etapa de derivatización en caso de que se quieran determinar por GC-MS, y este proceso no siempre es satisfactorio. Cabe destacar que es cada vez más común el empleo de contaminantes, en concreto plaguicidas, de mayor polaridad, ya que se ha comprobado que son más respetuosos con el medio ambiente, siendo degradados y eliminados con mayor facilidad. Este motivo hace que las técnicas de LC-MS que permiten la determinación de este tipo de compuestos sin etapa previa de derivatización se empleen cada vez más y estén desplazando a las técnicas de GC-MS. Sin embargo, no todos los compuestos pueden ser analizados por LC-MS; existen compuestos apolares como los organoclorados que sólo pueden ser analizados por GC-MS, aunque el empleo de estos pesticidas es cada vez más limitado debido a las distintas normativas que prohíben su uso. Esto explica que para el determinación del amplio número de contaminantes y dada la gran variedad de propiedades fisicoquímicas que presentan, es necesario tanto el empleo de GC-MS como de LC-MS. A pesar de que ambas técnicas son necesarias, estudios recientes han comprobado la mayor versatilidad de LC-MS, que cubre una mayor variedad de productos fitosanitarios [175]. Los resultados obtenidos en el trabajo de Alder y col. [175] quedan reflejados en el diagrama de Venn de la figura 17. De acuerdo con este estudio, realizado a un total de 500 pesticidas considerados como los más importantes en Alemania, usando LC-MS y GC-MS, el 64% pudieron ser determinados empleando ambas técnicas; de los compuestos que no era posible analizar empleando las dos técnicas (182), el 75% fueron analizados sólo por LC-MS, mientras que sólo un 25% fueron analizados por GC-MS.

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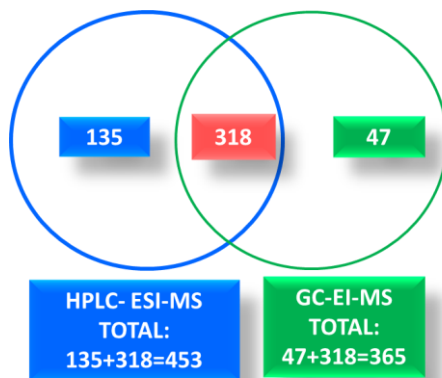


Figura 17. Diagrama de Venn para el análisis de 500 pesticidas mediante HPLC-ESI-MS y GC-EI-MS, de acuerdo con los resultados obtenidos en el trabajo de Alder et al. [175]

En resumen, aunque GC-MS continúa empleándose para el análisis de compuestos volátiles y moderadamente apolares, los avances en LC-MS han desembocado en el desarrollo de una eficiente y poderosa instrumentación para el análisis de compuestos más polares e iónicos, incluyendo pesticidas, drogas veterinarias, toxinas, contaminantes emergentes y otros contaminantes a nivel de trazas, en la que la fuente de ionización más empleada es electrospray (ESI)[179]. En concreto, la cromatografía de líquidos de alta resolución (HPLC) acoplada a espectrometría de masas (HPLC-MS) ha sido seleccionada como la técnica más popularmente empleada en la última década en el desarrollo de métodos multiresiduo/multiclase para la determinación de productos agroquímicos y micotoxinas [180].

La tendencia a incluir en un mismo método multiresiduo no sólo un amplio número de compuestos sino también diferentes clases de contaminantes (pesticidas, micotoxinas, plastificantes, drogas veterinarias, etc.), así como a disminuir al máximo el tiempo de análisis, hacen que el desarrollo de nuevas metodologías mediante LC-MS con diferentes analizadores se investigue con especial interés. Existen numerosos trabajos en los que se hace una revisión

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profunda de los métodos multiresiduo que se han desarrollado hasta la fecha para la determinación de pesticidas y otros contaminantes utilizando LC-MS con diferentes analizadores [179-185]. De acuerdo con los métodos desarrollados, dos aproximaciones pueden emplearse en LC-MS:

-Espectrometría de masas de Alta Resolución (High Resolution Mass Spectrometry, HRMS): esta aproximación proporciona alta resolución, valores de masa exacta y elevada sensibilidad y selectividad en modo full scan. Puede ser empleada para el análisis de compuestos conocidos y desconocidos y permite trabajar en modo full scan y MS/MS [186].

-Espectrometría de masas en tándem (MS/MS): para aumentar la selectividad y sensibilidad, así como para conseguir fragmentos de las moléculas de analito que conduzcan a una confirmación inequívoca de su presencia en la muestra sometida a análisis se emplea este tipo de espectrometría. Un ión precursor es seleccionado en una celda de colisión y se mide el valor de m/z de los iones producto. Se puede trabajar con un único analizador de masas o con combinación de varios analizadores.

Los analizadores disponibles hasta la fecha que pueden ser acoplados a un cromatógrafo de líquidos son:

- Cuadrupolo sencillo (Q)
- Trampa de iones (IT)
- Triple cuadrupolo (QQQ)
- Tiempo de vuelo (TOF)
- Cuadrupolo-tiempo de vuelo (Q-TOF)
- Orbitrap sencillo (Exactive)
- Q-Orbitrap (Q-Exactive)
- Trampa de iones-Orbitrap (IT-Orbitrap)
- Resonancia de ión-ciclotrón por transformada de Fourier (FT-ICR)

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En la tabla 15 se detalla la resolución que proporciona cada uno de ellos, los modos de trabajo que presentan (modo *full scan*, selected reaction monitoring (SIM), multiple reaction monitoring (MRM), product-ion scan, precursor-ion scan) así como algunas de sus características más destacadas. Los requerimientos de la *DG Sanco 12571/2013* para la identificación de los analitos en función del analizador empleado quedan descritos en la tabla 16.

En lo que concierne a la aplicación de LC-MS con alta resolución y espectrometría de masas en tándem, son múltiples los trabajos que aplican estas metodologías para la determinación de pesticidas y otros contaminantes a muestras de alimentos y agua.

Tabla 15. Analizadores de espectrometría de masas que pueden ser acoplados a cromatografía de líquidos.

Analizador	¹ Resolución	Modos de trabajo	Características
Q	<2x10 ³ (Baja)	- <i>Full scan</i> - SIM	- Baja selectividad - Sensibilidad baja (<i>full scan</i>) y moderada (SIM) - Bajo coste
IT	<3x10 ³ (Baja-media)	- <i>Full scan</i> - MS/MS (precursor-ion scan)	- Alta sensibilidad en modo <i>full scan</i> - Posibilidad de hacer MS ⁿ .
QQQ	<2x10 ³ (Baja)	- <i>Full scan</i> - MS/MS (precursor-ion scan, product-ion scan) - MRM - Pérdida neutra	- El más empleado para análisis de trazas - Muy sensible y selectivo en modo MRM

¹ Valor de resolución estimado. Este valor depende del rango de m/z del cálculo y del fabricante.

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TOF	5×10^3 - 6×10^3 (Media-alta)	- <i>Full scan</i>	- Medida de masa exacta - Muy sensible 2-3 órdenes de intervalo lineal
Q-TOF	5×10^3 - 6×10^3 (Media-alta)	- <i>Full scan</i> - MS/MS (product ion scan, con y sin aislamiento de precursor)	- Medida de masa exacta - MS/MS con masa exacta - Muy sensible en <i>full scan</i> 2-3 órdenes de intervalo lineal
Orbitrap (Exactive)	$>1 \times 10^5$ (Alta)	- <i>Full scan</i> - MS/MS (sin aislamiento de precursor si va incluida la celda de colisión)	- Masa exacta - Elevada sensibilidad 3-4 órdenes de intervalo lineal
Q-Orbitrap (Q-Exactive)	$>1 \times 10^5$ (Alta)	- <i>Full scan</i> - MS/MS (product ion scan, con y sin aislamiento de precursor)	- Masa exacta - Elevada sensibilidad 3-4 órdenes de intervalo lineal - MS/MS dedicado
IT-Orbitrap (LTQ-Orbitrap)	$>1 \times 10^5$ (Alta)	- <i>Full scan</i> - MS/MS (product ion scan, con y sin aislamiento de precursor) - MS^n	- Masa exacta - Elevada sensibilidad 3-4 órdenes de intervalo lineal - MS/MS dedicado - Posibilidad de MS^n
FT-ICR	1×10^5 - 5×10^6 (Ultra-alta)	- <i>Full scan</i> - MS/MS (product ion scan, con y sin aislamiento de precursor) - MS^n	- Medida de masa exacta - Posibilidad de incorporar IT (IT-FT-ICR) para hacer MS^n y MS/MS

Tabla 16. Requerimientos de la DG SANCO 12571/2013 que deben cumplir los diferentes analizadores de masas para la identificación de analitos.

Modo MS	Sistemas típicos	Modo de adquisición	Requerimientos para la identificación
MS	Q IT TOF	-Full scan -Rango limitado de m/z -SIM	≥ 3 iones diagnóstico, incluyendo el ión molecular
HRMS	TOF Orbitrap FT-ICR Sector magnético	-Full scan -Rango limitado de m/z -SIM	≥ 2 iones diagnóstico, incluyendo el ión molecular - Exactitud de masas < 5 ppm - Al menos un fragmento

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MS/MS	QQQ IT Q-TOF Q-TRAP	-SIM/MRM -Full scan -Espectro del ión producto	≥ 2 iones producto
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En las tablas 17 y 18 se resumen los métodos multiresiduo más recientes aplicados con tal fin, detallando en ellas el tipo de alimento al que han sido aplicados, el procedimiento de extracción empleado, las características del método desarrollado así como la sensibilidad obtenida.

De acuerdo con la tabla 17, en la que se hace un resumen de los métodos multiresiduo recientemente desarrollados empleando LC-HRMS, los métodos presentan tiempos de análisis comprendidos entre 5 y 40 minutos. Los volúmenes de inyección oscilan entre 3 y 50 μL . En todos ellos, las columnas empleadas son apolares (C_{18} ó C_8). El flujo empleado varía entre 0.3 y 0.6 ml/min. Las fases móviles, por lo general, son a) agua con un pequeño porcentaje de acetonitrilo o metanol, así como con o sin un pequeño porcentaje de ácido, y b) un disolvente orgánico, que suele ser acetonitrilo o metanol, en algunas ocasiones con un pequeño porcentaje de agua. Los métodos descritos en esta tabla emplean como analizadores TOF, Q-TOF en modo full scan y Orbitrap. Se emplea para la mayoría de los métodos descritos en esta tabla, QuEChERS como método de tratamiento de muestra, por lo general, empleando acetonitrilo con un porcentaje de ácido acético y con posterior etapa de clean up.

En la tabla 18, que recoge los métodos multiresiduo más recientes desarrollados con espectrometría de masas en tándem, los tiempos de análisis, como ocurría con alta resolución, son, generalmente, inferiores a 40 minutos. Los volúmenes de inyección empleados también suelen ser de 50 μL o inferiores, excepto en dos trabajos en los que se llegan a emplear hasta 100 μL . Las columnas empleadas son apolares (C_{18} ó C_8), salvo en un trabajo

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en el que se emplea cromatografía de líquidos de dos dimensiones y se compara el empleo de columna en fase reversa y en fase normal. Por lo general, estos métodos emplean como analizadores QQQ, QTRAP y QTOF en modo MS/MS. Por lo que respecta a la sensibilidad empleando analizadores de alta resolución y espectrometría de masas en tándem, los resultados indican que los métodos multiresiduo desarrollados con el segundo tipo de analizadores proporcionan valores de límites de cuantificación inferiores. En cuanto al método de tratamiento de muestra más empleado en los trabajos descritos cabe destacar el uso de QuEChERS empleando acetonitrilo, así como extracción líquido-líquido con disolventes como acetona, acetato de etilo o diclorometano.

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Tabla 17. Resumen de métodos multiresiduo con LC-MS de alta resolución para la determinación de pesticidas y otros contaminantes en alimentos y agua.

Compuestos	Muestra	Procedimiento extracción	Características del método	Sensibilidad	Ref. Año
Más de 350 pesticidas y fármacos	Potitos de carne, pescado y verdura	Extracción con agua/0.1% HCOOH en ACN	<i>UPLC-Orbitrap-MS (+ y -)</i> T.A. 14 min; V.I. 10µL; C ₁₈ (100 x 2.1 mm, 1.7µm); F. 0.3ml/min; F.M. A: agua; B: metanol, ambas con 0.1%HCOOH y 4mM NH ₄ COOH	Intervalo LOQs 10-100 µg/kg	[187] 2015
101 pesticidas	Pimiento verde, tomate, pepino, naranja, agua.	<i>Fruta y verdura:</i> QuEChERS: LLE con ACN seguida de clean up con PSA <i>Agua:</i> SPE	<i>LC-TOFMS (+)</i> T.A. 40 min; V.I. 50µL; C ₈ (150 x 4.6 mm, 5µm); F. 0.6ml/min; F.M. A: 0.1%HCOOH en agua; B: ACN	Media LOQs 10 µg/kg	[188] 2007
100 pesticidas y metabolitos	Frutas y verduras	QuEChERS: LLE con ACN seguida de clean up con PSA	<i>LC-ESI-TOFMS (+) y LC-ESI-QTRAP (+)</i> T.A. 40 min; V.I. 50µL; C ₈ (150 x 4.6 mm, 5µm); F. 0.6ml/min; F.M. A:0.1%HCOOH en agua; B: ACN	Media LOQs 10 µg/kg	[189] 2007
212 pesticidas	Manzana, fresa, tomate y espinaca	LLE con ACN	<i>UHPLC-ESI-TOFMS (+ y -)</i> T.A. 11.5 min; V.I. 2µL; C ₁₈ (100 x 2.1 mm, 1.8µm); F. 0.3-0.6-0.45ml/min; F.M. A: metanol; B: 0.005M NH ₄ COOH en agua	LOQs <10 µg/kg	[190] 2010
100 pesticidas	Fresa	Extracción con acetato de etilo	<i>UPLC-ESI-TOFMS (+)</i> T.A. 6.5 min; V.I. 3µL; C ₁₈ (50 x 2.1 mm, 1.7µm); F.0.6 ml/min; F.M. A: Metanol:agua (95:5); B:metanol, ambas con 5mM NH ₄ COOH	Media LOQs 10 µg/kg	[191] 2008
300 pesticidas y metabolitos.	Frutas y verduras	QuEChERS: extracción con 1% CH ₃ COOH en ACN seguida de clean up con PSA.	<i>HPLC-ESI-TOFMS (+)</i> T.A. 15 min; V.I. 20µL; C ₁₈ (150 x 4.6 mm, 5µm); F. 0.6ml/min; F.M. A: ACN: agua (95:5);B: ACN: agua (5:95), ambas con 0.1% HCOOH	Media LOQs 10 µg/kg	[192] 2011
60 pesticidas	Berenjena, coliflor, cebolla, patata, manzana, plátano, uva, mango, naranja, granada	LLE con ACN:MeOH (90:10) Etapa de clean up: SPE con GCB y PSA	<i>UPLC-TOFMS</i> T.A. 5 min; V.I. 5µL; C ₁₈ (50 x 2.1 mm, 1.7µm); F. 0.5ml/min; F.M.: A: metanol; B: agua, ambas con 0.1% HCOOH	Intervalo LOQs 0.8-11.8 µg/kg	[193] 2014

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510 pesticidas	Espinaca	QuEChERS: extracción con 1% CH ₃ COOH en ACN seguida de clean up con PSA.	<i>LC-Orbitrap MS</i> T.A. 14 min; V.I. 10µL; C ₁₈ (100 x 2.1 mm, 1.9µm); F. 0.3ml/min; F.M. A: agua; B: metanol, ambas con 0.1% HCOOH y 4mM NH ₄ COOH	LOQs <1µg/kg	[194] 2014
100 pesticidas	Alimentos y agua	QuEChERS: extracción con 1% CH ₃ COOH en ACN seguida de clean up con PSA.	<i>HPLC-TOFMS (+)</i> T.A. 30 min; V.I. 50µL; C ₈ (150 x 4.6 mm, 5µm); F. 0.6ml/min; F.M. A: 0.1% HCOOH en agua; B: ACN	Media LODs Alimentos: <0.1mg/kg Agua: <0.3mg/L	[195] 2006
850 pesticidas, 447 fragmentos y 99 metabolitos	Fruta y verdura	QuEChERS: extracción con 1% CH ₃ COOH en ACN seguida de clean up con PSA.	<i>HPLC-TOFMS (+)</i> T.A. 31 min; V.I. 20µL; C ₁₈ (50 x 4.6 mm, 1.8µm); F. 0.5ml/min; F.M. A: 0.1% HCOOH en agua; B: ACN	-	[140] 2012
300 pesticidas y metabolitos	Fruta y verdura	QuEChERS: Extracción con 1% CH ₃ COOH en ACN seguida de clean up con PSA.	<i>HPLC-ESI-TOFMS (+)</i> T.A. 18 min; V.I. 20µL; C ₁₈ (50 x 4.6 mm, 1.8µm); F.0.6ml/min; F.M. A: agua:ACN (95:5, v/v); B: ACN:agua (95:5, v/v), ambas con 0.1% HCOOH	Media LOQs 10µg/kg	[196] 2009
350 pesticidas y drogas veterinarias	Miel	QuEChERS: LLE sin etapa de clean up	<i>HPLC-Orbitrap-MS (+ and -)</i> T.A. 14 min; V.I.10µL; C ₁₈ (100 x 2.1 mm, 1.7µm); F. 0.3ml/min; F.M. A: agua; B: metanol, ambas con 0.1% HCOOH y 4mM NH ₄ COOH	Intervalo LOQs 1-50µg/kg	[197] 2012
170 pesticidas.	Tomate, pimiento, naranja y té verde	QuEChERS: Extracción con 1% CH ₃ COOH en ACN seguida de clean up con PSA y C ₁₈ ó cloruro cálcico	<i>UPLC-Orbitrap-MS (+)</i> T.A. 13 min; V.I.10µL; C ₁₈ (150 x 2.1 mm, 2.6µm); F.M. A: agua:metanol (98:2, v/v); B: metanol: agua (98:2, v/v), ambas con 0.1% HCOOH y 5mM NH ₄ COOH	-	[198] 2014
>350 pesticidas, drogas veterinarias y biopesticidas	Carne de pollo, ternera y cerdo	LLE con 1% HCOOH en ACN	<i>UPLC-ESI-Orbitrap-MS (+ y -)</i> T.A. 14 min; C ₁₈ (100 x 2.1 mm, 1.7µm); F. 0.3 ml/min; F.M: A: agua; B: metanol, ambas con 0.1% HCOOH y 4mM NH ₄ COOH	Intervalo LOQs 2-16 µg/kg	[199] 2014
Pesticidas, micotoxinas, drogas de abuso, antibióticos.	Agua residual, orina, naranja, plátano y maíz.	SPE (OASIS HLB); extracción con agua:MeOH ó ACN:agua, dependiendo de la muestra	<i>UPLC-QTOF-MS (+ and -) full scan</i> T.A. 18 min; V.I. 50µL; C ₁₈ (150 x 2.1 mm, 2.6µm); F. 0.3ml/min; F.M. A: agua; B:metanol, ambas con 0.1% HCOOH	-	[200] 2012

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<p>297 pesticidas y más de 400 fragmentos</p>	<p>Lechuga Aplicación de base de datos con 148 compuestos 60 muestras de alimentos (usando LC- TOFMS y LC-MS/MS)</p>	<p>QuEChERS: LLE con 1% CH₃COOH en ACN, seguida de clean up con PSA</p>	<p><i>LC-ESI-TOFMS (+)</i> T.A.: 17 min; V.I. 20µL; C₁₈ (4.6 x 50mm, 1.8µm); F. 0.6ml/min; F.M. A: agua:ACN (95:5, v/v) y B: ACN:agua (95:5, v/v), ambas con 0.1%HCOOH</p>	<p>LODs 20%: <5µg/kg 40%: 5-10µg/kg; 20%: 10-50µ/kg 20%: >50µg/kg</p>	<p>[201] 2009</p>
<p>130 pesticidas</p>	<p>Fruta y verdura</p>	<p>QuEChERS: LLE con 1% CH₃COOH en ACN, seguida de clean-up con PSA</p>	<p><i>LC-ESI-Orbitrap-MS</i> T.A. 25 min; V.I. 5µL; C₁₈ (3 x 100mm, 3µm); F. 0.3ml/min; F.M. A:agua; B:metanol:agua (95:5, v/v), ambas con 0.002% HCOOH y 2 mM NH₄COOH</p>	<p>Intervalo LODs 10-50 µg/kg</p>	<p>[141] 2012</p>

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Tabla 18. Resumen de métodos multiresiduo para la determinación de pesticidas y otros contaminantes en alimentos y agua usando analizadores de masas en tandem (MS/MS)

Compuestos	Muestra	Procedimiento extracción	Características del método	Sensibilidad	Ref. Año
100 pesticidas	Pimiento verde, tomate y naranja	QuEChERS: extracción con 1% CH ₃ COOH en ACN seguida de etapa de clean up con PSA.	<i>LC-ESI-QqQ-MS/MS (+)</i> T.A. 41 min; V.I. 10µL; C ₁₈ (150 x 4.6 mm, 1.8µm); F.0.6ml/min; F.M. A: ACN ; B: 0.1% HCOOH en agua	Intervalo LODs 0.3-50µg/kg	[202] 2007
99 pesticidas	Fruta, verdura y cereales	QuEChERS seguida de clean up con PSA	<i>LC-ESI-QqQ-MS/MS (+)</i> T.A. 40 min; V.I. 5µL; C ₈ (100 x 2.1 mm, 3µm); F.0.2ml/min; F.M. A: 0.1% HCOOH en agua; B: metanol	Media LOQs <20µg/kg	[203] 2008
183 pesticidas	Fruta y verdura	Extracción con acetato de etilo	<i>LC-ESI-QTRAP-MS/MS (+ y -)</i> V.I. 5µL; C ₈ (100 x 3 mm, 4µm); F.0.3ml/min; F.M. A: 0.1mM NH ₄ COOH en agua; B: metanol	Media LOQs: <20µg/kg	[204] 2007
316 pesticidas (en 3 laboratorios diferentes)	Pera, tomate y lechuga	QuEChERS : LLE con ACN (0.1% HCOOH) seguida de clean up usando SPE en columna	<i>LC-QqQ-MS/MS</i> T.A. 27 min; V.I. 10µL; C ₈ (150 x 2 mm); F. 0.2ml/min; F.M. A: ACN; B: agua, ambas con 0.1%HCOOH y 10mM NH ₄ COOH	-	[205] 2008
10 micotoxinas	Huevo	QuEChERS: LLE con MeOH/agua (80/20, v/v) con 0.1%HCOOH. Evaluación etapa de clean up (SPE con Oasis HLB y C ₁₈)	<i>UPLC-QqQ-MS/MS (+ y -)</i> T.A. 6.5 min; V.I. 5µL; F.0.3ml/min; F.M. A: metanol; B: 5mM NH ₄ COOH en agua	Intervalo LODs: 0.5-5µg/kg Intervalo LOQs: 1-10µg/kg	[206] 2011
160 pesticidas	Tomate, pera y naranja	QuEChERS: LLE con ACN, seguida de clean up con PSA.	<i>LC-ESI-QQQ-MS/MS (+)</i> T.A. 33 min; V.I. 10µL; C ₈ (150 x 4.6 mm, 5µm); F.0.6ml/min; F.M. A: 0.1%HCOOH en agua; B: ACN	Media LODs ≤5µg/kg	[207] 2008
90 pesticidas	Zumo de manzana, melocotón, piña y multifrutas.	QuEChERS: LLE con 1% CH ₃ COOH. Extractos de ACN diluidos con agua (1:1). Evaluación de SPE con cartuchos C ₁₈ , Oasis and Strata-X.	<i>UPLC-ESI-QqQ-MS/MS (+)</i> T.A. 11 min; V.I. 5µL; C ₁₈ (100 x 2.1 mm, 1.7µm); F.0.35ml/min; F.M. A: metanol; B: 0.01% HCOOH en agua	Media LOQs ≤5µg/L	[208] 2008
~90 compuestos (pesticidas, biopesticidas y micotoxinas)	Trigo, pepino y vino tinto	QuEChERS: LLE con 1% CH ₃ COOH	<i>UHPLC-ESI-QqQ-MS/MS (+)</i> T.A. 13 min; V.I. 5µL; C ₁₈ (100 x 2.1 mm, 1.7µm); F.0.45ml/min; F.M. A: metanol; B: 5mM NH ₄ COOH en agua	LOQs ≤10µg/kg	[209] 2011

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300 pesticidas	Limón, pepino, harina de trigo, rúcula y té negro	QuEChERS: LLE con ACN. Previamente se añadió agua a las muestras de harina de trigo y té negro.	<i>2D-LC-ESI-QqQ-MS/MS</i> F. 0.2ml/min; T.A. 30 min; V.I. 5µL. <i>Condiciones HILIC:</i> Diol (100 x 2.1 mm, 5µm); F.M. A: agua; B: ACN: agua (90:10), ambas con 5mM NH ₄ COOH y 0.1% CH ₃ COOH <i>Condiciones fase reversa:</i> C ₁₈ (100 x 2.1 mm, 2.7µm); F.M. A: agua; B: metanol; ambas con 5mM NH ₄ COOH y 0.1% CH ₃ COOH	Media LODs 10µg/kg	[210] 2013
43 pesticidas y 9 metabolitos de pesticidas	Limón, tomate, aguacate y uvas pasas.	LLE con 0.1% HCOOH en MeOH:agua (80:20,v/v). Etapa de clean-up: SPE con cartuchos Oasis HLB.	<i>LC-ESI-QqQMS/MS</i> T.A. 29 min; C ₁₈ (100 x 2.1 mm, 5µm); F. 0.2ml/min; F.M. A: metanol; B: agua, ambas con 0.01%HCOOH	Media LOQs 10µg/kg	[211] 2006
144 pesticidas	Naranja y lechuga	QuEChERS: LLE con ACN, seguida de clean up con PSA	<i>LC-ESI-QqQ-MS/MS (+)</i> T.A.30 min; V.I. 5µL; C ₁₈ (3 x 150 mm, 5µm); F. 0.3ml/min; F.M. A:metanol:agua (25:75, v/v), ambas con 5mM NH ₄ COOH; B: metanol:agua (95:5, v/v), ambas con 5mM NH ₄ COOH	Media LOQs 10µg/kg	[212] 2005
90 pesticidas	Manzana	Extracción con ACN-acetato amónico, seguida de clean up usando SPE (cartuchos empleados, Oasis HLB).	<i>LC-ESI-MS/MS (+)</i> T.A. 34 min; C ₁₈ (100 x 2.1mm, 3µm); V.I.10µl; F.M. A: ACN; B: 0.1M NH ₄ COOH en ACN:agua (20:80); C: agua. F. 0.2-0.3ml/min	LODs <1µg/kg	[213] 2007
82 pesticidas	Uva	Extracción con acetato de etilo, seguida de etapa de clean up SPE dispersiva.	<i>LC-ESI-QTRAP-MS/MS (+)</i> T.A. 18 min; V.I. 5µL; F. 0.3ml/min; F.M. A: metanol:agua (20:80, v/v), ambas con 5mM NH ₄ COOH; B: metanol:agua (90:10, v/v), ambas con 5mM NH ₄ COOH	Media LOQs 10µg/kg	[214] 2007
169 pesticidas	Semillas de soja	Extracción con acetona, diclorometano y disolventes derivados de petróleo (1:1:1)	<i>LC-ESI-QqQ-MS/MS (+ and -)</i> T.A. 32.5 min; V.I. 5µL; F. 0.3ml/min; C ₁₈ (3.2 x 150 mm, 5µm); F.M. A: metanol; B: 5mM NH ₄ COOH en agua	Intervalo LODs: 0.1-0.25 µg/kg Intervalo LOQs: 10-100 µg/kg	[215] 2007
171 pesticidas	Lechuga, naranja, manzana, repollo y harina de trigo	Extracción con acetona, diclorometano y mezcla de disolventes derivados del petróleo (1:1:1)	<i>LC-ESI-QqQ-MS/MS (+)</i> T.A. 32.5 min; V.I. 5µL; F. 0.3ml/min; C ₁₈ (3.2 x 150 mm, 5µm); F.M. A: metanol; B: 5mM NH ₄ COOH en agua	Media LOQs 10µg/kg	[216] 2007

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11 colorantes, 11 micotoxinas y 20 pesticidas	Pimentón, curry, pimienta blanca y negra, chili, cúrcuma, nuez moscada, jengibre	Extracción con ACN. Dilución de los extractos con agua.	<i>LC-ESI-QTRAP-MS/MS (QTRAP) (+)</i> T.A. 35 min; V.I. 10µL; F. 0.2ml/min; C ₁₈ (50 x 2mm, 4µm); F.M. A: agua:metanol (80:20, v/v), B: metanol:agua (90:10, v/v), ambas con 5mM NH ₄ COO	Intervalo LOQs 0.2-10 µg/kg	[217] 2010
30 pesticidas (positivos en muestras confirmados con UPLC-QTOF-MS)	Naranja, lechuga, cacahuete y aguacate	dSPE con C ₁₈ como agente dispersante y diclorometano como eluyente.	V.I. 20µL; F. 0.4ml/min; F.M. A: agua; B: metanol, ambas con 10mM NH ₄ COOH <i>LC-QqQ-MS/MS (+)</i> T.A. 30 min; C ₁₈ (150 x 4.6 mm, 5µm) <i>UPLC-QTOF-MS</i> T.A. 7 min; C ₁₈ (5 x 2.1mm, 1.7µm)	Intervalo LOQs 0.5-10 µg/kg	[218] 2009
108 pesticidas	Fruta, verdure y cereales	Extracción con MeOH/agua; etapa de clean up con columna, usando diclorometano como eluyente	<i>LC-ESI-QqQ-MS/MS(+ y -)</i> T.A. 38 min; V.I. 20µL; F. 0.2ml/min; C ₁₈ (3 x 150mm, 5µm); F.M. A: metanol:agua (80:20, v/v); B: Metanol:agua (10:90, v/v), ambas con 5mM NH ₄ COOH	Media LOQs ~10 µg/kg	[219] 2003
300 pesticidas	Agua mineral	Filtración e inyección directa	<i>LC-ESI-QqQ-MS/MS(+)</i> T.A. 38 min; V.I. 100µL; F. 0.3ml/min; C ₁₈ (2 x 50mm, 5µm); F.M. A: metanol:agua (20:80, v/v); B: metanol:agua (10:90, v/v), ambas con 5mM NH ₄ COOH	Media LOQs 0.1µg/L	[220] 2008
53 pesticidas	Muestras no grasas: pepino, naranja. Muestra grasa: aceituna	QuEChERS: LLE con 1% CH ₃ COOH en ACN. -Muestras no grasas: Sin etapa de clean up. -Aceituna: después de QuEChERS, etapa de clean-up con cartuchos Fluorisil	<i>UPLC-ESI-QqQ-MS/MS (+)</i> T.A. 10 min; V.I. 5µL; F. 0.35ml/min; C ₁₈ (100 x 2.1 mm, 1.7µm); F.M. A: 0.01% HCOOH en agua; B: metanol	Media LODs <3µg/kg Media LOQs <10µg/kg	[221] 2008
400 pesticides	Mango, aguacate y potitos de frutas	QuEChERS: LLE con 1% CH ₃ COOH en ACN, seguida de etapa de clean up con PSA	<i>UPLC-ESI-QqQ-MS/MS(+)</i> T.A. 10 min; V.I. 20µL; F. 0.45ml/min; C ₁₈ (2.1 x 100mm, 1.7µm); F.M. A: agua:metanol (98:2); B: metanol, ambas con 0.1% HCOOH	-	[222] 2008

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136 pesticidas	Fruta y verdura	Extracción con acetato de etilo	<i>LC-ESI-QqQ-MS/MS (+)</i> T.A. 34 min; V.I. 20µl; F. 0.3ml/min; C ₁₈ (100 x 3 mm, 5µm); F.M. A: metanol:agua:1M NH ₄ COO (90:9.5:0.5); B: methanol:agua:1M NH ₄ COO (20:79.5:0.5)	Media LOQs 10µg/kg	[223] 2007
277 pesticidas	Malta y cerveza	Malta: adición de ACN: agua (3:1, v/v). Cerveza y malta: LLE con acetato de etilo, seguido de clean up (SPE)	<i>LC-ESI-QqQ-MS/MS (+)</i> T.A. 35 min; V.I. 5µl; F. 0.2ml/min; C ₁₈ (100 x 3 mm, 5µm); F.M. A: agua; B: metanol, ambas con 10 mM NH ₄ COOCH ₃	Media LOQs 10µg/kg	[224] 2006
55 pesticidas (screening para 300 pesticidas; confirmación y cuantificación solo para 55)	Fruta y verdura	QuEChERS: LLE con 1% CH ₃ COOH en ACN, de clean up con PSA	<i>LC-ESI-QTRAP-MS/MS (+)</i> T.A. 45 min; V.I. 10µL; F. 0.6ml/min; C ₈ (150 x 4.6, 5µm); F.M. A: 0.1%HCOOH en agua; B: ACN	LOQs <0.04µg/kg	[225] 2012
446 pesticidas (383 con GC/MS y 63 con LC-MS/MS)	Fruta y verdura	Extracción con ACN seguida de SPE usando dos cartuchos diferentes en serie	<i>LC-ESI-Q-MS/MS (+)</i> T.A. 55 min; columna: 150 x 2.1 mm, 3µm; F. 0.2ml/min; V.I. 20µL; F.M. A: agua; B: ACN	LOQs <0.25mg/kg	[226] 2006
20 pesticidas usando LC-MS/MS and GC-MS (studio interlaboratorio)	Uva, naranja y lechuga	QuEChERS: LLE con 1% CH ₃ COOH en ACN, seguido de clean up con PSA	<i>LC-ESI-QqQ-MS/MS (+)</i> T.A. 30 min; V.I. (5-100µl, dependiendo del espectrómetro de masas empleado); C ₁₈ (150 x 3 mm, 3 µm); F. 0.3ml/min; F.M. A: agua; B: metanol, ambas con 5mM HCOOH	LOQs <10µg/kg	[227] 2007
136 Pesticidas, 36 micotoxinas y 86 drogas veterinarias	Pienso y miel	QuEChERS: LLE con 1% HCOOH en acetonitrilo	<i>UPLC-QqQ-MS/MS</i> T.A. 20 min; V.I. 5µl; C ₁₈ (100 x 2.1 mm, 1.7µm); F. 0.4ml/min; F.M. A: agua; B: agua: metanol (5/95, v/v), ambas con 1mM NH ₄ COOH y 20µl/L HCOOH	LODs <10-50µg/kg	[228] 2008
148 pesticidas	Manzana, plátano, melón, naranja y zumo de naranja, zanahoria, maíz, cebolla, guisante	QuEChERS: extracción con 1% CH ₃ COOH en ACN con etapa de clean up.	<i>LC-ESI-MS/MS (+)</i> T.A. 35 min; V.I. 5µL; C ₁₈ (100 x 2.1 mm, 3µm); F. 0.2-0.3ml/min; F.M. A: ACN; B: 10mM NH ₄ CH ₂ COOH y 2% ACN en agua <i>UPLC-QqTOF-MS (+)</i> T.A. 14 min; V.I. 10µL; C ₁₈ (100 x 2.1 mm, 1.7µm); F. 0.4ml/min; F.M. A: ACN; B: 10mM NH ₄ CH ₂ COOH en agua	LC-ESI-MS/MS: Media LOQs 5µg/kg UPLC-QqTOFMS LODs 5µg/kg	[229] 2010

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138 pesticidas	Alimentos infantiles con verdura y fruta	QuEChERS: extracción con 1% CH ₃ COOH en ACN seguida de clean up con PSA.	<i>UPLC-QqTOFMS</i> T.A. 14 min; V.I. 10µL; C ₁₈ (100 x 2.1 mm, 1.7µm); F. 0.4ml/min; F.M. A: ACN; B: 10mM amonio en agua	Media LOQ 10µg/kg	[230] 2009
116 drogas veterinarias	Pienso aves de corral, cabra, vaca, cerdo y conejo.	Extracción con 1% HCOOH en ACN	<i>UPLC-ESI-QTOFMS (+ and -)</i> T.A. 18 min; V.I. 50µL; C ₁₈ (100 x 2.1 mm, 1.7µm); F.0.3ml/min; F.M. A: agua; B: metanol, ambas con 0.1% HCOOH	-	[231] 2014

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[100] *Directiva 96/23/CE del Consejo*, de 29 de abril de 1996 relativa las medidas de control aplicables respecto de determinadas sustancias y sus residuos en los animales vivos y sus productos y por la que se derogan las *Directivas 85/358/CEE y 86/469/CEE* y las *Decisiones 89/187/CEE y 91/664/CEE*.

[101] *Real Decreto 2178/2004*, de 12 de noviembre de 2004, por el que se prohíbe utilizar determinadas sustancias de efecto hormonal y tireostático y sustancias beta-agonistas de uso en la cría de ganado. BOE número 274.

[102] *Reglamento (CE) 282/2008 de la Comisión*, de 27 de marzo de 2008, sobre los materiales y objetos de plástico reciclado destinados a entrar en contacto con alimentos y por el que se modifica el *Reglamento (CE) 2023/2006*.

[103] *Reglamento (CE) 2023/2006 de la Comisión*, de 22 de diciembre de 2006, sobre buenas prácticas de fabricación de materiales y objetos destinados a entrar en contacto con alimentos.

[104] *Real Decreto 866/2008*, de 23 de Mayo de 2008, por el que se aprueba la lista de sustancias permitidas para la fabricación de materiales y objetos plásticos destinados a entrar en contacto con los alimentos y se regulan determinadas condiciones de ensayo.

[105] *Real Decreto 103/2009*, de 6 de febrero, por el que se modifica el *Real Decreto 866/2008*, de 23 de mayo, por el que se aprueba la lista de sustancias permitidas para la fabricación de materiales y objetos plásticos

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destinados a entrar en contacto con los alimentos y se regulan determinadas condiciones de ensayo.

[106] *Reglamento (CE) 975/2009 de la Comisión*, de 19 de octubre de 2009 por la que se modifica la *Directiva 2002/72/CE* relativa a los materiales y objetos plásticos destinados a entrar en contacto con productos alimenticios.

[107] *Orden PRE/628/2011*, de 22 de marzo, por la que se modifica el Anexo II del *Real Decreto 866/2008*, de 23 de mayo, por el que se aprueba la lista de sustancias permitidas para la fabricación de materiales y objetos plásticos destinados a entrar en contacto con los alimentos y se regulan determinadas condiciones de ensayo.

[108] *Directiva 85/572/CEE del Consejo*, de 19 de diciembre de 1985, por la que se determina la lista de los simulantes que se deben utilizar para controlar la migración de los componentes de los materiales y objetos de material plástico destinados a entrar en contacto con los productos alimenticios.

[109] *Real Decreto 846/2011*, de 17 de junio, por el que se establecen las condiciones que deben cumplir las materias primas a base de materiales poliméricos reciclados para su utilización en materiales y objetos destinados a entrar en contacto con alimentos.

[110] *Real Decreto 517/2013*, de 5 de julio, por el que se modifica el *Real Decreto 846/2011*, de 17 de junio, por el que se establecen las condiciones que deben cumplir las materias primas a base de materiales poliméricos reciclados para su utilización en materiales y objetos destinados a entrar en contacto con alimentos.

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[111] *Reglamento 1331/2008 del Parlamento Europeo y del Consejo*, de 16 de diciembre de 2008, por el que se establece un procedimiento de autorización común para los aditivos, las enzimas y los aromas alimentarios.

[112] *Reglamento (UE) 231/2012 de la Comisión*, de 9 de marzo de 2012, por el que se establecen especificaciones para los aditivos alimentarios que figuran en los anexos II y III del *Reglamento (CE) 1333/2008 del Parlamento Europeo y del Consejo*

[113] *Real Decreto 2001/1995*, de 7 de diciembre de 1995, por el que se aprueba la lista positiva de colorantes autorizados para su uso en la elaboración de productos alimenticios así como sus condiciones de utilización.

[114] *Real Decreto 2002/1995*, de 7 de diciembre de 1995, por el que se aprueba la lista positiva de aditivos edulcorantes autorizados para su uso en la elaboración de productos alimenticios, así como sus condiciones de utilización.

[115] *Real Decreto 142/2002*, de 1 de febrero de 2002, por el que se aprueba la lista positiva de aditivos distintos de colorantes y edulcorantes para su uso en la elaboración de productos alimenticios, así como sus condiciones de utilización.

[116] *Directiva 94/35/CE [116]*, de 30 de junio de 1994, relativa a los edulcorantes utilizados en los productos alimenticios.

[117] *Reglamento (UE) 1258/2011 de la Comisión*, de 2 de diciembre de 2011 que modifica el *Reglamento (CE) 1881/2006* por lo que respecta al contenido máximo de nitratos en los productos alimenticios.

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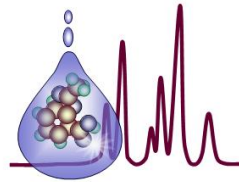
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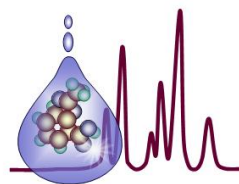
Objetivos

II. OBJETIVOS

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Las metodologías analíticas, principalmente LC-HRMS, están focalizadas en el desarrollo de métodos de *screening* que permiten la determinación de cientos de compuestos en un único análisis. Una de las razones por las que es importante el uso de este tipo de metodologías es debido al amplio número y gran variedad de contaminantes orgánicos que son susceptibles de ser encontrados en muestras de alimentos. Los principales objetivos de la presente Tesis Doctoral son:

1. Estudiar la aplicabilidad de la cromatografía de líquidos-espectrometría de masas de alta resolución para el análisis exhaustivo de un amplio número de contaminantes orgánicos en muestras de alimentos. Para ello, se desarrollará una base de datos de masas exactas de iones incluyendo pares de valores de tiempo de retención y m/z para más de 600 compuestos.
2. Desarrollar métodos de tratamiento de muestra genéricos para muestras de alimentos, con el objeto de obtener extractos de la muestra que contengan el menor número de interferentes posible, pero proporcionando una recuperación adecuada para la mayoría de los compuestos estudiados.
3. Evaluar y demostrar la utilidad de los métodos de *screening* para la determinación de contaminantes orgánicos en muestras reales.



Resultados y Discusión

*III.1. ESTUDIO DE LAS PRINCIPALES VENTAJAS
E INCONVENIENTES DE LA CROMATOGRAFÍA DE
LÍQUIDOS DE ULTRAELEVADA EFICACIA
ACOPLADA A ESPECTROMETRÍA DE MASAS CON
ANALIZADOR DE TIEMPO DE VUELO (UHPLC-
TOFMS) EN EL DESARROLLO DE MÉTODOS DE
SCREENING PARA LA DETECCIÓN DE MÁS DE 600
CONTAMINANTES ORGÁNICOS.*

III.1. Estudio de las principales ventajas e inconvenientes de la cromatografía de líquidos de ultraelevada eficacia acoplada a espectrometría de masas con analizador de tiempo de vuelo (UHPLC-TOFMS) en el desarrollo de métodos de *screening* para la detección de más de 600 contaminantes orgánicos

III.1.1. Resumen

La seguridad alimentaria es un campo de interés para el gran público. Se trata de una aplicación de la espectrometría de masas muy compleja, ya que requiere la determinación simultánea de un gran número de analitos con propiedades físico-químicas muy variadas. La determinación de residuos de pesticidas y otros contaminantes tanto de origen animal como vegetal es de gran relevancia para la protección del consumidor por lo que se encuentra legislada en detalle en todo el mundo. Por ejemplo la Directiva Europea 396/2005 y sus posteriores actualizaciones incluyen mas de 150000 valores de límites de concentraciones permitidas de pesticidas para frutas y verduras.

Aparte de los productos frescos, existen otros productos derivados que pueden contener frutas y verduras dentro de su composición, así como carne o pescado. Un ejemplo significativo son los productos infantiles, para los cuales además de controlar los plaguicidas, es necesario controlar también productos veterinarios, micotoxinas, residuos de envases alimentarios y otros contaminantes. Esto indica que el número de potenciales contaminantes es demasiado elevado como para implementar los métodos de análisis basados en aproximaciones convencionales, basadas en el empleo de patrones primarios. Éstos métodos actualmente sólo cubren los analitos que se detectan con mayor frecuencia, por lo que otros que en principio no deben estar contaminando la muestra no son ni siquiera examinados.

En los últimos años, el empleo de la cromatografía de líquidos/espectrometría de masas de alta resolución (LC-HRMS) ha ganado aceptación en el campo del análisis de contaminantes por sus características adecuadas para el desarrollo de métodos que permitan el análisis de un elevado número de analitos e incluso la detección de nuevos contaminantes previamente desconocidos. Este tipo de métodos suele estar basado en el desarrollo de bases de datos que contengan las masas exactas de iones de los analitos objeto de estudio.

En este capítulo, se ha desarrollado un estudio detallado sobre la viabilidad de este tipo de métodos, examinando en detalle las principales fortalezas y limitaciones que presentan. Para ello, se ha puesto a punto una base de datos que incluyen datos de más de 625 contaminantes orgánicos (426 pesticidas, 117 productos veterinarios, 42 residuos de envases alimentarios, 21 micotoxinas, 10 compuestos perfluorados, 9 nitrosaminas and 5 edulcorantes) y los parámetros necesarios para su análisis mediante LC-HRMS.

Los aspectos más relevantes que se han estudiado han sido la separación cromatográfica y la necesidad de la misma, la selectividad global del método y aspectos relacionados con análisis cualitativo y cuantitativo empleando la base de datos, incluyendo los modos de adquisición más apropiados para el tipo de aplicación teniendo en cuenta la fragmentación y aspectos prácticos como efectos de supresión de señal (efectos matriz) entre analitos. Se encontró que debido al gran número de analitos en la base de datos, junto con las especies que ya de por sí incluye la muestra, es necesario realizar una separación exhaustiva con cromatografía de líquidos de ultraelevada eficacia (UHPLC) con un gradiente suficientemente amplio que permita la secuenciación de los analitos a lo largo del cromatograma para así, evitar solapamientos y coeluciones para poder minimizar efectos indeseables como

los efectos de supresión de señal. Por otra parte, se encontró que el empleo de columnas estándar tipo C₁₈ no permite la separación en condiciones apropiadas (de acuerdo con los requisitos establecidos por organismos oficiales (DG SANCO) de las especies más polares, que inevitablemente salen en el frente del disolvente. Por otra parte, se encontró que debido al elevado número de compuestos, hay muchas especies isobáricas/isoméricas que necesitan ser resueltas con otros medios distintos a la separación cromatográfica. Por este motivo, se propone el uso de métodos de adquisición que permitan incorporar información de la fragmentación característica de cada uno de los analitos para su confirmación inequívoca. El método que mostró ser más eficaz para este propósito es el modo de adquisición *all ion mode collision induced dissociation (CID)*, que permite la fragmentación de varias especies en una cámara de colisión sin necesidad de llevar a cabo aislamiento del ión precursor. Se encontró que la efectividad era próxima al 100 % y que la mayoría de compuestos proporcionaban información suficiente para su identificación inequívoca. Este rendimiento es muy superior al de la fragmentación en la fuente (*in-source CID*), que sólo obtenía dicha información para el 85 % de los compuestos. El uso combinado de este modo de adquisición y UHPLC generan una selectividad suficiente para el análisis cualitativo y confirmación de todas las especies en muestras complejas. No obstante, que por afinar los métodos y las herramientas de informática para poder llevar a cabo las distintas tareas de forma automatizada.

Por otra parte, en lo que respecta a análisis cuantitativo, se encontraron varias limitaciones de este método. Entre ellas, la escasa sensibilidad ofrecida por algunos compuestos cuya estructura y grupos funcionales no los hace muy apropiados para su detección empleando ionización electrospray. Esta limitación es independiente de la sofisticación o sensibilidad del equipo

y se suele dar para un porcentaje de compuestos reducido en torno al 5 %. Por último, y dejando aparte el efecto matriz y las limitaciones a las que da lugar en cuanto a cuantificación, otro aspecto que limitan la eficacia del método propuesto son las interacciones entre analitos que coeluyen, y el efecto de competencia que entre ellos se ejercen durante la etapa de ionización y la preparación y conservación de multipatrones considerando las diferentes propiedades fisicoquímicas de los analitos que se suelen incluir.

III.1.2. Artículo

Abstract

In this article, the feasibility of an accurate-mass multi-residue screening method using liquid chromatography high-resolution mass spectrometry has been examined for the determination of over 625 multiclass food contaminants (426 pesticides, 117 veterinary drugs, 42 plasticizers, 21 mycotoxins, 10 perfluorinated compounds, 9 nitrosamines and 5 sweeteners). The proposed approach was based on the use of ultra-high performance liquid chromatography electrospray (quadrupole)time-of-flight mass spectrometry, operated in positive and/or negative ionization mode, and with data acquired in full-scan mode. Compelling aspects such as chromatographic separation and the selectivity and confirmation capability provided by HRMS with different acquisition modes (full-scan or full-scan combined with collision induced dissociation (CID) with no precursor ion isolation), along with caveats such as sensitivity or automated data processing are examined and discussed. The identification of compounds was carried out using retention time matching and accurate mass measurements of the targeted ions for each analyte (mainly (de)protonated molecules). Compounds with the same nominal mass (isobaric species) were very frequent due to the wide number of compounds used. 76% of database compounds were involved in isobaric groups and 99% of isobaric species were distinguished by retention time, resolving power, isotopic profile or fragment ions. Only four pairs could not be resolved using the proposed methodology. In-source CID fragmentation was evaluated in depth, varying fragmentor voltages from 160 to 250V. The results obtained in terms of fragmentation information were not as thorough as those obtained using CID MS/MS experiments without precursor ion isolation (*all ion mode*). This acquisition mode is definitely the best suited for this type of large-scale

screening method instead of classic product ion scan, as provides excellent fragmentation information for confirmatory purposes for an unlimited number of compounds. The main weaknesses of the approach are basically the relatively low sensitivity for selected compounds which does not map well against electrospray ionization and also quantitation issues such as those produced by signal suppression effects due to either matrix effects from coeluting matrix components or from coeluting analytes present in the standards solutions which often occur as they contain hundreds of the analytes included in the database.

Introduction

Food safety testing is a societally relevant and challenging application of mass spectrometry, which requires simultaneous trace analysis for a large range of species belonging to a wide variety of compound classes [1-5]. The determination of pesticide residues and other contaminants in a wide range of different foods, both of plant and animal origin is of great interest for the protection of human health, and is thoroughly controlled worldwide with a span of regulations [6-16]. For instance, Regulation (EC) 396/2005 lists more than 150000 MRLs for pesticides in 380 defined commodities. Other derivate food products such as baby food combine different matrices: cereal-based food, meat-based food, powdered milk based infant formulae and fruit and vegetable-based food [17]. Thus, they should be tested keeping in mind the potential simultaneous presence of both pesticides and veterinary drugs. Furthermore, the presence of emerging contaminants such as parabens and musk compounds, human pharmaceuticals and antibiotics, and veterinary drugs has been recently reported in processed food due to contamination either during farming/ crop production [18] or in the food-producing scenarios [19]. To deal with these huge numbers of contaminants/

commodity combinations, residue laboratories are forced to employ multi-residue methods.

For the examination of pesticides and other organic contaminants in food, official laboratories methodologies rely on targeting a list of priority substances, typically those more often detected or more widely used. A list of around 100-150 of LC and GC-amenable compounds is usually examined. The approach selected to cover the majority of the analytes is liquid chromatography-tandem mass spectrometry (LC-MS/MS) operated in the multiple reaction monitoring (MRM) mode, which offers unsurpassed quantitative performance for typically from 100 to 200 compounds (depending on the instrument scan speed/dwell-time) using a carefully optimized acquisition method [20]. The implementation of LC-MS/MS multi-residue methods with triple quadrupole equipment no longer constitute a technical challenge thanks to advances in instrumentation (dwell time per transition (≤ 5 milliseconds) with high sensitivity makes possible the simultaneous screening of dozens of coeluting species) or in software (automated MS/MS optimization and dynamic time windows for enhanced acquisition [21]). Yet, one of the main weaknesses of the approach is the previous knowledge of both retention time and optimized MS/MS transition conditions of each analyte sought, required to set-up the acquisition method. MS/MS MRM acquisition lacks the flexibility of full-scan acquisition methods for instance in terms of analyte scope modification. Consequently, LC-MS/MS multi-residue methods are blind to compounds not defined in the MRM method (non-targeted analysis), so that none or scarce information on possible non-target or unknown pesticides or their degradation products are available when using these techniques. Besides, handling and preservation within a quality control (QC) environment of standard mixtures containing hundred of compounds, which are barely stable over long periods, constitute

a compelling effort required. Actually, the shelf life of mixed standard solutions is obviously determined by the most labile species. This forces the storage of standard solutions at very low temperature, which may prompt the partial precipitation of poorly soluble compounds. This is a really strong limitation, given the fact that in monitoring programs most positive results are usually reported for a limited number of pesticides (Pareto's rule). Therefore, screening methods skipping such reference materials and all ongoing QC measurements required are desirable.

The need for a thorough examination of hundreds of pesticides in food has recently prompted the inception of the concept of screening methods. Screening methods may desirably be used to extend the scope of the methods used in official laboratories in a cost-effective fashion, thus, enabling the detection/ identification of unexpected pesticides at levels at, or above 0.01 mg kg^{-1} , included in and/or in addition to the laboratories' quantitative methods used for frequently-detected pesticides.

Liquid chromatography combined with full-scan high-resolution mass spectrometry (LC-full-scan HRMS) has shown to be an effective approach to screen food samples for the presence of high number of analytes [22-24]. The use of high resolution mass spectrometers (HRMS) such as Orbitrap and time-of-flight (TOF) instruments provide both high mass accuracy and resolution in full scan mode, enabling accurate mass screening of a theoretically unlimited number of polar organic pollutants. This feature maps well against the current requirements in food safety testing. Since LC-HRMS has the ability to record an unlimited number of compounds as it operates in full scan mode, it is very convenient for the development of screening strategies based on the use of accurate-mass databases [6, 22-24] of substances. Such databases are powerful for practical screening of compounds when reference standards are commercially available. In these

cases, the interrogation of the data is performed against the list of compounds included in the database or library, retrospective evaluation is always possible as data for all compounds that have given sufficient detector response was acquired.

The development of accurate-mass LC-HRMS screening methods has been addressed in recent years by different authors, using either time-of-flight [25,26] or Orbitrap mass spectrometers [27-29]. Methodologies described so far include typically between 200 and 450 pesticides, although there are also a few examples covering other contaminants such as veterinary drugs. The qualitative information regarding fragmentation for confirmation purposes is not addressed in most of these previous works. In this article, the feasibility of an accurate-mass multi-residue screening method using liquid chromatography high-resolution mass spectrometry has been examined for the determination of over 625 multiclass food contaminants (pesticides, veterinary drugs and mycotoxins). Compelling aspects such as chromatographic separation and the selectivity and confirmation capability provided by HRMS with different acquisition modes (full-scan or full-scan combined with collision induced dissociation (CID) with no precursor ion isolation), along with caveats such as sensitivity or automated data processing are examined and discussed.

Experimental Section

Ultra-high Performance Liquid Chromatography-Electrospray-(Quadrupole)-Time-of-Flight Mass Spectrometry. The separation of the analytical standards was carried out in a high speed reversed phase C₁₈ analytical column of 50 mm x 2.1 mm and 1.8 µm particle size (Zorbax Rapid Resolution High Definition (RRHD) Eclipse-Plus C₁₈) by means an Agilent UHPLC system (Agilent 1290 Infinity, Agilent Technologies, Santa Clara, CA, USA), consisting

of vacuum degasser, auto-sampler and a binary pump. Typical operating pressure of this HPLC column varied from 150 psi (100% acetonitrile) to 360 psi (5% acetonitrile). Mobile phases A and B were water and acetonitrile respectively, both with 0.1% formic acid. The chromatographic method held the initial mobile phase composition (5% B) constant for 2 min. Then, it was followed by a linear gradient to 100 % B at 8 min and held constant for a 2 min at 100 % B. The flow-rate used was 0.5 mL min⁻¹. 20µL of extract were injected in each study. A 5-min post-time was used for each analysis.

The HPLC system was connected to a time-of-flight mass spectrometer Agilent TOF 6220 (Agilent Technologies, Santa Clara, CA, USA) equipped with an electrospray interface operating in positive and negative ion mode, using the following operation parameters: capillary voltage, 4000 V; nebulizer pressure, 40 psig; drying gas, 9 L min⁻¹; gas temperature, 325 °C; fragmentor voltage (in-source CID fragmentation), 190 V. 160, 190, 220 and 250V were used for fragments evaluation. LC-MS accurate mass spectra were recorded across the range 50-1000 m/z. 1.5 spectra per second acquisition rate was employed. To perform CID experiments with a dedicated collision cell, an Agilent 1260 Infinity HPLC system was connected to a hybrid quadrupole time-of-flight (Q-TOF) mass spectrometer Agilent 6530 (Agilent Technologies, Santa Clara, CA), equipped with the same dual spray interface, applying the same chromatographic method and MS parameters described for the TOF instrument except fragmentor voltage, set at 90 V. "All-ion mode" full-scan acquisition was used at different collision energy conditions (0, 10, 20 and 30 V). All data was recorded with Agilent Mass Hunter Data Acquisition software (version B.04.00) and processed with Agilent Mass Hunter Qualitative Analysis software (version B.04.00), which included both "Molecular Feature Extractor" and "Find by Formula" applications used. Accurate mass measurements of each peak from the total ion chromatograms were

obtained by means of an automated calibrant delivery system using a dual-nebulizer electrospray source that introduces the flow from the outlet of the chromatograph together with a low flow of a calibrating solution (calibrant solution A, Agilent Technologies), which contains the internal reference masses (purine ($C_5H_4N_4$ at m/z 121.050873 and HP-0921 [hexakis-(1H,1H,3H-tetrafluoropentoxo)-phosphazene] ($C_{18}H_{18}O_6N_3P_3F_{24}$) at m/z 922.009798). Agilent MassHunter Data Acquisition software was used for method development and full-scan data acquisition. Agilent MassHunter Qualitative Analysis (version B.04.00) software were used for data processing.

Chemicals and Reagents. Pesticides, veterinary drugs, food-packaging contaminants, perfluorinated compounds, mycotoxins, nitrosamines and sweeteners analytical-grade standards were purchased from Fluka (Pestanal quality) (Madrid, Spain), Sigma-Aldrich (Madrid, Spain) or Dr. Ehrenstorfer (Augsburg, Germany). Individual stock solutions (ca. 500 mg L^{-1} each) were prepared in different solvents depending on compound solubility and stability (acetonitrile, metanol MeOH, and/or water in basic or acidic media) and were stored at -20°C . Working solutions containing ca. 30 compounds each were prepared by appropriate dilution of the stock solutions with MeOH at concentration levels in the range from 0.01 to 1 mg L^{-1} . HPLC-grade acetonitrile and methanol were obtained from Merck (Darmstadt, Germany). Formic acid was obtained from Fluka (Buchs, Switzerland). Primary-secondary amine (PSA) Bond Elut was obtained from Varian, Inc. (Palo Alto, CA, USA). Acetic acid was from Panreac (Barcelona, Spain). Anhydrous magnesium sulfate anhydrous ($MgSO_4$) and sodium acetate ($NaCOOCH_3$) were from Sigma-Aldrich (Madrid, Spain). A Milli-Q-Plus ultrapure water system from Millipore (Milford, MA, USA) was used throughout the study to obtain the HPLC-grade water used during the analyses.

The 630 compounds included in the study were carefully selected considering different lists established by official bodies from the European Union and The United States, previous relevant literature, and thus, their potential presence in different types of foodstuffs and water. Up to 426 pesticides, 117 veterinary drugs and pharmaceutical, 43 food-packaging contaminants, 10 perfluorinated compounds 21 mycotoxins, 9 nitrosamines and 5 sweeteners were included. From the 426 pesticides included, most of them are covered in Annex 1 of Directive 396/2005 for several commodities [30]. A significant number (over 130 species), considered as priority pesticides according to Annex I of Commission Implementing Regulation 788/2012 due to their usage and frequency of detection, were also included in the targeted list [31]. Most of the selected food-packaging contaminants and perfluorinated compounds are regulated by different EU Directives [32,33]. With regards to the veterinary drugs and pharmaceuticals, most of the selected substances are US FDA approved veterinary drugs for animal use [34] or authorized products in the European Union. It should be noted that some of the species are included in **Table 1** as pesticides although they can be classified as veterinary drugs such as albendazole, fenbendazole, fenthion, ivermectin, lufenuron, spinosad, sulfaquinoxaline, thiabendazole and trichlorfon, all of them included in US FDA approved list for animal use. Along with the veterinary drugs, other human pharmaceuticals were included due to their ubiquitous presence in the environment as described elsewhere [19]. Besides, all the main mycotoxins including those regulated in Commission Regulation EC 1881/2006 [35] are amongst the 21 substances selected. The 11 nitrosamines selected are included in US EPA final Drinking Water Contaminant Candidate lists (CCL-3) [36,37]. Finally, all the sweeteners included are DG SANCO authorized food additives [38].

Sample treatment. Different baby food samples from different local markets containing meat and vegetables were pooled and used as model matrix. Extraction was accomplished using QuEChERS approach described elsewhere and detailed in the Annex [39].

Results and discussion

Screening method development and considerations. Several requirements from DG SANCO were taken into account to develop the screening method [40]. In first place, given the complexity of the application, that is to measure trace amounts of hundreds of species at the $\mu\text{g Kg}^{-1}$ level in complex mixtures with around 5000-20000 matrix components that may potentially interfere [23] demands for high selective approaches able to separate and unambiguously confirm these species. UHPLC-TOFMS was used for this purpose. Preliminary studies showed the need for a dedicated chromatographic gradient. The use of short (*eg.* 5-min run) methods could easily results in multiple issues and related problems such as interferences due to overlapping and also major matrix effects. Given the large number of analytes in such large-scale methods, it is advisable to provide thorough separation conditions. A 10-min gradient was finally selected as it provided appropriate separation conditions for most of the species tested. Average peak width were in the range of 6-10 seconds, so that acquisition method cycle times slightly below 1 scan per second could fit well with the separation conditions. **Figure 1** includes a histogram with the distribution of the analytes throughout the entire LC run, and also a 2D-plot of the analytes distribution (retention time (RT) and m/z values) to provide a glimpse of such complexity, that only can be unraveled with advanced methods such as UHPLC-HRMS. As illustrated in the histogram, most of the analytes included in the database are concentrated in the middle section of the chromatogram. Consequently, and leaving aside the matrix components present in samples,

there were several cases of isobaric coeluting species that need additional tools for appropriate resolution.

Another issue that could be easily interpreted from **Figure 1** is the presence of early eluting compounds. Amongst the plethora of contaminants with such wide range of physicochemical properties, there are some highly polar species that are not retained in the standard column used (C₁₈, 2.1 mm x 50 mm., 1.8 µm particle size). From the 2D-plot, and considering the void volume (t₀ = 0.27 minutes), up to 33 compounds were found with capacity factors (k) < 1, so that the criterion set by DG SANCO for pesticide testing (the analyte RT should be at least twice the RT corresponding to the void volume) was not fulfilled in these cases. Some of the analytes are *eg.* quaternary ammonium herbicides (diquat, paraquat, chlormequat), polar species such as glyphosate and its metabolites or small molecules such as amitrol. In these cases, the use of the so-called single residue methods would be requested, using other chromatographic approaches such as HILIC, which would not work with the majority of the compounds included in the study.

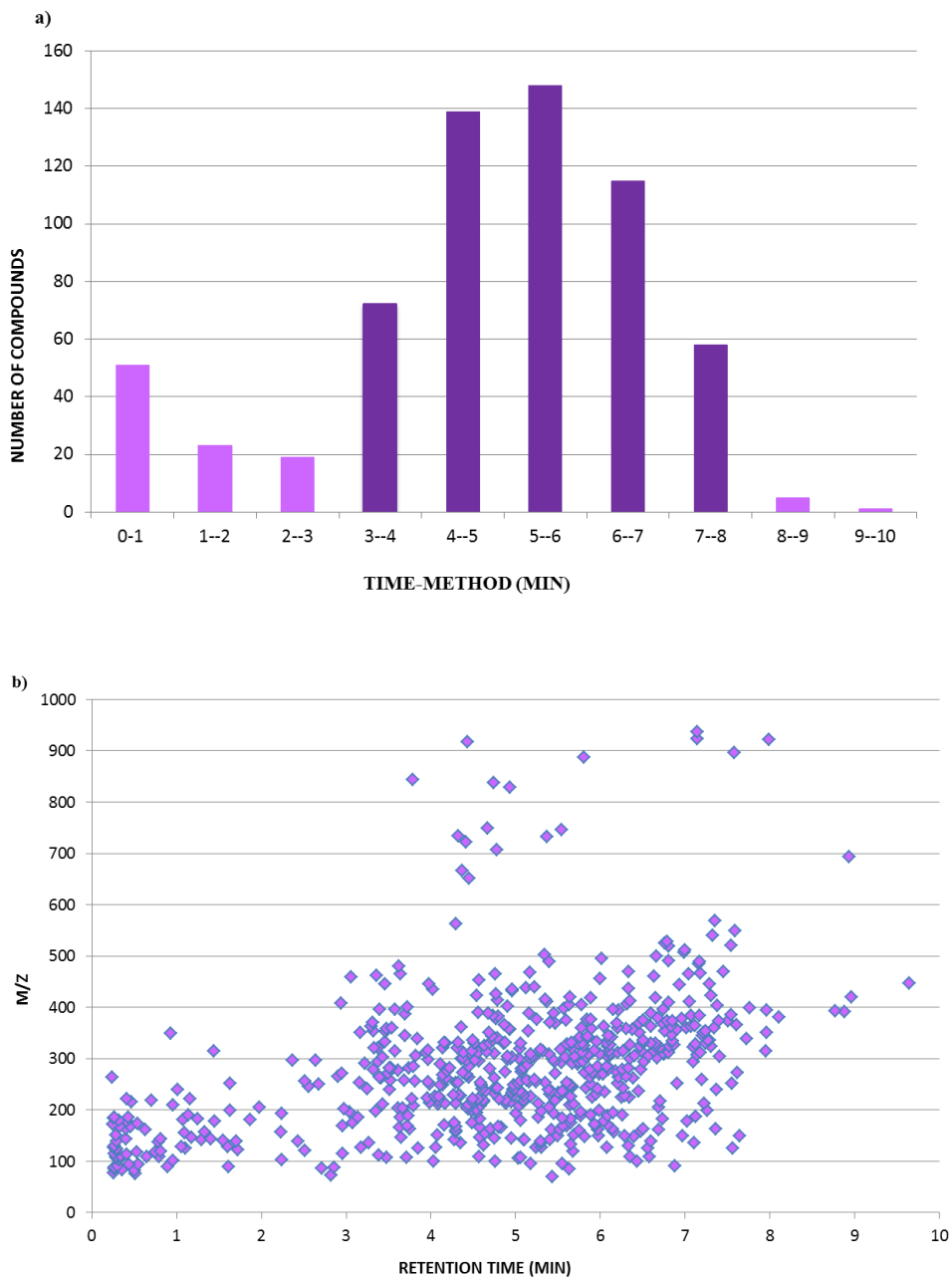


Figure 1 a) Distribution of database compounds according to their retention time; b) 2D-plot retention time/ m/z for compounds included in the database developed.

The identification of selected compounds was performed by RT matching combined with accurate mass measurements of the targeted species -

generally the (de)protonated molecules-, except some analytes which displayed adducts (sodium, ammonium or methanol), or they were fragmented during ion transportation in the mass spectrometer (in-source CID) so that the more abundant ion was a fragment instead. The combined information of RT and accurate masses of the ion(s) characteristic for each analyte enabled their unambiguous confirmation. Additionally, isotopic pattern matching could be used for further confirmatory purposes, particularly when the molecules contain chlorine, bromine or sulphur atoms (A+2 signals).

Once mixtures of standards were prepared and injected in the UHPLC-(Q) TOFMS system, the relevant information required for each compound was collected. **Table S1** contains information for the identification of the 625 compounds included in the database (Annex). **Table S2** (Annex) includes the detailed fragmentation of (both in-source CID and all ion mode CID MS/MS experiments.) of the species.

Protonated or deprotonated molecule, fragment or adduct (sodium, ammonium or methanol) were showed as the main ion for database compounds. 93% of pesticides, 94% of veterinary drugs, 83% food packaging contaminants, and 100% of nitrosamines and mycotoxins were identified in positive ion mode. $[M+H]^+$ was showed as the more abundant ion for 63% pesticides, 74% veterinary drugs, 48% food packaging contaminants food packaging contaminants, 81% mycotoxins and 89% nitrosamines. However, 26 pesticides, 5 veterinary drugs, 6 food packaging contaminants, 10 perfluoroorganic compounds and 5 sweeteners had deprotonated molecules ($[M-H]^-$) as the most abundant ion. For 10 pesticides, 2 veterinary drugs, 1 food packaging contaminants and 2 mycotoxins, sodium adducts were used for identification. Ammonium adducts were employed to identify 3 pesticides and 2 food packaging contaminants. Methanol adducts were the

most abundant ion for 4 veterinary drugs. Besides, fragments were identified as the main ion for 111 pesticides, 20 veterinary drugs, 11 food packaging contaminants, 2 mycotoxins, 9 perfluorinated compounds and 1 nitrosamine.

Selectivity of the accurate-mass database screening approach

Isobaric coeluting species. Despite one should expect that the strong selectivity provided by HRMS instrumentation itself is enough for the application, the role of chromatography must not be underrated. Actually, when considering the complexity of the samples and the high number of species, it turns out that the role of chromatography is remarkable in many cases. Due to the high number of compounds, coelutions and species with the same nominal mass (isobaric species) are very common as highlighted in the 2D-Plot with such density of compounds concentrated in a small section of the chromatogram. The m/z value itself is not enough to obtain reliable screening results. In the studied database, there were a lot of compounds with the same nominal mass (isobaric species), which cannot be distinguished when low-resolution mass spectrometry is used. The term isobaric is used to describe compounds with the same nominal mass but different elemental composition. The high number of database compounds makes possible the presence of isobaric species and it is obvious the possibility of encountering isobaric species when the number of compounds included in the database is extended. Table 1 includes a high number of these species. 172 sets of compounds constituted from 2 to 7 compounds were identified as isobars. It means that 76% of database compounds were somewhat involved in isobaric groups. The vast majority of cases (383 compounds) were clearly resolved by retention time, as shown in **Table 1**. This fact demonstrates the need of providing retention time data when such a large database is developed. Otherwise, one should expect many potential false positives when applying the database to actual samples. **Figure S1**

(Annex) shows examples of group of isobaric compounds that could be clearly distinguished solely by means of RT; in spite of having the same nominal masses, differences in retention times were significantly higher than 0.20 min, so this criterion was employed to resolve these compounds.

Table 1. Table with groups of isobaric species of the database. Elucidation criteria for each group.

Group	Compound	Theoretical m/z	RT (min)	Comments
1	Methidation	85.0396	5.63	Distinguished by RT
	Amitrol	85.0509	0.27	
2	Methomyl	88.0215	2.86	Distinguished by RT and resolving power
	Morpholin	88.0757	0.27	
3	Aldicarb sulfoxide	89.0419	1.61	Distinguished by RT
	N-nitrosomethylenthylamine	89.0709	0.89	
4	Methamidophos	94.0052	0.55	Distinguished by resolving power
	Aniline	94.0651	0.44	
5	Fenobucarb	95.0491	5.55	Distinguished by RT
	Isoprocarb	95.0491	5.18	
6	Tributyl phosphate	98.9842	6.43	Distinguished by RT
	Triethyl phosphate	98.9842	4.03	
7	Ethylthiourea	103.0324	0.32	Distinguished by RT and resolving power
	N-nitrosodiethylamine	103.0866	2.24	
8	Ethiofencarb	107.0491	5.06	Distinguished by RT
	Ethiofencarb sulfone	107.0491	3.71	
	Ethiofencarb sulfoxide	107.0491	3.48	
9	Cyazofamid	108.0114	6.35	Distinguished by RT and resolving power
	o-Toluidine	108.0808	0.79	
10	Fonofos	108.9871	6.58	Distinguished by RT
	o-Anisidine	109.0522	0.65	
	Metolcarb	109.0648	4.57	
	1,3-Phenylenediamine	109.0760	0.29	
11	Propylene thiourea	117.0481	0.53	Distinguished by RT
	N-nitrosomorpholine	117.0659	0.75	
12	Pentafluoropropionic acid	118.9926	0.81	Distinguished by RT and resolving power
	Iprovalicarb	119.0855	5.68	
13	Chlormequat chloride	122.0370	0.28	Distinguished by RT and resolving power
	2,4-Dimethylaniline	122.0964	1.72	
14	2,4-Diaminotoluene	123.0917	0.29	They cannot be distinguished by RT, resolving power, isotopic profile or additional ions
	2,6-Diaminotoluene	123.0917	0.29	
15	Dimethoate	124.9821	3.85	Distinguished by RT
	Omethoate	124.9821	1.10	
	Orbencarb	125.0153	6.56	
	Fenpropathrin	125.0960	7.56	
16	Clofibric Acid	126.9951	5.24	Distinguished by RT, with the exception of dibrom and clofibric acid, which are distinguished by resolving power, isotopic profile and additional ions (fragment ions: dibrom, m/z 378; clofibric acid, m/z 213)
	Dibrom	127.0155	5.31	
	Mevinphos	127.0155	4.06	
	Monocrotophos	127.0155	3.18	
	Tetrachovinphos	127.0155	6.08	
17	Melamine	127.0727	0.26	Distinguished by RT and isotopic profile
	4-Chloroaniline	128.0262	1.60	
	Metronidazole	128.0456	1.06	
18	Benzothiazole	136.0215	4.35	Distinguished by RT and resolving power
	2,4,5-Trimethylaniline	136.1121	3.27	

19	Clofentezine	138.0105	6.60	Distinguished by RT and resolving power
	Propham	138.0550	5.30	
	2-Methoxy-5-methylalanine	138.0913	1.70	
20	2,4-Diaminoanisole	139.0866	0.29	Distinguished by RT
	Pentylentetrazole	139.0978	2.43	
21	4-Chloro-2-methylphenol	141.0113	5.10	Distinguished by RT, which the exception of 4-Chloro-o-tolyoxyacetic acid and 4-chloro-2-methylphenol, which are distinguished by additional ion of 4-chloro-o-tolyoxiacetic acid (m/z 199)
	4-Chloro-o-tolyoxyacetic acid	141.0113	5.11	
	Mecoprop	141.0113	5.41	
	1-Naphtalene-Acetamide	141.0699	4.28	
22	Ethephon	142.9670	1.40	Distinguished by RT
	Acephate	142.9926	0.81	
	Daminozide	143.0815	0.40	
23	Cadusafos	158.9698	6.48	Distinguished by RT and resolving power
	N-nitrosodi-n-dibutylamine	159.1492	5.75	
24	Clopyralid	145.9559	1.18	Distinguished by RT and resolving power
	Desethyl Terbutylazine	146.0227	4.58	
	Vamidothion	146.0634	3.65	
25	Mefenacet	148.0757	5.82	Distinguished by RT and resolving power
	Propisochlor	148.1121	6.40	
26	Dicyclohexyl phthalate	149.0233	7.64	Distinguished by RT
	Diethyl phthalate	149.0233	5.50	
	Di-N-butyl phthalate	149.0233	6.97	
	Dipropyl phthalate	149.0233	6.29	
	Methoxyfenozide	149.0597	5.98	
27	Methyl paraben	151.0401	4.08	Distinguished by RT and resolving power
	Promecarb	151.1117	5.69	
28	Asulam	156.0114	2.23	Distinguished by RT
	Sulfabenzamide	156.0114	4.30	
	Sulfacetamide	156.0114	1.33	
	Propetamphos	156.0243	6.16	
29	Irgasan	160.9555	6.69	Distinguished by RT
	Dichlorprop	160.9566	5.42	
	Ibuprofen	161.1325	5.97	
30	Acesulfame-K	161.9867	0.63	Distinguished by RT
	3,5-Dichloroaniline	161.9872	5.52	
31	Transfluthrin	163.0165	7.36	Distinguished by RT
	Dimethyl phthalate	163.0390	4.71	
	Carbofuran 3-Hydroxy	163.0754	3.75	
	Phenthoate	163.0754	6.51	
	Nicotine	163.1230	0.4	
32	Methabenzthiazuron	165.0481	4.86	Distinguished by RT, with the exception of 1-Naphthyl-N-methylcarbamate and methabenzthiazuron, which are distinguished by resolving power
	Ethyl 4-hydroxybenzoate	165.0557	4.58	
	1-Naphthyl-N-methylcarbamate	165.0910	4.86	
	Fenuron	165.1022	3.63	
	Bendiocarb	167.0703	4.80	
33	Diphenhydramine	167.0855	4.30	Distinguished by RT

	Cyromazine	167.1040	0.46	
34	Glyphosate	168.0067	0.33	Distinguished by RT and resolving power
	Phenmedipham	168.0655	5.61	
35	Perfluorobutyric acid	168.9894	2.96	Distinguished by RT
	Clothianidin	169.0541	3.72	
	Methiocarb	169.0682	5.56	
	N-nitroso-n-diphenylamine	169.0886	5.94	
37	Diphenylamine	170.0964	6.09	Distinguished by RT
	4-Aminobiphenyl	170.0964	4.16	
38	Atrazine Desisopropyl	174.0541	3.08	Distinguished by RT and resolving power
	Pyroquilon	174.0913	4.28	
39	Dicamba	174.9723	4.49	Distinguished by RT
	Tcpp	174.9923	5.65	
40	Piperonyl Butoxide	177.0910	7.03	Distinguished by RT
	Cotinine	177.1022	0.41	
41	Barban	178.0418	6.04	Distinguished by RT
	Cyclamate-Na	178.0538	1.45	
42	Theobromine	181.0720	1.08	Distinguished by RT and additional ions (fragment ions: theophylline, m/z 124; theobromine, m/z 138)
	Theophylline	181.0720	1.87	
43	Saccharin	181.9917	1.25	Distinguished by RT and resolving power
	Phosalone	182.0003	6.73	
	Desmedipham	182.0812	5.65	
44	2,4-Dinitrophenol	183.0047	4.58	Distinguished by RT
	Azobenzene	183.0917	5.55	
	Diquat dibromide	183.0917	0.26	
45	Methiocarb Sulfoxide	185.0631	3.64	Distinguished by RT
	Fuberidazol	185.0709	3.14	
	Naproxen	185.0961	5.27	
	Benzidine	185.1073	0.43	
46	Atrazine Desethyl	188.0697	3.73	Distinguished by RT and resolving power
	Molinate	188.1104	5.77	
47	Isoprothiolane	188.9675	6.09	Distinguished by RT and resolving power
	Propamocarb	189.1598	1.14	
48	Propyzamid	189.9821	5.89	Distinguished by RT and resolving power
	Eptc	190.126	6.26	
49	Carbendazim	192.0768	2.24	Distinguished by RT and resolving power
	Deet	192.1383	5.01	
	Fluroxypyr	194.9534	4.54	
50	Caffeine	195.0877	3.04	Distinguished by RT and resolving power
	4-Hexylresorcinol	195.1380	5.77	
51	DNOC	197.0204	5.31	Distinguished by RT and resolving power
	Chlordimeform	197.0840	3.35	
	Ethion	199.0011	7.26	
52	Monuron	199.0633	4.48	Distinguished by RT
	Cymoxanil	199.0826	1.63	
53	Thiabendazole	202.0433	2.98	Distinguished by RT and resolving power
	Simazine	202.0854	4.44	
54	Quinmerac	204.0211	3.67	Distinguished by RT and resolving

	Pebulate	204.1417	6.69	power
55	Dicloran	204.9577	5.40	Distinguished by RT
	Bromacil	204.9607	4.42	
	Levamisole	205.0794	1.98	
56	Quinoclamine	208.0160	4.59	Distinguished by RT
	Ethidimuron	208.0209	3.80	
57	Methacrifos	209.0032	5.64	Distinguished by RT
	Bisphenol A 2,3-dihydroxypropyl ether	209.1172	4.44	
	Aminocarb	209.1285	0.96	
58	Acibenzolar S-Methyl	210.9994	5.69	Distinguished by RT
	Prohexadione	211.0612	4.09	
	Thiamethoxam	211.0648	3.43	
59	Pendimethalin	212.0666	7.23	Distinguished by RT
	Propachlor	212.0837	5.27	
60	Aldicarb	213.0668	4.30	Distinguished by RT, with the exception of aldicarb and butocarboxim, which are distinguished by additional ions (fragment ions: aldicarb, m/z 89; butocarboxim, m/z 75)
	Butocarboxim	213.0668	4.17	
	Chlorotoluron	213.0789	4.89	
61	Monolinuron	215.0582	5.10	Distinguished by retention time, with the exception of terbacil and metribuzin, which are distinguished by isotopic profile and fragment ions (terbacil, m/z 158; metribuzin, m/z 187)
	Terbacil	215.0593	4.50	
	Sulfaguanidine	215.0597	0.47	
	Metribuzin	215.0961	4.62	
62	Atrazine	216.1011	4.95	Distinguished by RT and resolving power
	Cycloate	216.1417	6.71	
63	Propanil	218.0134	5.47	Distinguished by RT
	Pymetrozin	218.1036	0.70	
	Pyracarbolid	218.1176	4.89	
	Ethoxyquin	218.1539	4.62	
64	2,4-Dichlorophenoxyacetic acid	218.9621	5.10	Distinguished by RT
	Perfluoropentanoic acid	218.9862	4.09	
	Oxadixyl	219.1128	4.55	
65	Dichlorvos	220.9532	4.56	Distinguished by resolving power, additional ions (fragment ions: dichlorvos, m/z 109; m/z 102) and isotopic profile
	Thidiazuron	221.0492	4.50	
66	Chloridazon	222.0429	3.78	Distinguished by RT
	Glufosinate N-acetyl	222.0537	0.41	
	Carbofuran	222.1125	4.81	
	Formetanate	222.1237	1.16	

67	Dichlofluanid	223.9498	6.34	Distinguished by RT, with the exception of dichlofluanid and mefenamic acid, which are distinguished by additional ions (dichlofluanid, m/z 123; mefenamic acid, m/z 242)
	Mefenamic Acid	224.1070	6.25	
	Mepanipyrim	224.1182	5.91	
68	Diethofencarb	226.1074	5.65	Distinguished by RT, with the exception of prometon, which is distinguished by additional ion (m/z 142) at higher fragmentor voltage. Secbumeton and terbumeton cannot be distinguished by RT, resolving power, isotopic profile or fragment ions.
	Cyprodinil	226.1339	5.18	
	Prometon	226.1662	4.05	
	Secbumeton	226.1662	4.05	
	Terbumeton	226.1662	4.10	
69	Mecarbam	226.9961	6.29	Distinguished by RT and resolving power
	Bisphenol A	227.1078	5.10	
70	Fosthiazate	227.9912	4.98	Distinguished by RT and resolving power
	Ametryn	228.1278	4.35	
71	Metoxuron	229.0738	4.33	Distinguished by resolving power and additional ions (fragment ions: methoxuron, m/z 72; tebuthiuron, m/z 172) at higher fragmentor voltage
	Tebuthiuron	229.1118	4.27	
72	Propazine	230.1167	5.41	Distinguished by RT, with the exception of propazine and terbuthylazine, which are distinguished by additional ions (fragment ions: propazine, m/z 188; terbuthylazine, m/z 174) at higher fragmentor voltage
	Terbuthylazine	230.1167	5.54	
	Trietazine	230.1167	5.95	
73	Diuron	233.0243	5.08	Distinguished by RT, with the exception of diuron and fluomethuron, which are distinguished by resolving power and isotopic profile
	Fluomethuron	233.0896	4.96	
	Siduron	233.1648	5.51	
74	Parathion	235.9777	6.45	Distinguished by RT and resolving power
	Carboxine	236.0740	5.05	
75	Fenpiclonil	236.9981	5.55	Distinguished by RT, with the exception of fenpiclonil and buturon, which are distinguished by resolving power
	Buturon	237.0789	5.42	
	Carbamazepine	237.1022	4.65	
76	Bentazone	239.0496	4.97	Distinguished by RT and resolving power
	Pirimicarb	239.1503	3.51	
77	Clomazone	240.0786	5.39	Distinguished by RT
	Butralin	240.0979	7.37	
	Salbutamol	240.1594	1.01	
78	Picloram	240.9333	3.25	Distinguished by RT
	Ethofumesate	241.0529	5.97	
	Cyanazine	241.0963	4.61	
	Thiofanox	241.0981	4.99	

79	Vinclozolin	242.0134	6.27	Distinguished by RT, with the exception of prometryn and terbutryn, which are distinguished by additional ions (fragment ions: prometryn, m/z 158; terbutryn, m/z 186)
	Prometryn	242.1434	4.76	
	Terbutryn	242.1434	4.79	
80	Paraoxon methyl	248.0319	4.60	Distinguished by RT
	Triazoxide	248.0334	4.14	
	Forchlorfenuron	248.0585	4.98	
81	Linuron	249.0192	5.64	Distinguished by RT and resolving power
	Difenzoquat	249.1392	4.11	
82	Diclofenac	250.0196	5.89	Distinguished by RT and resolving power
	Sulfapyridine	250.0645	2.68	
	Oxybendazole	250.1186	3.99	
83	2-Ethylhexyl diphenyl phosphate	251.0468	7.55	Distinguished by RT
	Sulfadiazine	251.0597	1.63	
	Citrinin	251.0914	5.03	
84	Prosulfocarb	252.1417	6.91	Distinguished by RT
	Furmecycloz	252.1594	6.21	
85	3,3-Dichlorobenzidine	253.0294	5.61	Distinguished by RT, with the exception of hexazinone and thiacloprid, which are distinguished by resolving power and isotopic profile
	Demeton-S-Methyl	253.0092	4.59	
	Hexazinone	253.1659	4.32	
	Menadione	253.0171	3.16	
	Thiacloprid	253.0309	4.30	
	Trinexapac-Ethyl	253.1071	5.35	
86	Ketoprofen	255.1016	5.24	Distinguished by resolving power
	B-Estradiol	255.1743	5.16	
87	Sulfathiazole	256.0209	2.51	Distinguished by RT and resolving power
	Imidacloprid	256.0596	3.81	
	Dimethametryn	256.159	5.06	
88	Trichlorfon	256.9299	3.52	Distinguished by resolving power and isotopic profile
	Imazalil metabolite	257.0243	3.69	
89	Dichlofenthion	258.9147	7.20	Distinguished by RT and resolving power
	Metobromuron	259.0077	5.22	
90	Tolfenamic Acid	262.0629	6.39	Distinguished by RT
	Oxolinic Acid	262.0710	4.19	
	Flumequine	262.0874	4.75	
	Imazapyr	262.1186	3.41	
91	Carbadox	263.0775	3.40	Distinguished by RT
	Gliotoxin	263.1026	4.45	
	Streptomycin	263.1462	0.24	
92	Parathion-Methyl	264.0090	5.88	Distinguished by RT and resolving power
	Flufenamic Acid	264.0631	6.22	
93	Aclonifen	265.0374	6.31	Distinguished by RT and resolving power
	Sulfamerazine	265.0754	2.90	
94	Mephosfolam	270.0382	4.42	Distinguished by RT and resolving power
	Mepronil	270.1489	6.03	
95	Sulfamethizole	271.0318	3.49	Distinguished by RT and resolving

	Nitenpyram	271.0956	2.95	power
	Estrone	271.1693	5.47	
96	Methoprotryne	272.1540	4.38	
	N,N-Diethyl-2-Naphtoloxypromide	272.1645	5.91	Distinguished by RT
97	Anilazine	272.9507	5.82	Distinguished by RT and resolving power
	Spiromesifen	273.1485	7.62	
98	Bromoxynil	273.8509	5.07	Distinguished by resolving power
	Fenpropidine	274.2529	4.88	
99	Meclofenamic Acid	278.0134	6.26	Distinguished by RT, with the exception of meclofenamic acid and fenitrothion, which are distinguished by isotopic profile and additional ion (meclofenamic acid, m/z 243; fenitrothion, m/z 246)
	Fenitrothion	278.0247	6.10	
	Triflumizole	278.0554	5.88	
100	Fenthion	279.0273	6.48	Distinguished by RT and resolving power
	Sulfamethazine	279.0910	3.32	
101	Metalaxyl	280.1543	5.07	Distinguished by RT
	Karbutilate	280.1656	4.70	
102	Sulfameter	281.0703	3.51	Distinguished by RT, with the exception of sulfameter and sulfamethoxy-pyridazine, that cannot be distinguished by RT, resolving power, isotopic profile or fragment ions
	Sulfamethoxy-pyridazine	281.0703	3.53	
	Sulfamonomethoxine	281.0703	3.74	
103	Ofurace	282.0891	5.10	
	Albendazole sulfoxide	282.0907	3.51	Distinguished by RT
	Kresoxim Methyl	282.1125	6.33	
	Cycloheximid	282.1700	4.22	
104	Procymidone	284.0240	6.09	Distinguished by resolving power, isotopic profile and additional ions (fragments ions: procymidone, m/z 256; penconazole, m/z 159; metolachlor, m/z 252) at higher fragmentor voltage
	Penconazole	284.0716	5.97	
	Metolachlor	284.1412	6.08	
105	Sulfachloropyridazine	285.0208	3.80	Distinguished by RT and resolving power
	Promethazine	285.1420	4.45	
106	Myclobutanil	289.1215	5.73	Distinguished by RT
	Imazamethabenz-Methyl	289.1547	4.11	
107	Chloroxuron	291.0895	5.67	Distinguished by RT and resolving power
	Trimethoprim	291.1452	3.22	
	Chlorbromuron	292.9687	5.74	
108	Etrimphos	293.0719	6.52	Distinguished by RT and resolving power
	Aspartame	293.1143	3.38	
	Triadimefon	294.1004	5.80	
109	Paclobutrazol	294.1368	5.46	Distinguished by RT and resolving power
	Amitraz	294.1965	7.10	
110	Hydrochlorothiazide	295.9572	2.64	Distinguished by RT and resolving power
	Mebendazole	296.1030	4.42	

111	Imazalil	297.0556	4.52	Distinguished by RT and resolving power
	Deoxynivalenol	297.1333	2.37	
	Albendazole sulfone	298.0856	3.97	
112	Spiroxamine	298.2741	4.91	Distinguished by RT and resolving power
	Tridemorph	298.3105	5.44	
113	Azaconazole	300.0301	5.04	Distinguished by RT, with the exception of azaconazole and fenbendazole, which are distinguished by resolving power and isotopic profile
	Phosphamidon	300.0762	4.36	
	Fenbendazole	300.0801	4.94	
114	Tolclofos Methyl	300.9616	6.67	Distinguished by RT and resolving power
	Sulfaquinoxaline	301.0754	4.38	
	Nordihydroguaiaretic acid	301.1445	5.17	
115	Robenidine	302.1751	3.43	Distinguished by RT and resolving power
	Flutriafol	302.1099	4.96	
	Furalaxyl	302.1387	5.59	
	Fenhexamid	302.0709	5.84	
	Fenoxycarb	302.1387	6.10	
116	Triallat	304.0091	7.41	Distinguished by RT and resolving power
	Norflurazone	304.0459	5.20	
	Fenamiphos	304.1131	5.70	
	Fenpropimorph	304.2635	4.91	
117	Pirimiphos Methyl	306.1036	6.41	Distinguished by RT
	Imazamox	306.1448	3.82	
	Buprofezin	306.1635	6.08	
118	Prochloraz	308.0006	5.4	Distinguished by RT
	Quinoxifen	308.004	6.75	
	Tebuconazole	308.1524	5.86	
119	Diflubenzuron	309.0248	6.00	Distinguished by RT, with the exception of diflubenzuron and phenylbutazone, which are distinguished by isotopic profile and additional ions (fragment ions: diflubenzuron, m/z 113; phenylbutazone, m/z 120) at higher fragmentor voltage
	Fensulfothion	309.0379	5.18	
	Phenylbutazone	309.1598	6.12	
120	Bifenox	309.9668	6.74	Distinguished by RT and resolving power
	Fluoxetine	310.1413	4.75	
	Benzydamine	310.1914	4.47	
121	Edifenphos	311.0324	6.21	Distinguished by RT
	Sulfadoxine	311.0809	3.94	
	Sulfadimethoxyn	311.0809	4.39	
122	Fenamidone	312.1165	5.79	Distinguished by RT
	Imazaquin	312.1343	4.56	
	Pretilachlor	312.1725	6.81	
	Butachlor	312.1725	7.18	

123	Bensulide	313.9739	6.49	Distinguished by RT, with the exception of isazophos and triazophos, which are distinguished by additional ions (fragment ions: isazophos, m/z 120; triazophos, m/z 162), at higher fragmentor voltage
	Isazophos	314.0490	6.27	
	Triazophos	314.0723	6.11	
124	Hydroflumethiazide	314.9716	3.58	Distinguished by RT
	Triclocarban	314.9853	6.63	
	Nuarimol	315.0695	5.32	
	Aflatoxin B2	315.0863	4.49	
	Ranitidine	315.1485	1.44	
125	Dibutyl sebacate	315.2530	7.95	Distinguished by RT and resolving power
	Oxfendazole	316.0751	3.97	
126	Flusilazole	316.1076	5.93	Distinguished by RT and resolving power
	Perfluoroheptanoic acid	318.9798	5.05	
127	Zearalenone	319.1540	5.66	Distinguished by RT and resolving power
	Fenamiphos Sulfoxide	320.1080	4.31	
128	Norfloxacin	320.1405	3.38	Distinguished by RT and resolving power
	Chloramphenicol	321.0051	4.14	
129	Enoxacin	321.1357	3.33	Distinguished by RT and resolving power
	Chlorpyrifos Methyl	321.9023	6.71	
130	Pyriproxifen	322.1438	7.10	Distinguished by RT, with the exception of sulfotep and pyranocoumarin, which are distinguished by resolving power
	Sulfotep	323.0300	6.65	
	Sulprofos	323.0358	7.31	
131	Pyranocoumarin	323.1278	6.47	Distinguished by RT and resolving power
	Epn	324.0454	6.82	
132	Flutolanil	324.1206	6.09	Distinguished by RT and resolving power
	Azamethiphos	324.9809	4.63	
133	Sterigmatocystin	325.0707	5.81	Distinguished by RT, with the exception of diniconazole and benalaxyl, which are distinguished by resolving power and isotopic profile
	Famphur	326.0280	5.64	
	Diniconazole	326.0821	6.12	
	Benalaxyl	326.1751	6.35	
134	Cycloxydim	326.1784	6.87	Distinguished by RT and resolving power, with the exception of etaconazol and fluazifop, which are distinguished by additional ion (fragment ions: fluazifop, m/z 282; etaconazol, m/z 159) at higher fragmentor voltage
	Etaconazol	328.0614	5.74	
	Fluazifop	328.0791	5.61	
135	Sethoxydim	328.1941	7.13	Aflatoxin M1, pencycuron and malachite green distinguished by RT; aflatoxin G1 and furosemide are distinguished by resolving power; furosemide and sulcotrione are distinguished by isotopic profile and additional ions (fragment ions: furosemide, m/z
	Furosemide	329.0040	4.70	
	Sulcotrione	329.0245	4.86	
	Aflatoxin M1	329.0656	4.18	
	Aflatoxin G1	329.0656	4.51	
135	Pencycuron	329.1415	6.65	Distinguished by resolving power; furosemide and sulcotrione are distinguished by isotopic profile and additional ions (fragment ions: furosemide, m/z
	Malachite Green	329.2012	5.06	

				285; sulcotrione, m/z 139)
136	Iprodione	330.0407	6.60	
	Epoxiconazole	330.0804	5.79	Distinguished by RT and resolving power
	Tralkoxidym	330.2064	7.24	
137	Fenarimol	331.0399	5.66	
	Malathion	331.0433	6.07	Distinguished by RT, with the exception of febantel 1 and Aflatoxin G2, which are distinguished by resolving power
	Aflatoxin G2	331.0812	4.32	
	Febantel ₁	331.1223	4.16	
	Famoxadone	331.1441	6.51	
138	Leucomalachite Green	331.2169	4.88	
	Zoxamide	336.0319	6.51	Distinguished by RT and resolving power, with the exception of benfluralin and trifluralin, which are distinguished by additional ion of benfluralin (m/z 236) at higher fragmentor voltage. The absence of m/z 236 can be used to distinguish this compounds
	Fenamiphos Sulfone	336.1029	4.73	
	Benfluralin	336.1166	7.29	
139	Trifluralin	336.1166	7.27	
	3-Acetyldeoxynivalenol	339.1438	3.84	Distinguished by RT and resolving power
140	Resmethrin	339.1955	7.73	
	Tembotrione	341.0245	5.76	Distinguished by resolving power, isotopic profile and additional ions (fragment ions: pyridaphention, m/z 189; tembotrione, m/z 262, at higher fragmentor voltage)
141	Pyridaphenthion	341.0719	5.86	
	Propiconazole	342.0771	6.13	Distinguished by RT and resolving power
142	Tepraloxydim	342.1467	5.84	
	Boscalid	343.0399	5.85	Distinguished by RT
143	Thiophanate Methyl	343.0529	4.72	
	Oxadiazon	345.0757	7.21	
	Oryzalin	345.0874	6.10	Distinguished by RT
	Gibberellic acid	345.1344	3.70	
144	Chlorpyrifos	349.9336	7.22	
	Clodinafop-Propargyl	350.059	6.46	Distinguished by RT and resolving power
145	Ampicillin	350.1169	3.17	
	Fentin chloride	351.0196	4.69	Distinguished by RT and resolving power
	Phenothrin	351.1955	7.96	
146	Griseofulvin	353.0786	5.15	Distinguished by RT
	Hexythiazox	353.1085	7.24	
147	Thiamphenicol	353.9975	3.32	Distinguished by RT and resolving power
	Piperophos	354.1321	6.76	
148	Triflumuron	357.0259	6.38	Distinguished by RT and resolving power
	Sulindac	357.0955	4.93	
149	Chlorsulfuron	358.0371	4.92	
	Indomethacine	358.0841	5.9	Distinguished by RT and resolving power
	Danofloxacin	358.1561	3.48	
	Bisphenol A diglycidyl ether	358.2013	6.31	
150	Isoxaflutole	360.0512	5.78	Distinguished by RT

	Clethodim	360.1395	7.02	
	Enrofloxacin	360.1718	3.54	
	Etoazole	360.1770	7.34	
151	Haloxifop	362.0401	6.04	Distinguished by RT; fenoxaprop-p-ethyl can also be distinguished by resolving power
	Oxyfluorfen	362.0401	7.07	
	Fenoxaprop P-Ethyl	362.0790	6.83	
152	Coumaphos	363.0217	6.60	Distinguished by RT and resolving power
	Marbofloxacin	363.1463	3.30	
153	Bromophos Methyl	364.8565	7.12	Distinguished by RT and resolving power
	Sulfometuron Methyl	365.0914	4.87	
	Pyridaben	365.1449	7.61	
154	Azinphos Ethyl	368.0263	6.20	Distinguished by RT and isotopic profile
	Anilofos	368.0305	6.46	
155	Perfluorooctanoic acid	368.9766	5.47	Distinguished by RT and resolving power
	Azocyclotin	369.1604	6.73	
156	loxynil	369.8231	5.41	Distinguished by RT and resolving power
	Fleroxacin	370.1373	3.31	
157	Profenofos	372.9424	6.79	Distinguished by RT and resolving power, with the exception of: 1) profenofos and quizalofop-p-ethyl (distinguished by resolving power) and 2) propargite and proquinazid (distinguished by resolving power)
	Proquinazid	373.0407	7.51	
	Quizalofop-P-Ethyl	373.0950	6.85	
	Propargite	373.1444	7.40	
158	Pyrazophos	374.0934	6.51	Distinguished by RT and resolving power
	Spirotetramat	374.1962	5.60	
159	Bromuconazole Isomer 1	375.9614	5.84	Distinguished by RT and resolving power, with the exception of bromuconazole and fluquinconazole, which are distinguished by resolving power and isotopic profile
	Fluquinconazole	376.0163	5.89	
	Bisphenol A 2,3-dihydroxypropyl glycidyl ether	376.2118	5.25	
160	Thiodicarb	377.0382	4.77	Distinguished by RT and resolving power
	Picolinafen	377.0908	6.96	
161	Penicillin V	383.1271	4.73	Distinguished by RT and resolving power
	Furathiocarb	383.1635	7.07	
162	Triforine	387.9106	5.16	Distinguished by RT
	Thifensulfuron methyl	388.0380	4.68	
	Pyraclostrobin	388.1059	6.60	
	Dimethomorph Isomer 1	388.1310	5.45	
163	Bisphenol A 3-chloro,2-hydroxypropyl glycidyl ether	394.1780	6.22	Distinguished by RT and resolving power
	Etofenprox	394.2377	7.96	
	Sucralose	395.0073	3.40	
164	Diflufenican	395.0813	6.74	Distinguished by RT and resolving power
	Rotenone	395.1489	6.15	
165	Ochratoxin A	404.0895	5.63	Distinguished by resolving power, isotopic profile and additional ions (fragment ions: ochratoxin A, m/z 239; azoxystrobin, m/z 372) at higher fragmentor voltage
	Azoxystrobin	404.1241	5.78	

166	Bensulfuron Methyl	411.0969	5.37	Distinguished by RT and resolving power
	Benfuracarb	411.1948	7.05	
	Endosulfan sulfate	418.8045	6.65	
167	Perfluorononanoic acid	418.9734	5.89	Distinguished by RT and resolving power
	Diisononyl phthalate	419.3156	8.96	
	Doxycycline	445.1605	3.98	
168	Tetracycline	445.1605	3.46	Distinguished by RT
	Difenacoum	445.1798	7.29	
	Hexaflumuron	460.9889	6.63	
169	Oxytetracycline	461.1555	3.36	Distinguished by RT and resolving power
	Fluazinam	464.9587	7.04	
170	Demeclocycline	465.1059	3.64	Distinguished by RT and resolving power
	Perfluorodecanoic acid	468.9702	6.33	
171	Flucythrinate	469.1933	7.45	Distinguished by RT and resolving power
	Flufenoxuron	489.0435	7.17	
172	T2-Toxin	489.2095	5.40	Distinguished by RT and resolving power

In the remaining cases with isobaric species involved, at least two compounds eluted relatively close (within 0.2-0.25 minutes RT shift), so additional criteria was necessary to resolve them. At this point, the resolution of the instrument on the m/z axis could be used to distinguish between some of the isobaric species. Thus, using this feature, 47 pairs of compounds could be distinguished. **Figure S2** (Annex) illustrates an example of two isobaric species which were resolved using resolving power is shown. In this figure, extracted ion chromatograms (EICs) and mass spectrums of methabenzthiazuron fragment and 1-naphthyl-n-methylcarbamate fragment are shown. Retention time difference was lower than 0.20 min, so resolving power was used to distinguish them. Mass difference in this case was high enough to use resolving power as elucidation criteria.

The TOF and Q-TOF instruments used displayed a resolution of *ca.* 15000 in the mass range studied which can resolve interferences in the range of *ca.* 15-20 mDa (Δm) (for the range of masses common to most of our target compounds). Resolving power is an important tool to distinguish isobaric compounds that cannot be resolved by retention time but its utility depends

on the resolution of the instrument used. Advances in instrumentation recently introduced provide values of 50000 (for TOF technology) or higher than 140000 (Orbitrap). When species with the same nominal mass cannot be solved by retention time or resolving power, LC-HRMS systems provide additional tools for further differentiation: the use of isotopic pattern and fragmentation experiments. 25 pairs of isobaric compounds could be distinguished by additional fragment ions, which reveal the importance of using fragmentation in this type of methodologies. In **Figure S3** (Annex) extracted ion chromatograms and mass spectrums of metribuzin and terbacil are shown. Firstly, retention time values could not be used for distinguishing those compounds ($\Delta RT < 0.20$ min). Secondly, mass difference was close to 30 ppm. Not only resolving power could be used to distinguish those compounds, but also additional ions. Fragment ions for metribuzin (m/z 187) and for terbacil (m/z 158) were useful for identify that compounds. In conclusion, 99% of isobaric species could be distinguished by retention time, resolving power or characteristic fragmentation and only 3 pairs could not be resolved. These pairs were: 2,4 and 2,6-diaminotoluene; terbumeton and secbumeton; sulfameter and sulfamethoxy-piridazine. **Table S3** (Annex) includes the theoretical m/z and retention times for those compounds. As the differences between retention times of each pair were lower than 0.05 min, they could not be distinguished by retention time. Exact masses of each pair (isomeric species) are the same so that they could not be resolved solely by MS instrument resolving power. **Figure 2** shows examples of group of isobaric compounds distinguished by retention time; in spite of having the same nominal masses, differences in retention times were close to 0.20 min, so this criterion was employed to identify those compounds. Fragmentation of each pair was tested using both in-source CID and dedicated CID MS/MS experiments in a collision cell (UHPLC-QTOFMS). However, as shown in

Figure 2, they could not be distinguished by fragmentation. Overlapped extracted ion chromatograms and mass spectra of each pair of isobaric species are illustrated. Only slight differences of retention time may eventually enable their resolution.

Fragmentation studies for confirmation purposes and the choice of the more appropriate acquisition mode. DG SANCO guidelines for identification of pesticides in food [40] were considered with the aim to evaluate UHPLC-(Q)TOFMS capabilities for confirmatory purposes, setting the measurement of 2 HR ions (within 5 ppm error) as criterion for unambiguous confirmation. For effective fragmentation, tandem mass spectrometry instrumentation using dedicated collision cell is usually the preferred and more effective option. The product ion scan is the typical experiment accomplished. However, there is one major problem affecting the typical product ion scan experiment used after precursor ion isolation. As described in **Figure 1**, nearly over 300 hundred analytes elutes in a very short time period, so that the development of such dedicated MS/MS acquisition methods would not be feasible as there is no time to register such number of experiments with appropriate sensitivity and providing an appropriate number of acquisition points per chromatographic peak.

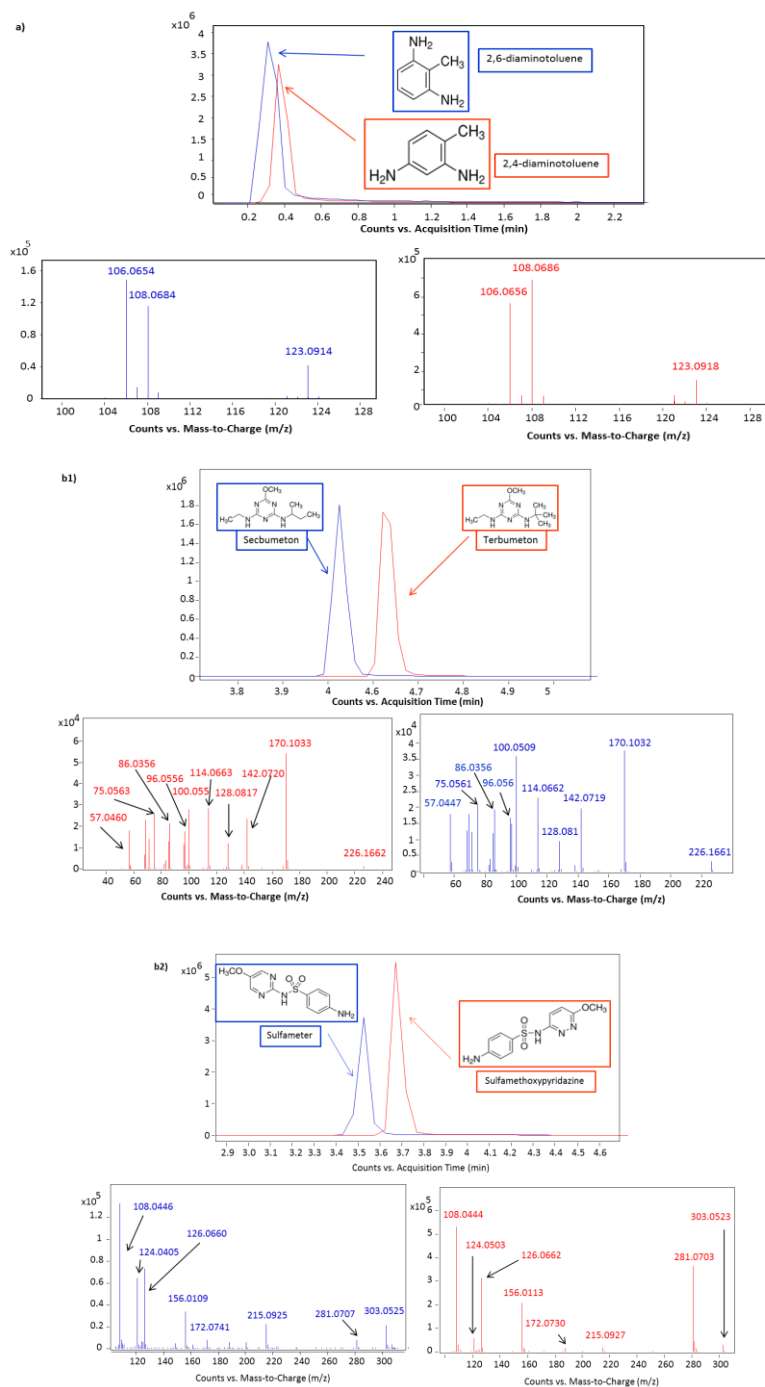


Figure 2. Overlapped extracted ion chromatograms (EICs) and mass spectrums of controversial isobaric species included in the database; a) 2,4 and 2,6-diaminotoluene; b1) secbumeton and terbumeton; b2) sulfameter and sulfamethoxyypyridazine.

For instance, *ca.* between 20-50 millisecond would be required to perform MS/MS for each analytes. Consequently, only 10-20 compounds could be simultaneously acquired at the same time, thus requiring a lot of effort to arrange the different time segment of acquisition method. For this reason, only two different acquisition approaches were examined: (a) *In-source CID fragmentation using two different fragmentor voltages* (190 and 220V), and;(b) *CID MS/MS fragmentation without precursor ion isolation* (commercially called “*all ion mode*” or “*MS^E*”), an approach analogous to in-source CID carried out in a dedicated collision cell (instead of the ion transportation region), fully compatible with full-scan acquisition of LC-TOFMS instruments.

In-source CID fragmentation [41] is an alternative approach to dedicated MS/MS instruments, in single-stage MS instruments. In-source CID fragmentation occurs in an intermediate pressure section of the mass spectrometer, between the atmospheric pressure source and the high vacuum of the mass analyzer. Ions generated in the source that enter the vacuum region can be accelerated by applying voltages, prompting collisions with surrounding species which can produce sufficient energy to yield (diagnostic) fragment ions [41]. Fragmentation patterns obtained are consistent with those attained in dedicated collision cells (in which an auxiliary collision gas is used at controlled pressure and conditions), although is not as efficient because of collision energy limitations. For confirmatory purposes, in-source CID fragmentation of the 625 database compounds was examined. As it was described in experimental section, isobaric species are very frequent in these situations. Fragmentation offers the possibility of distinguishing isobaric compounds when retention time, resolving power or isotopic patterns do not succeed. In this work, fragmentation features and abundances relatives to the most abundant ion of each compound were

studied. Four different fragmentor voltages (160, 190, 220 and 250V) were assayed. **Table S2** (Annex) includes the fragmentation for each family of compounds, listed by alphabetical order. Abbreviations such as F₁, F₂, F₃ are used to referring to fragments of each compound. Relative abundances of each fragment were calculated using the most abundant ion as reference (protonated or deprotonated molecule, adduct or fragment). In general, if the absolute value of the fragmentor voltage is increased, more fragments ions with increasing signal intensity will appear, but it depends on the behavior of each compound. Small molecules such as amitrol (C₂H₄N₄), maleic hydrazide (C₄H₄N₂O₂), AMPA (CH₆NPO₃), phosphonic acid (H₃O₃P), N-nitrosodimethylamine (C₂N₂H₆O), N-nitrosopyrrolidine (C₄H₈N₂O) or trimethylsulfonium (C₃H₈S) did not show any fragmentation. In spite of their tiny size, other small molecules such as aniline (C₂N₂H₆O), N-nitrosodiethylamine (C₄H₁₀N₂O), o-toluidine (C₇H₉N) or phenyendiamine (C₆H₈N₂) showed fragments. When molecule size increased, fragmentation in-source was more possible. However, there were examples of large molecules that did not show any fragment using this methodology (josamycin (C₄₂H₆₉NO₁₅), fumonisins B₁ (C₃₄H₅₉NO₁₅), heptadecafluorooctanesulfonic acid (C₈HO₃F₁₇S)).

As it is detailed in **Table S2** (Supplementary data), over 1200 fragments were obtained when 220V was used as fragmentor voltage, with relative abundances higher than 10%. In this sense, 794 fragments were identified for pesticides, 269 for veterinary drugs, 77 for food packaging contaminants, 33 for mycotoxins, 7 for nitrosamines, 25 for perfluorinated compounds and 7 for sweeteners. 14% of compounds did not present fragments or their relative abundances were lower than 10% (at 220V). These compounds are summarized in **Table S4** (Supplementary data), which includes 61 pesticides, 11 veterinary drugs, 2 food packaging contaminants, 3 mycotoxins, 1

perfluorinated compound, 6 nitrosamines and 1 sweetener. When fragments are not available, isotopic pattern can be useful for identification or confirmatory purposes. In this sense, 41% of pesticides shown in **Table S4** could be identified due to the presence of bromine or chlorine atoms in their structure. Compounds that did not show any useful fragmentation with in-source CID, were evaluated in detail using liquid chromatography quadrupole time-of-flight mass spectrometry (QTOF) in MS/MS using *all ion mode* fragmentation using different collision energies (0, 10, 20 and 30 V). Results are also included in **Table S1** (Annex).

At this point it is important to mention that the use of “all ion mode” preserves full-scan acquisition flexibility and benefits of acquiring all the information all the time without time window boundaries (scheduled precursor ion lists), but also adding the ability to cleave molecules which requires high energy to provide fragmentation due to the use of a dedicated collision cell. Given the number of potentially coeluting analytes, and considering the fact that 80% of the targeted species are concentrated on the middle section of the chromatographic run, the use of all ion mode seems to be better suited than dedicated CID MS/MS with precursor isolation, since several MS/MS features can be collected from coeluting species without loss of sensitivity. A dedicated MS/MS method development would be required instead, and eventually may produce a significant loss of sensitivity and also of information of the sample. Without precursor selection, this is no longer a problem, although at the expense of an inherent loss of specificity compared to precursor ion isolation MS/MS spectra. In most cases, except low-molecular weight species, the fragmentation of the species which were difficult to cleave with in-source CID were satisfactorily accomplished, providing at least an additional fragment ion in all cases with the exception of 17 pesticides (those with low molecular weight difficult to

cleave such as amitrol and other polar species, 1 mycotoxin and 2 veterinary drugs, which did not show any fragments using LC-QTOF-MS or their abundances related to the main ion were lower than 10% even with the highest collision energy tested (30 V). As a conclusion, UHPLC-TOFMS using in-source CID provided information for 80-85 %, a value reasonably high, but not as comprehensive as results obtained with “all ion mode” CID MS/MS fragmentation without precursor isolation. The use of two experiments at for instance 0 and 20 V (collision energy) provided detailed information for confirmation purposes in a single run.

Current caveats of screening methods

Sensitivity. Sensitivity is a parameter related somewhat to selectivity, since the acquisition mode selected, and the experiments and details required (fragmentation mode, acquisition time, etc) have an impact on the sensitivity of the method. Consequently, the use of high-end instrumentation minimizes some quantitative issues associated such as matrix effects, since diluted samples and lower sample volumes will definitely increase the ruggedness of screening methods. To examine the sensitivity, compounds were classified according to their sensitivity using solvent standard (20% methanol). As a criterion from previous experience with the instrumentation used and the typical signal-to-noise ratio expected, analytes were considered very sensitive when peak counts in extracted ion chromatograms were higher than 10^6 with standards at $100 \mu\text{g L}^{-1}$ ($\text{LOQ} > 1 \mu\text{g L}^{-1}$ would be e) when peak counts were lower than 10^5 at $100 \mu\text{g L}^{-1}$, compounds were considered low sensitive. According to those criteria, peak counts of each compound were divided by 10^6 and compounds were labeled as high sensitive when results were higher than 1 and as low sensitive when results were lower than 0.1. In general, 59% and 10% of database compounds showed high sensitivity and

low sensitivity, respectively, when they were injected in UHPLC-TOFMS system with the screening method developed. Other 31% of compounds showed medium sensitivity peak counts between 10^5 and 10^6 when concentration of $100\mu\text{gL}^{-1}$ was injected. Taking into consideration each class of compounds, 60% pesticides, 64% veterinary drugs, 42% food packaging contaminants, 62% mycotoxins, 70% perfluorinated compounds, 11% nitrosamines and 40% sweeteners showed high sensitivity (peak counts higher than 10^6). 11% of pesticides, 6% veterinary drugs, 19% food packaging contaminants, 9% mycotoxins and 44% nitrosamines had peak counts lower than 10^5 , so they were considered as low sensitive.

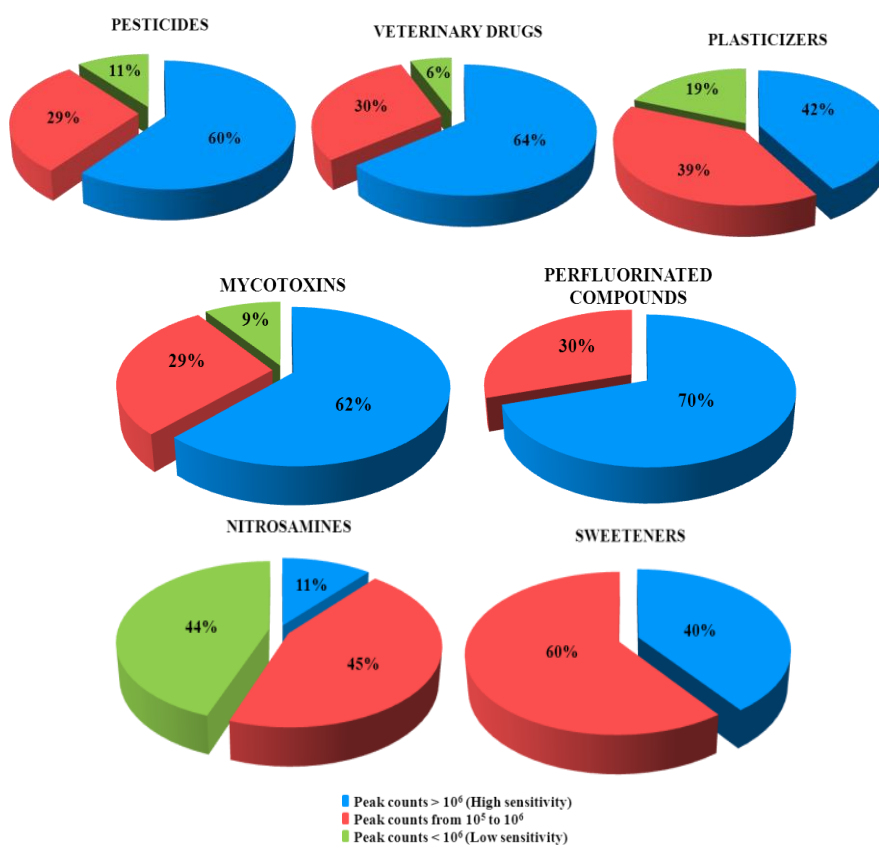


Figure 3. Percentages of pesticides, veterinary drugs, mycotoxins, plasticizers, perfluorinated compounds, nitrosamines and sweeteners according to their sensitivity using LC-TOF-MS.

The overall results in terms of sensitivity are consistent with previous studies. There are always some compounds ([26 out of 220 [42]; over 50 out of 500 [28]) which will not fulfill the MRLs. The percentage of compounds that do not fulfill the MRLs value is usually in the range from 5 to 20 % depending on the matrix. In our study with 630 compounds, leaving aside particular cases such as highly polar species (quats) requiring specific conditions, about 10-15 % were not sensitive enough even with pure solvents standards (with LOQs over 0.2 mg/L). Some of these pesticides are not frequently used so they are not even included in the 396/2005 so they are subjected to the default 10 $\mu\text{g Kg}^{-1}$ threshold difficult to meet. An interesting example is shown in **Figure 4** for selected compounds. They have such low proton affinity that can hardly be ionized (linearly) even at huge concentration. No matter which analyzer or instrument/ionization source is used, they will have problems to be detected.

Quantitation issues and automated detection limitations. As noted above, both selectivity and sensitivity are closely related to matrix effects. Besides matrix effects, other compelling aspects affecting the performance of screening methods are the preservation and handling of standards with a high number of analytes included. In fact, suppression signal effects can occur in neat solvent standards considering such amount of species that needs to be included in the same solution for screening method quality control purposes. An example of this aspect is shown in **Tables 2 and 3**, where two selected groups of coeluting species were examined in the entire mixture and in separated standard, observing remarkable suppression effects.

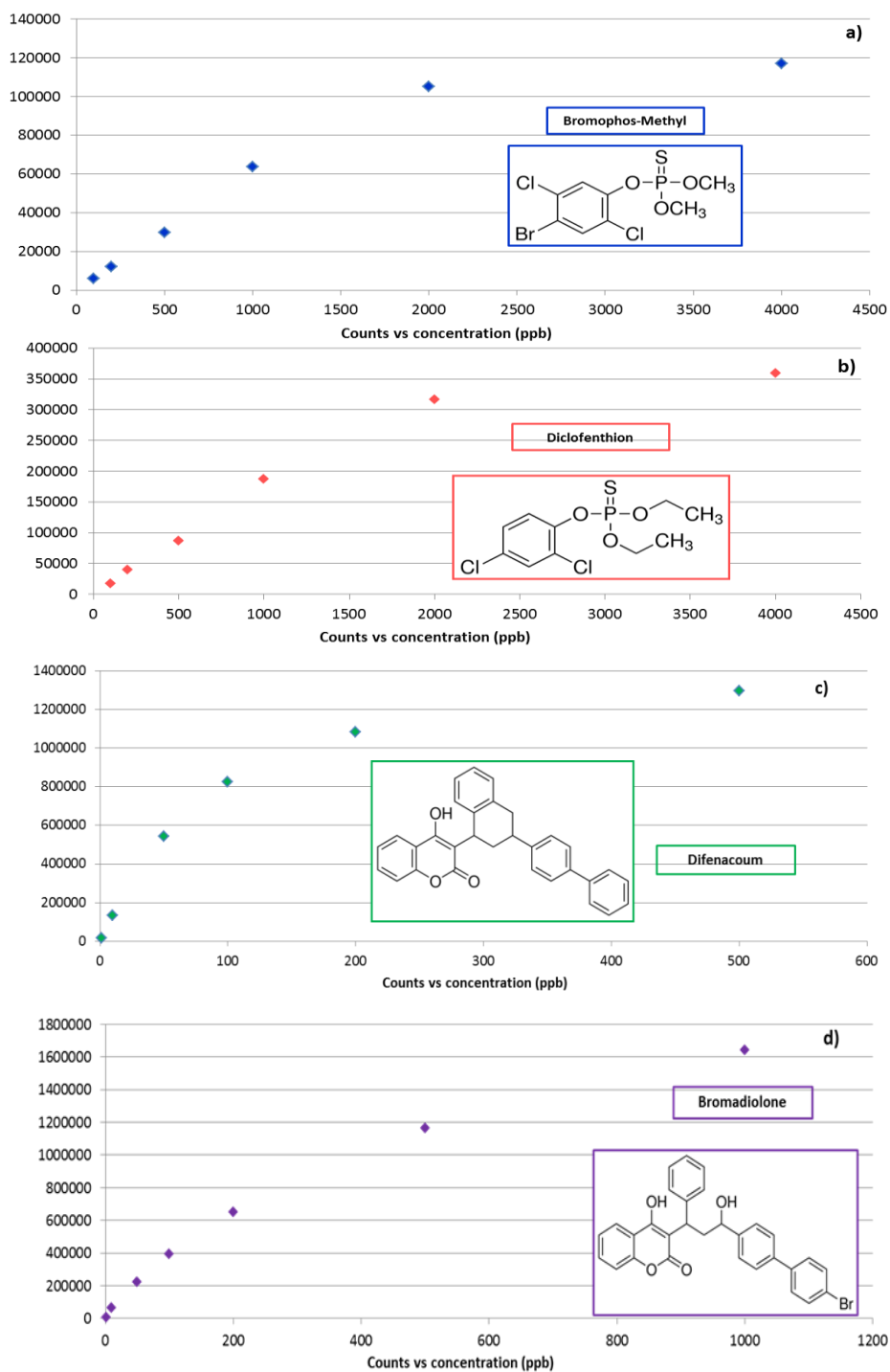


Figure 4. Calibration curves in solvent (20% methanol) for low sensitivity compounds: a) bromophos-methyl; b) diclofenthion; c) difenacoum; d) bromadiolone.

Table 2. Results of calibration curve slopes of group A compounds in mixture (slope 1) and individual solutions (slope 2). Matrix effect (%) = [(slope1/slope2)-1] x 100.

Compound	RT (min)	Slope 1	Slope 2	Matrix Effect (%)
Alachlor	6.11	5127	7110	-28
Diniconazole	6.09	7687	10223	-25
Fenitrothion	6.09	300	500	-40
Fenoxycarb	6.07	815	1248	-35
Flufenacet	6.13	351	766	-54
Neburon	6.17	11431	10249	12
Propetamphos	6.14	1058	1680	-37
Propiconazole	6.1	10443	11244	-7
Rotenone	6.13	3722	4755	-22
Triazophos	6.08	11556	12319	-6

Table 3. Results of calibration curve slopes of group B compounds in mixture (slope 1) and individual solutions (slope 2). Matrix effect (%) = [(slope1/slope2)-1] x 100.

Compound	RT (min)	Slope 1	Slope 2	Matrix Effect (%)
Allethrin	7.07	735	995	-26
Butachlor	7.16	1269	1604	-21
Eprinomectin	7.14	857	1524	-44
Fenazaquin	7.14	43974	51202	-14
Fluazifop-Butyl	7.13	15953	31881	-50
Pyriproxifen	7.12	23694	37768	-37
Sethoxydim	7.12	13356	19488	-31

Finally, the software tools used for the automated detection are also one of the weakest aspects of screening methods [23,28,42]. There is room for improvement concerning the tools for data mining and effective extraction of data for the identification of compounds.

Conclusions

In this article, the main features of the performance of large-scale screening methods using accurate-mass databases and ultra-high performance liquid

chromatography electrospray (quadrupole) time-of-flight mass spectrometry has been examined. Main aspects such as the chromatography and the fragmentation obtained using with different acquisition modes (full-scan or full-scan combined with collision induced dissociation (CID) with no precursor ion isolation), along with caveats such as sensitivity or automated data processing were discussed. The results obtained in terms of fragmentation information were not as appropriate as those obtained using *all ion mode* CID MS/MS experiments, probably the best suited for this type of application. The main weaknesses of the approach are basically the relatively low sensitivity for selected compounds which does not map well against electrospray ionization and also quantitation issues such as those produced by signal suppression effects due to either matrix effects from coeluting matrix components or from coeluting analytes present in the standards solutions which often occur as they contain hundreds of the analytes included in the database.

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III.1.3. Anexo

Sample Treatment. A representative 10-g portion of homogenized sample was weighed in a 50-mL PTFE centrifuge tube and mixed with 10mL of 0.1% acetic acid in acetonitrile, being the tube vigorously shaken for 1 minute. Then, 1g of NaCOOCH₃ and 4g of MgSO₄ anhydrous were added, and the tube was shaken again to prevent coagulation of MgSO₄. The extract was centrifuged (3700 rpm) for 3 minutes. A 5 mL aliquot of supernatant (acetonitrile phase) was taken with a pipette and transferred to a 15 mL centrifuge tube containing 250mg of PSA and 750mg of MgSO₄ anhydrous that was energetically shaken for 20 seconds. The extract was centrifuged again (3700rpm) for 3 minutes. 3 mL of supernatant were taken and evaporated to near dryness and reconstituted to 3mL of 20% MeOH. Prior UHPLC–MS analysis, the extract was filter through a 0.45µm PTFE filter and transfer into a vial. Tomato, orange and baby food extracts were obtained. These extracts were used for method performance evaluation by appropriate spiking with the compounds mixtures.

Table S1. Accurate-mass database of selected pesticides, veterinary drugs, plasticizers, mycotoxins, perfluorinated compounds and sweeteners, including retention times (RT), theoretical accurate masses and elemental composition of the detected ions.

Compound	RT (min)	Theoretical m/z	Ion	Elemental Composition M
Pesticides				
1-Naphtalene-Acetamide	4.28	141.0699	C ₁₁ H ₉ ⁺	C ₁₂ H ₁₁ NO
1-Naphtyl-N-methylcarbamate	4.83	165.0910	C ₁₀ H ₁₃ O ⁺	C ₁₂ H ₁₅ NO ₃
2,4-Dichlorophenoxyacetic acid	5.10	218.9621	[M-H] ⁻	C ₈ H ₆ Cl ₂ O ₃
2,4-Dinitrophenol	4.58	183.0047	[M-H] ⁻	C ₆ H ₄ N ₂ O ₅
3,3-Dichlorobenzidine	5.61	253.0294	[M+H] ⁺	C ₁₂ H ₁₀ Cl ₂ N ₂
3,5-Dichloroaniline	5.52	161.9872	[M+H] ⁺	C ₆ H ₃ NH ₂ Cl ₂
4-Chloro-2-methylphenol	5.1	141.0113	[M-H] ⁻	C ₇ H ₆ N ₂ O ₅
4-Chloro-o-tolyoxyacetic acid	5.11	141.0113	C ₇ H ₆ ClO ⁻	C ₉ H ₉ ClO ₃
Acephate	0.81	142.9926	C ₂ H ₉ O ₃ PS ⁺	C ₄ H ₁₀ NO ₃ PS
Acetamiprid	3.96	223.0745	[M+H] ⁺	C ₁₀ H ₁₁ ClN ₄
Acibenzolar S-Methyl	5.69	210.9994	[M+H] ⁺	C ₈ H ₆ N ₂ OS ₂
Aclonifen	6.31	265.0374	[M+H] ⁺	C ₁₂ H ₉ ClN ₂ O ₃
Alachlor	6.14	162.1277	C ₁₁ H ₁₆ N ⁺	C ₁₄ H ₂₀ ClNO ₂
Albendazole	4.42	266.0958	[M+H] ⁺	C ₁₂ H ₁₅ N ₃ O ₂ S
Aldicarb	4.30	213.0668	[M+H] ⁺	C ₇ H ₁₄ N ₂ O ₂ S
Aldicarb Sulfone	2.71	86.0600	C ₄ H ₈ NO ⁺	C ₇ H ₁₄ N ₂ O ₄ S
Aldicarb Sulfoxide	1.61	89.0419	C ₄ H ₉ S ⁺	C ₇ H ₁₄ N ₂ O ₃ S
Allethrin isomer ₁	7.11	135.0804	C ₉ H ₁₁ O ⁺	C ₁₉ H ₂₆ O ₃
Allethrin isomer ₂	7.07	135.0804	C ₉ H ₁₁ O ⁺	C ₁₉ H ₂₆ O ₃
Ametryn	4.35	228.1278	[M+H] ⁺	C ₉ H ₁₇ N ₅ S
Aminocarb	0.96	209.1285	[M+H] ⁺	C ₁₁ H ₁₆ N ₂ O ₂
Amitraz	7.1	294.1965	[M+H] ⁺	C ₁₉ H ₂₃ N ₃
Amitrol	0.27	85.0509	[M+H] ⁺	C ₂ H ₄ N ₄
Ampa	0.34	110.0013	[M-H] ⁻	CH ₆ NO ₃ P
Anilazine	5.82	272.9507	[M-H] ⁻	C ₉ H ₅ Cl ₃ N ₄
Anilofos	6.46	368.0305	[M+H] ⁺	C ₁₃ H ₁₉ ClNO ₃ PS ₂
Antimycin A	7.59	549.2807	[M+H] ⁺	C ₂₈ H ₄₀ N ₂ O ₉
Asulam	2.23	156.0114	C ₆ H ₆ NO ₂ S ⁺	C ₈ H ₁₀ N ₂ O ₄ S
Atrazine	4.95	216.1011	[M+H] ⁺	C ₈ H ₁₄ ClN ₅
Atrazine Desethyl	3.73	188.0697	[M+H] ⁺	C ₆ H ₁₀ ClN ₅
Atrazine Desisopropyl	3.08	174.0541	[M+H] ⁺	C ₅ H ₈ ClN ₅
Azaconazole	5.04	300.0301	[M+H] ⁺	C ₁₂ H ₁₁ Cl ₂ N ₃ O ₂
Azamethiphos	4.63	324.9809	[M+H] ⁺	C ₉ H ₁₀ ClN ₂ O ₅ PS
Azinphos Ethyl	6.20	368.0263	[M+Na] ⁺	C ₁₂ H ₁₆ N ₃ O ₃ PS ₂
Azinphos Methyl	5.65	132.0444	C ₈ H ₆ NO ⁺	C ₁₀ H ₁₂ N ₃ O ₃ PS
Azobenzene	5.55	183.0917	[M+H] ⁺	C ₁₂ H ₁₀ N ₂
Azocyclotin	6.73	369.1604	[M-C ₂ H ₂ N ₃] ⁺	C ₂₀ H ₃₅ N ₃ Sn

Azoxystrobin	5.78	404.1241	[M+H] ⁺	C ₂₂ H ₁₇ N ₃ O ₅
Barban	6.04	178.0418	C ₁₀ H ₉ ClN ⁺	C ₁₁ H ₉ Cl ₂ NO ₂
Benalaxyl	6.35	326.1751	[M+H] ⁺	C ₂₀ H ₂₃ NO ₃
Bendiocarb	4.80	167.0703	C ₉ H ₁₁ O ₃ ⁺	C ₁₁ H ₁₃ NO ₄
Benfluralin	7.29	336.1166	[M+H] ⁺	C ₁₃ H ₁₆ F ₃ N ₃ O ₄
Benfuracarb	7.05	411.1948	[M+H] ⁺	C ₂₀ H ₃₀ N ₂ O ₅ S
Bensulfuron Methyl	5.37	411.0969	[M+H] ⁺	C ₁₆ H ₁₈ N ₄ O ₇ S
Bensulide	6.49	313.9739	C ₈ H ₁₃ NO ₄ PS ₃ ⁺	C ₁₄ H ₂₄ NO ₄ PS ₃
Bentazone	4.97	239.0496	[M-H] ⁻	C ₁₀ H ₁₂ N ₂ O ₃ S
Benzidine	0.43	185.1073	[M+H] ⁺	C ₁₂ H ₁₂ N ₂
Bifenazate	5.99	198.0913	C ₁₃ H ₁₂ NO ⁺	C ₁₇ H ₂₀ N ₂ O ₃
Bifenox	6.74	309.9668	C ₁₃ H ₆ Cl ₂ NO ₄ ⁺	C ₁₄ H ₉ Cl ₂ NO ₅
Bitertanol	5.99	269.1536	C ₁₈ H ₂₁ O ₂ ⁺	C ₂₀ H ₂₃ N ₃ O ₂
Boscalid	5.85	343.0399	[M+H] ⁺	C ₁₈ H ₁₂ Cl ₂ N ₂ O
Brodifacoum isomer 1	7.54	521.0758	[M-H] ⁻	C ₃₁ H ₂₃ BrO ₃
Brodifacoum isomer 2	7.67	521.0758	[M-H] ⁻	C ₃₁ H ₂₃ BrO ₃
Bromacil	4.42	204.9607	C ₅ H ₆ BrN ₂ O ₂ ⁺	C ₉ H ₁₃ BrN ₂ O ₂
Bromadiolone isomer 1	6.76	525.0707	[M-H] ⁻	C ₃₀ H ₂₃ BrO ₄
Bromadiolone isomer 2	6.82	525.0707	[M-H] ⁻	C ₃₀ H ₂₃ BrO ₄
Bromophos Methyl	7.12	364.8565	[M+H] ⁺	C ₈ H ₈ BrCl ₂ O ₃ PS
Bromoxynil	5.07	273.8509	[M-H] ⁻	C ₇ H ₃ ONBr ₂
Bromuconazole Isomer 1	5.84	375.9614	[M+H] ⁺	C ₁₃ H ₁₂ BrCl ₂ N ₃ O
Bromuconazole Isomer 2	5.66	375.9614	[M+H] ⁺	C ₁₃ H ₁₂ BrCl ₂ N ₃ O
Bupirimate	5.30	317.1642	[M+H] ⁺	C ₁₃ H ₂₄ N ₄ O ₃ S
Buprofezin	6.08	306.1635	[M+H] ⁺	C ₁₆ H ₂₃ N ₃ OS
Butachlor	7.18	312.1725	[M+H] ⁺	C ₁₇ H ₂₆ ClNO ₂
Butocarboxim	4.17	213.0668	[M+Na] ⁺	C ₇ H ₁₄ N ₂ O ₂ S
Butoxycarboxim	2.56	245.0564	[M+Na] ⁺	C ₇ H ₁₄ N ₂ O ₄ S
Butralin	7.37	240.0979	C ₁₀ H ₁₄ N ₃ O ₄ ⁺	C ₁₄ H ₂₁ N ₃ O ₄
Buturon	5.42	237.0789	[M+H] ⁺	C ₁₂ H ₁₃ ClN ₂ O
Cadusafos	6.48	158.9698	C ₂ H ₈ O ₂ PS ₂ ⁺	C ₁₀ H ₂₃ O ₂ PS ₂
Carbaryl	4.95	145.0648	C ₁₀ H ₉ O ⁺	C ₁₂ H ₁₁ NO ₂
Carbendazim	2.24	192.0768	[M+H] ⁺	C ₉ H ₉ N ₃ O ₂
Carbofuran	4.81	222.1125	[M+H] ⁺	C ₁₂ H ₁₅ NO ₃
Carbofuran 3-Hydroxy	3.75	163.0754	C ₁₀ H ₁₁ O ₂ ⁺	C ₁₂ H ₁₅ NO ₄
Carbosulfan	8.11	381.2206	[M+H] ⁺	C ₂₀ H ₃₂ N ₂ O ₃ S
Carboxine	5.05	236.0740	[M+H] ⁺	C ₁₂ H ₁₃ NO ₂ S
Carfentazone-ethyl	6.35	412.0437	[M+H] ⁺	C ₁₅ H ₁₄ Cl ₂ F ₃ N ₃ O ₃
Chlorbromuron	5.74	292.9687	[M+H] ⁺	C ₉ H ₁₀ BrClN ₂ O ₂
Chlordimeform	3.35	197.084	[M+H] ⁺	C ₁₀ H ₁₃ ClN ₂
Chlorfenvinfos	6.21	358.9768	[M+H] ⁺	C ₁₂ H ₁₄ Cl ₃ O ₄ P
Chlorfluzuron	7.33	539.9702	[M+H] ⁺	C ₂₀ H ₉ Cl ₃ F ₅ N ₃ O ₃
Chloridazon	3.78	222.0429	[M+H] ⁺	C ₁₀ H ₈ ClN ₃ O
Chlormequat chloride	0.28	122.0370	[M] ⁺	C ₅ H ₁₃ NCl ⁺
Chloroprotham	5.93	172.0160	C ₇ H ₇ ClNO ₂ ⁺	C ₁₀ H ₁₂ ClNO ₂

Chlorotoluron	4.89	213.0789	[M+H] ⁺	C ₁₀ H ₁₃ ClN ₂ O
Chloroxuron	5.67	291.0895	[M+H] ⁺	C ₁₅ H ₁₅ ClN ₂ O ₂
Chlorpyrifos	7.22	349.9336	[M+H] ⁺	C ₉ H ₁₁ Cl ₃ NO ₃ PS
Chlorpyrifos Methyl	6.71	321.9023	[M+H] ⁺	C ₇ H ₇ Cl ₃ NO ₃ PS
Chlorsulfuron	4.92	358.0371	[M+H] ⁺	C ₁₂ H ₁₂ ClN ₅ O ₄ S
Cinosulfuron	4.79	414.1078	[M+H] ⁺	C ₁₅ H ₁₉ N ₅ O ₇ S
Clethodim isomer E	7.02	360.1395	[M+H] ⁺	C ₁₇ H ₂₆ ClNO ₃ S
Clethodim isomer Z	5.7	360.1395	[M+H] ⁺	C ₁₇ H ₂₆ ClNO ₃ S
Clethodim sulfoxide	5.03	376.1344	[M+H] ⁺	C ₁₇ H ₂₆ ClNO ₄ S
Clethodim imine	5.01	270.1522	[M+H] ⁺	C ₁₄ H ₂₃ NO ₂ S
Clodinafop-Propargyl	6.46	350.0590	[M+H] ⁺	C ₁₇ H ₁₃ ClFNO ₄
Clofentezine	6.60	138.0105	C ₇ H ₅ ClN ⁺	C ₁₄ H ₈ Cl ₂ N ₄
Clomazone	5.39	240.0786	[M+H] ⁺	C ₁₂ H ₁₄ ClNO ₂
Clopyralid	1.18	145.9559	C ₅ H ₂ Cl ₂ N ⁺	C ₆ H ₃ Cl ₂ NO ₂
Clothianidin	3.72	169.0541	C ₆ H ₉ N ₄ S ⁺	C ₆ H ₈ ClN ₅ O ₂ S
Coumaphos	6.60	363.0217	[M+H] ⁺	C ₁₄ H ₁₆ ClO ₅ PS
Cyanazine	4.61	241.0963	[M+H] ⁺	C ₉ H ₁₃ ClN ₆
Cyazofamid	6.35	108.0114	C ₂ H ₆ NO ₂ S ⁺	C ₁₃ H ₁₃ ClN ₄ O ₂ S
Cycloate	6.71	216.1417	[M+H] ⁺	C ₁₁ H ₂₁ NOS
Cycloheximid	4.22	282.1700	[M+H] ⁺	C ₁₅ H ₂₃ NO ₄
Cycloxydim isomer 1	6.87	326.1784	[M+H] ⁺	C ₁₇ H ₂₇ NO ₃ S
Cycloxydim isomer 2	5.24	326.1784	[M+H] ⁺	C ₁₇ H ₂₇ NO ₃ S
Cymoxanil	1.63	199.0826	[M+H] ⁺	C ₇ H ₁₀ N ₄ O ₃
Cyphenothrin	7.76	398.1727	[M+Na] ⁺	C ₂₄ H ₂₅ NO ₃
Cyproconazole	5.54	292.1211	[M+H] ⁺	C ₁₅ H ₁₈ ClN ₃ O
Cyprodinil	5.18	226.1339	[M+H] ⁺	C ₁₄ H ₁₅ N ₃
Cyromazine	0.46	167.1040	[M+H] ⁺	C ₆ H ₁₀ N ₆
Daminozide	0.40	143.0815	C ₆ H ₁₁ O ₂ N ₂ ⁺	C ₆ H ₁₂ O ₃ N ₂
Dazomet	2.51	119.9936	C ₃ H ₆ NS ₂ ⁺	C ₅ H ₁₀ N ₂ S ₂
Deet	5.01	192.1383	[M+H] ⁺	C ₁₂ H ₁₇ NO
Demeton-S-Methyl	4.59	253.0092	[M+Na] ⁺	C ₆ H ₁₅ O ₃ PS ₂
Desethyl-terbutylazine	4.58	146.0227	C ₃ H ₅ ClN ₅ ⁺	C ₇ H ₁₂ ClN ₅
Desmedipham	5.65	182.0812	C ₉ H ₁₂ NO ₃ ⁺	C ₁₆ H ₁₆ N ₂ O ₄
Desmetryn	3.99	214.1121	[M+H] ⁺	C ₈ H ₁₅ N ₅ S
Diafenthiuron	7.54	385.2308	[M+H] ⁺	C ₂₃ H ₃₂ N ₂ OS
Diazinon	6.57	305.1083	[M+H] ⁺	C ₁₂ H ₂₁ N ₂ O ₃ PS
Dibrom	5.31	127.0155	C ₂ H ₈ O ₄ P ⁺	C ₄ H ₇ Br ₂ Cl ₂ O ₄ P
Dicamba	4.49	174.9723	C ₇ H ₆ Cl ₂ O ⁻	C ₈ Cl ₂ H ₆ O ₃
Dichlofenthion	7.20	258.9147	C ₆ H ₆ Cl ₂ O ₃ PS ⁺	C ₁₀ H ₁₃ Cl ₂ O ₃ PS
Dichlofluanid	6.34	223.9498	C ₇ H ₅ Cl ₂ FNS ⁺	C ₉ H ₁₁ Cl ₂ FN ₂ O ₂ S ₂
Dichlorprop	5.42	160.9566	C ₆ H ₃ Cl ₂ O ⁻	C ₉ H ₈ Cl ₂ O ₃
Dichlorvos	4.56	220.9532	[M+H] ⁺	C ₄ H ₇ Cl ₂ O ₄ P
Dicloran	5.400	204.9577	[M-H] ⁻	C ₆ H ₄ N ₂ O ₂ Cl ₂
Dicrotophos	3.39	112.0757	C ₆ H ₁₀ NO ⁺	C ₈ H ₁₆ NO ₅ P
Diethanolamine	0.27	88.07570	C ₄ H ₁₀ NO ⁺	C ₄ H ₁₁ NO ₂

Diethofencarb	5.65	226.1074	$C_{11}H_{16}NO_4^+$	$C_{14}H_{21}NO_4$
Difenacoum isomer 1	7.29	445.1798	$[M+H]^+$	$C_{31}H_{24}O_3$
Difenacoum isomer 2	7.15	445.1798	$[M+H]^+$	$C_{31}H_{24}O_3$
Difenoconazole	6.32	406.0720	$[M+H]^+$	$C_{19}H_{17}Cl_2N_3O_3$
Difenoconazole	5.14	287.1390	$[M+H]^+$	$C_{16}H_{18}N_2O_3$
Difenzoquat	4.11	249.1392	$[M]^+$	$C_{17}H_{17}N_2$
Diflubenzuron	6.00	309.0248	$[M-H]^-$	$C_{14}H_9ClF_2N_2O_2$
Diflufenican	6.74	395.0813	$[M+H]^+$	$C_{19}H_{11}F_5N_2O_2$
Dimethametryn	5.06	256.1590	$[M+H]^+$	$C_{11}H_{21}N_5S$
Dimethenamid	5.67	244.0557	$C_{11}H_{15}ClNOS^+$	$C_{12}H_{18}ClNO_2S$
Dimethoate	3.85	124.9821	$C_2H_6O_2PS^+$	$C_5H_{12}NO_3PS_2$
Dimethomorph Isomer 1	5.45	388.1310	$[M+H]^+$	$C_{21}H_{22}ClNO_4$
Dimethomorph Isomer 2	5.37	388.1310	$[M+H]^+$	$C_{21}H_{22}ClNO_4$
Diniconazole	6.12	326.0821	$[M+H]^+$	$C_{15}H_{17}Cl_2N_3O$
Diphenylamine	6.09	170.0964	$[M+H]^+$	$C_{12}H_{11}N$
Diquat dibromide	0.26	183.0917	$[M-Br_2-H]^+$	$C_{12}H_{12}Br_2N_2$
Diuron	5.08	233.0243	$[M+H]^+$	$C_9H_{10}Cl_2N_2O$
Dmst	5.03	106.0651	$C_7H_9N^+$	$C_9H_{14}N_2O_2S$
DNOC	5.31	197.0204	$[M-H]^-$	$C_7H_6N_2O_5$
Edifenphos	6.21	311.0324	$[M+H]^+$	$C_{14}H_{15}O_2PS_2$
Emamectin isomer 1	5.81	886.5311	$[M+H]^+$	$C_{49}H_{75}NO_{13}$
Emamectin isomer 2	5.74	886.5311	$[M+H]^+$	$C_{49}H_{75}NO_{13}$
Endosulfan sulfate	6.65	418.8045	$[M-H]^-$	$C_9H_6Cl_6O_4S$
Epn	6.82	324.0454	$[M+H]^+$	$C_{14}H_{14}NO_4PS$
Epoxiconazole	5.79	330.0804	$[M+H]^+$	$C_{17}H_{13}ClFN_3O$
Eptc	6.26	190.1260	$[M+H]^+$	$C_9H_{19}NOS$
Etaconazol	5.74	328.0614	$[M+H]^+$	$C_{14}H_{15}Cl_2N_3O_2$
Ethephon	1.40	142.9670	$[M-H]^-$	$C_2H_6ClO_3P$
Ethidimuron	3.80	208.0209	$C_5H_{10}N_3O_2S_2^+$	$C_7H_{12}N_4O_3S_2$
Ethiofencarb	5.06	107.0491	$C_7H_7O^+$	$C_{11}H_{15}NO_2S$
Ethiofencarb sulfone	3.71	107.0491	$C_7H_7O^+$	$C_{11}H_{15}NO_4S$
Ethiofencarb sulfoxide	3.48	107.0491	$C_7H_7O^+$	$C_{11}H_{15}NO_3S$
Ethion	7.26	199.0011	$C_5H_{12}O_2PS_2^+$	$C_9H_{22}O_4P_2S_4$
Ethiprole	5.57	396.9899	$[M+H]^+$	$C_{13}H_9Cl_2F_3N_4OS$
Ethofumesate	5.97	241.0529	$C_{11}H_{12}O_4S^+$	$C_{13}H_{18}O_5S$
Ethoprophos	5.83	243.0637	$[M+Na]^+$	$C_8H_{19}O_2PS_2$
Ethoxyquin	4.62	218.1539	$[M+H]^+$	$C_{14}H_{19}NO$
Ethylthiourea isomer 1	0.32	103.0324	$[M+H]^+$	$C_3H_6N_2S$
Ethylthiourea isomer 2	0.41	103.0324	$[M+H]^+$	$C_3H_6N_2S$
Etofenprox	7.96	394.2377	$[M+NH_4]^+$	$C_{25}H_{28}O_3$
Etoazole	7.34	360.1770	$[M+H]^+$	$C_{21}H_{23}F_2NO_2$
Etrimphos	6.52	293.0719	$[M+H]^+$	$C_{10}H_{17}N_2O_4PS$
Famoxadone	6.51	331.1441	$C_{21}H_{19}N_2O_2^+$	$C_{22}H_{18}N_2O_4$
Famphur	5.64	326.0280	$[M+H]^+$	$C_{10}H_{16}NO_5PS_2$
Fenamidone	5.79	312.1165	$[M+H]^+$	$C_{17}H_{17}N_3OS$

Fenamiphos	5.70	304.1131	[M+H] ⁺	C ₁₃ H ₂₂ NO ₃ PS
Fenamiphos Sulfone	4.73	336.1029	[M+H] ⁺	C ₁₃ H ₂₂ NO ₅ PS
Fenamiphos Sulfoxide	4.31	320.1080	[M+H] ⁺	C ₁₃ H ₂₂ NO ₄ PS
Fenarimol	5.66	331.0399	[M+H] ⁺	C ₁₇ H ₁₂ Cl ₂ N ₂ O
Fenazaquin	7.14	307.1805	[M+H] ⁺	C ₂₀ H ₂₂ N ₂ O
Fenbendazole	4.94	300.0801	[M+H] ⁺	C ₁₅ H ₁₃ N ₃ O ₂ S
Fenhexamid	5.84	302.0709	[M+H] ⁺	C ₁₄ H ₁₇ Cl ₂ NO ₂
Fenhexamid 4-O-Glucoside	4.76	464.1237	[M+H] ⁺	C ₂₀ H ₂₇ NO ₇ Cl ₂
Fenitrothion	6.10	278.0247	[M+H] ⁺	C ₉ H ₁₂ NO ₅ PS
Fenobucarb	5.55	95.0491	C ₆ H ₇ O ⁺	C ₁₂ H ₁₇ NO ₂
Fenoxaprop-P-Ethyl	6.83	362.079	[M+H] ⁺	C ₁₈ H ₁₆ ClNO ₅
Fenoxycarb	6.10	302.1387	[M+H] ⁺	C ₁₇ H ₁₉ NO ₄
Fenpiclonil	5.55	236.9981	[M+H] ⁺	C ₁₁ H ₆ Cl ₂ N ₂
Fenpropathrin	7.56	125.0960	C ₈ H ₁₃ O ⁺	C ₂₂ H ₂₃ NO ₃
Fenpropidine	4.88	274.2529	[M+H] ⁺	C ₁₉ H ₃₁ N
Fenpropimorph	4.91	304.2635	[M+H] ⁺	C ₂₀ H ₃₃ NO
Fenpyroximate	7.31	422.2074	[M+H] ⁺	C ₂₄ H ₂₇ N ₃ O ₄
Fensulfothion	5.18	309.0379	[M+H] ⁺	C ₁₁ H ₁₇ O ₄ PS ₂
Fenthion	6.48	279.0273	[M+H] ⁺	C ₁₀ H ₁₅ O ₃ PS ₂
Fentin chloride	4.69	351.0196	[M-Cl] ⁺	C ₁₈ H ₁₅ SnCl
Fenuron	3.63	165.1022	[M+H] ⁺	C ₉ H ₁₂ N ₂ O
Fipronil	6.33	436.9460	[M+H] ⁺	C ₁₂ H ₄ Cl ₂ F ₆ N ₄ OS
Fluazifop	5.61	328.0791	[M+H] ⁺	C ₁₅ H ₁₂ F ₃ NO ₄
Fluazifop-Butyl	7.17	384.1417	[M+H] ⁺	C ₁₉ H ₂₀ F ₃ NO ₄
Fluazinam	7.04	464.9587	[M+H] ⁺	C ₁₃ H ₄ Cl ₂ F ₆ N ₄ O ₄
Fluchloralin	6.91	356.0619	[M+H] ⁺	C ₁₂ H ₁₃ ClF ₃ N ₃ O ₄
Flucythrinate	7.45	469.1933	[M+NH ₄] ⁺	C ₂₆ H ₂₃ F ₂ NO ₄
Fludioxonil	5.66	247.0325	[M-H] ⁻	C ₁₂ H ₆ F ₂ N ₂ O ₂
Flufenacet	6.15	194.0976	C ₁₁ H ₁₃ FNO ⁺	C ₁₄ H ₁₄ F ₄ N ₃ O ₂ S
Flufenoxuron	7.17	489.0435	[M+H] ⁺	C ₂₁ H ₁₁ ClF ₆ N ₂ O ₃
Fluomethuron	4.96	233.0896	[M+H] ⁺	C ₁₀ H ₁₁ F ₃ N ₂ O
Fluquinconazole	5.89	376.0163	[M+H] ⁺	C ₁₆ H ₈ Cl ₂ FN ₅ O
Fluroxypyr	4.54	194.9534	C ₅ Cl ₂ H ₂ FN ₂ O ⁻	C ₇ H ₅ Cl ₂ FN ₂ O ₃
Flusilazole	5.93	316.1076	[M+H] ⁺	C ₁₆ H ₁₅ F ₂ N ₃ Si
Flutolanil	6.09	324.1206	[M+H] ⁺	C ₁₇ H ₁₆ F ₃ NO ₂
Flutriafol	4.96	302.1099	[M+H] ⁺	C ₁₆ H ₁₃ F ₂ N ₃ O
Fomesafen	6.00	456.0238	[M+NH ₄] ⁺	C ₁₅ H ₁₀ ClF ₃ N ₂ O ₆ S
Fonofos	6.58	108.9871	C ₂ H ₆ OPS ⁺	C ₁₀ H ₁₅ OPS ₂
Foramsulfuron	4.57	453.1187	[M+H] ⁺	C ₁₇ H ₂₀ N ₆ O ₇ S
Forchlorfenuron	4.98	248.0585	[M+H] ⁺	C ₁₂ H ₁₀ ClN ₃ O
Formetanate	1.16	222.1237	[M+H] ⁺	C ₁₁ H ₁₅ N ₃ O ₂
Fosetyl	0.36	82.9893	H ₄ PO ₃ ⁺	C ₂ H ₇ O ₃ P
Fosthiazate	4.98	227.9912	C ₅ H ₁₁ NO ₃ PS ₂ ⁺	C ₉ H ₁₈ NO ₃ PS ₂
Fuberidazol	3.14	185.0709	[M+H] ⁺	C ₁₁ H ₈ N ₂ O
Furalaxyl	5.59	302.1387	[M+H] ⁺	C ₁₇ H ₁₉ NO ₄

Furathiocarb	7.07	383.1635	[M+H] ⁺	C ₁₈ H ₂₆ N ₂ O ₅ S
Furmecyclox	6.21	252.1594	[M+H] ⁺	C ₁₄ H ₂₁ NO ₃
Gibberellic acid	3.7	345.1344	[M-H] ⁻	C ₁₉ H ₂₂ O ₆
Glufosinate ammonium	0.32	180.0431	[M-H] ⁻	C ₅ H ₁₂ NO ₄ P
Glufosinate N-acetyl	0.41	222.0537	[M-H] ⁻	C ₇ H ₁₄ NO ₅ P
Glyphosate	0.33	168.0067	[M-H] ⁻	C ₃ H ₈ NO ₅ P
Griseofulvin	5.15	353.0786	[M+H] ⁺	C ₁₇ H ₁₇ ClO ₆
Haloxfop	6.04	362.0401	[M+H] ⁺	C ₁₅ H ₁₁ ClF ₃ NO ₄
Hexaflumuron	6.63	460.9889	[M+H] ⁺	C ₁₆ H ₈ Cl ₂ F ₆ N ₂ O ₃
Hexazinone	4.32	253.1659	[M+H] ⁺	C ₁₂ H ₂₀ N ₄ O ₂
Hexythiazox	7.24	353.1085	[M+H] ⁺	C ₁₇ H ₂₁ ClN ₂ O ₂ S
Hydramethylnon	6.02	495.1978	[M+H] ⁺	C ₂₅ H ₂₄ F ₆ N ₄
Imazalil	4.52	297.0556	[M+H] ⁺	C ₁₄ H ₁₄ Cl ₂ N ₂ O
Imazalil metabolite	3.69	257.0243	[M+H] ⁺	C ₉ H ₁₀ Cl ₂ N ₂ O
Imazamethabenz-Methyl	4.11	289.1547	[M+H] ⁺	C ₁₆ H ₂₀ N ₂ O ₃
Imazamox	3.82	306.1448	[M+H] ⁺	C ₁₅ H ₁₉ N ₃ O ₄
Imazapyr	3.41	262.1186	[M+H] ⁺	C ₁₃ H ₁₅ N ₃ O ₃
Imazaquin	4.56	312.1343	[M+H] ⁺	C ₁₇ H ₁₇ N ₃ O ₃
Imidacloprid	3.81	256.0596	[M+H] ⁺	C ₉ H ₁₀ ClN ₅ O ₂
Indoxacarb	6.79	528.0780	[M+H] ⁺	C ₂₂ H ₁₇ ClF ₃ N ₃ O ₇
Ioxynil	5.41	369.8231	[M-H] ⁻	C ₇ H ₃ I ₂ NO
Iprodione	6.6	330.0407	[M+H] ⁺	C ₁₃ H ₁₃ N ₃ Cl ₂ O ₃
Iprovalicarb	5.68	119.0855	C ₉ H ₁₁ ⁺	C ₁₈ H ₂₈ N ₂ O ₃
Isazophos	6.27	314.0490	[M+H] ⁺	C ₉ H ₁₇ ClN ₃ O ₃ PS
Isocarbophos	5.54	230.9875	C ₈ H ₈ O ₄ PS ⁺	C ₁₁ H ₁₆ NO ₄ PS
Isofenphos	6.84	346.1236	[M+H] ⁺	C ₁₅ H ₂₄ NO ₄ PS
Isoprocarb	5.18	95.0491	C ₆ H ₇ O ⁺	C ₁₁ H ₁₅ NO ₂
Isoprothiolane	6.09	188.9675	C ₆ H ₅ O ₃ S ₂ ⁺	C ₁₂ H ₁₈ O ₄ S ₂
Isoproturon	5.04	207.1492	[M+H] ⁺	C ₁₂ H ₁₈ N ₂ O
Isoxaben	5.96	333.1809	[M+H] ⁺	C ₁₈ H ₂₄ N ₂ O ₄
Isoxaflutole	5.78	360.0512	[M+H] ⁺	C ₁₅ H ₁₂ F ₃ NO ₄ S
Ivermectin	7.58	895.4814	[M+Na] ⁺	C ₄₈ H ₇₂ O ₁₄
Karbutilate	4.7	280.1656	[M+H] ⁺	C ₁₄ H ₂₁ N ₃ O ₃
Kresoxim-methyl	6.33	282.1125	C ₁₇ H ₁₆ NO ₃ ⁺	C ₁₈ H ₁₉ NO ₄
Lactofen	7.16	484.0381	[M+Na] ⁺	C ₁₉ H ₁₅ ClF ₃ NO ₇
Lenacil	4.64	153.0659	C ₇ H ₉ N ₂ O ₂ ⁺	C ₁₃ H ₁₈ N ₂ O ₂
Linuron	5.64	249.0192	[M+H] ⁺	C ₉ H ₁₀ Cl ₂ N ₂ O ₂
Lufenuron	7.00	510.9857	[M+H] ⁺	C ₁₇ H ₈ Cl ₂ F ₈ N ₂ O ₃
Malaoxon	4.76	99.0077	C ₄ H ₃ O ₃ ⁺	C ₁₀ H ₁₉ O ₇ PS
Malathion	6.07	331.0433	[M+H] ⁺	C ₁₀ H ₁₉ O ₆ PS ₂
Maleic hydrazine	0.41	113.0346	[M+H] ⁺	C ₄ H ₄ N ₂ O ₂
Mecarbam	6.29	226.9961	C ₆ H ₁₄ O ₃ PS ₂ ⁺	C ₁₀ H ₂₀ NO ₅ PS ₂
Mecoprop	5.41	141.0113	C ₇ H ₆ ClO ⁻	C ₁₀ H ₁₁ ClO ₃
Mefenacet	5.82	148.0757	C ₉ H ₁₀ NO ⁺	C ₁₆ H ₁₄ N ₂ O ₂ S
Mepanipyrim	5.91	224.1182	[M+H] ⁺	C ₁₄ H ₁₃ N ₃

Mepfosfolam	4.42	270.0382	[M+H] ⁺	C ₈ H ₁₆ NO ₃ PS ₂
Mepiquat chloride isomer 1	0.27	114.1283	[M] ⁺	C ₇ H ₁₆ N ⁺
Mepiquat chloride isomer 2	0.4	114.1283	[M] ⁺	C ₇ H ₁₆ N ⁺
Mepronil	6.03	270.1489	[M+H] ⁺	C ₁₇ H ₁₉ NO ₂
Mesotrione	4.79	340.0485	[M+H] ⁺	C ₁₄ H ₁₃ NO ₇ S
Metaflumizone	6.99	507.1250	[M+H] ⁺	C ₂₄ H ₁₆ F ₆ N ₄ O ₂
Metalaxyl	5.07	280.1543	[M+H] ⁺	C ₁₅ H ₂₁ NO ₄
Metamitron	3.61	203.0927	[M+H] ⁺	C ₁₀ H ₁₀ N ₄ O
Metazachlor	5.30	134.0964	C ₉ H ₁₂ N ⁺	C ₁₄ H ₁₆ ClN ₃ O
Methabenzthiazuron	4.81	165.0481	C ₈ H ₉ N ₂ S ⁺	C ₁₀ H ₁₁ N ₃ OS
Methacrifos	5.64	209.0032	C ₆ H ₁₀ O ₄ PS ⁺	C ₇ H ₁₃ O ₅ PS
Methamidophos	0.55	94.0052	CH ₅ NO ₂ P ⁺	C ₂ H ₈ NO ₂ PS
Methidathion	5.63	85.0396	C ₃ H ₅ N ₂ O ⁺	C ₆ H ₁₁ N ₂ O ₄ PS ₃
Methiocarb	5.56	169.0682	C ₉ H ₁₂ OS ⁺	C ₁₁ H ₁₅ NO ₂ S
Methiocarb Sulfoxide	3.64	185.0631	C ₉ H ₁₃ O ₂ S ⁺	C ₁₁ H ₁₅ NO ₃ S
Methomyl	2.86	88.0215	C ₃ H ₄ NS ⁺	C ₅ H ₁₀ N ₂ O ₂ S
Methoprotrotryne	4.38	272.1540	[M+H] ⁺	C ₁₁ H ₂₁ N ₅ OS
Methoxyfenozide	5.98	149.0597	C ₁₈ H ₂₁ N ₂ O ₃ ⁺	C ₂₂ H ₂₈ N ₂ O ₃
Metobromuron	5.22	259.0077	[M+H] ⁺	C ₉ H ₁₁ BrN ₂ O ₂
Metolachlor	6.08	284.1412	[M+H] ⁺	C ₁₅ H ₂₂ ClNO ₂
Metolcarb	4.57	109.0648	C ₇ H ₉ O ⁺	C ₉ H ₁₁ NO ₂
Metoxuron	4.33	229.0738	[M+H] ⁺	C ₁₀ H ₁₃ ClN ₂ O ₂
Metribuzin	4.62	215.0961	[M+H] ⁺	C ₈ H ₁₄ N ₄ OS
Metsulfuron Methyl	4.80	382.0816	[M+H] ⁺	C ₁₄ H ₁₅ N ₅ O ₆ S
Mevinphos	4.06	127.0155	C ₂ H ₈ O ₄ P ⁺	C ₇ H ₁₃ O ₆ P
Molinate	5.77	188.1104	[M+H] ⁺	C ₉ H ₁₇ NOS
Monocrotophos	3.18	127.0155	C ₂ H ₇ O ₄ P ⁺	C ₇ H ₁₄ NO ₅ P
Monolinuron	5.10	215.0582	[M+H] ⁺	C ₉ H ₁₁ ClN ₂ O ₂
Monuron	4.48	199.0633	[M+H] ⁺	C ₉ H ₁₁ ClON ₂
Morpholin	0.27	88.0757	[M+H] ⁺	C ₄ H ₉ NO
Myclobutanil	5.73	289.1215	[M+H] ⁺	C ₁₅ H ₁₇ ClN ₄
Naptalam	4.75	144.0808	C ₁₀ H ₁₀ N ⁺	C ₁₈ H ₁₃ NO ₃
Neburon	6.18	275.0715	[M+H] ⁺	C ₁₂ H ₁₆ Cl ₂ N ₂ O
Nereistoxin isomer 1	0.29	104.9827	C ₃ H ₅ S ₂ ⁺	C ₅ S ₂ NH ₁₁
Nereistoxin isomer 2	0.49	104.9827	C ₃ H ₅ S ₂ ⁺	C ₅ S ₂ NH ₁₁
Nitenpyram	2.95	271.0956	[M+H] ⁺	C ₁₁ H ₁₅ ClN ₄ O ₂
N,N-Diethyl-2-Naphtoloxypromamide	5.91	272.1645	[M+H] ⁺	C ₁₇ H ₂₁ O ₂ N
Norflurazone	5.20	304.0459	[M+H] ⁺	C ₁₂ H ₉ ClF ₃ N ₃ O
Novaluron	6.81	491.0050	[M-H] ⁻	C ₁₇ H ₉ ClF ₈ N ₂ O ₄
Nuarimol	5.32	315.0695	[M+H] ⁺	C ₁₇ H ₁₂ ClFN ₂ O
Ofurace	5.10	282.0891	[M+H] ⁺	C ₁₄ H ₁₆ ClNO ₃
Omethoate	1.10	124.9821	C ₂ H ₆ O ₂ PS ⁺	C ₅ H ₁₂ NO ₄ PS
Orbencarb	6.56	125.0153	C ₇ H ₆ Cl ⁺	C ₁₂ H ₁₆ ClNOS
Oryzalin	6.1	345.0874	[M+H] ⁺	C ₁₂ H ₁₈ N ₄ O ₆ S
Oxadiazon	7.21	345.0757	[M+H] ⁺	C ₁₅ H ₁₈ Cl ₂ N ₂ O ₃

Oxadixyl	4.55	219.1128	$C_{12}H_{15}N_2O_2^+$	$C_{14}H_{18}N_2O_4$
Oxamyl	2.82	72.0444	$C_3H_6NO^+$	$C_7H_{13}N_3O_3S$
Oxfendazole	3.97	316.0751	$[M+H]^+$	$C_{15}H_{13}N_3O_3S$
Oxyfluorfen	7.07	362.0401	$[M+H]^+$	$C_{15}H_{11}ClF_3NO_4$
Paclobutrazol	5.46	294.1368	$[M+H]^+$	$C_{15}H_{20}ClN_3O$
Paraoxon methyl	4.60	248.0319	$[M+H]^+$	$C_8H_{10}NO_6P$
Paraquat dichloride	0.27	185.1073	$[M-Cl_2-H]^+$	$C_{12}H_{14}Cl_2N_2$
Parathion	6.45	235.9777	$C_6H_7NO_5PS^+$	$C_{10}H_{14}NO_5PS$
Parathion-Methyl	5.88	264.009	$[M+H]^+$	$C_8H_{10}NO_5PS$
Pebulate	6.69	204.1417	$[M+H]^+$	$C_{10}H_{21}NOS$
Penconazole	5.97	284.0716	$[M+H]^+$	$C_{13}H_{15}Cl_2N_3$
Pencycuron	6.65	329.1415	$[M+H]^+$	$C_{19}H_{21}ClN_2O$
Pendimethalin	7.23	212.0666	$C_8H_{10}N_3O_4^+$	$C_{13}H_{19}N_3O_4$
Phenmedipham	5.61	168.0655	$C_8H_{10}NO_3^+$	$C_{16}H_{16}N_2O_4$
Phenothrin	7.96	351.1955	$[M+H]^+$	$C_{23}H_{26}O_3$
Phenthoate	6.51	163.0754	$C_{10}H_{11}O_2^+$	$C_{12}H_{17}O_4PS_2$
Phosalone	6.73	182.0003	$C_8H_5ClNO_2^+$	$C_{12}H_{15}ClNO_4PS_2$
Phosmet	4.30	160.0393	$C_9H_6NO_2^+$	$C_{11}H_{12}NO_4PS_2$
Phosphamidon	4.36	300.0762	$[M+H]^+$	$C_{10}H_{19}ClNO_5P$
Phosphonic acid	0.50	80.9747	$[M-H]^-$	H_3O_3P
Picloram	3.25	240.9333	$[M+H]^+$	$C_6H_3Cl_3N_2O_2$
Picolinafen	6.96	377.0908	$[M+H]^+$	$C_{19}H_{12}F_4N_2O_2$
Piperonyl Butoxide	7.03	177.0910	$C_{11}H_{13}O_2^+$	$C_{19}H_{30}O_5$
Piperophos	6.76	354.1321	$[M+H]^+$	$C_{14}H_{28}NO_3PS_2$
Pirimicarb	3.51	239.1503	$[M+H]^+$	$C_{11}H_{18}N_4O_2$
Pirimiphos Methyl	6.41	306.1036	$[M+H]^+$	$C_{11}H_{20}N_3O_3PS$
Pretilachlor Isomer 1	6.81	312.1725	$[M+H]^+$	$C_{17}H_{26}ClNO_2$
Pretilachlor Isomer 2	6.73	312.1725	$[M+H]^+$	$C_{17}H_{26}ClNO_2$
Prochloraz	5.40	308.0006	$C_{12}H_{13}Cl_3NO_2^+$	$C_{15}H_{16}Cl_3N_3O_2$
Procymidone	6.09	284.0240	$[M+H]^+$	$C_{13}H_{11}Cl_2NO_2$
Profenofos	6.79	372.9424	$[M+H]^+$	$C_{11}H_{15}BrClO_3PS$
Prohexadione	4.09	211.0612	$[M-H]^-$	$C_{10}H_{12}O_5$
Promecarb	5.69	151.1117	$C_{10}H_{15}O^+$	$C_{12}H_{17}NO_2$
Prometon	4.05	226.1662	$[M+H]^+$	$C_{10}H_{19}N_5O$
Prometryn	4.76	242.1434	$[M+H]^+$	$C_{10}H_{19}N_5S$
Propachlor	5.27	212.0837	$[M+H]^+$	$C_{11}H_{14}ClNO$
Propamocarb	1.14	189.1598	$[M+H]^+$	$C_9H_{20}N_2O_2$
Propanil	5.47	218.0134	$[M+H]^+$	$C_9H_9Cl_2NO$
Propaquizafop	6.93	444.1321	$[M+H]^+$	$C_{22}H_{22}ClN_3O_5$
Propargite	7.40	373.1444	$[M+Na]^+$	$C_{19}H_{26}O_4S$
Propazine	5.41	230.1167	$[M+H]^+$	$C_9H_{16}ClN_5$
Propetamphos	6.16	156.0243	$C_3H_{11}NO_2PS^+$	$C_{10}H_{20}NO_4PS$
Propham	5.30	138.055	$C_7H_8NO_2^+$	$C_{10}H_{13}NO_2$
Propiconazole	6.13	342.0771	$[M+H]^+$	$C_{15}H_{17}Cl_2N_3O_2$
Propisochlor	6.4	148.1121	$C_{10}H_{15}N^+$	$C_{15}H_{22}ClNO_2$

Propoxur	4.75	232.0944	[M+H] ⁺	C ₁₁ H ₁₅ NO ₃
Propylene thiourea	0.53	117.0481	[M+H] ⁺	C ₄ H ₈ N ₂ S
Propyzamid	5.89	189.9821	C ₇ H ₆ Cl ₂ NO ⁺	C ₁₂ H ₁₁ Cl ₂ NO
Proquinazid	7.51	373.0407	[M+H] ⁺	C ₁₄ H ₁₇ IN ₂ O ₂
Prosulfocarb	6.91	252.1417	[M+H] ⁺	C ₁₄ H ₂₁ NOS
Prosulfuron	5.64	420.0948	[M+H] ⁺	C ₁₅ H ₁₆ F ₃ N ₅ O ₄ S
Pymetrozin	0.70	218.1036	[M+H] ⁺	C ₁₀ H ₁₁ N ₅ O
Pyracarbolid	4.89	218.1176	[M+H] ⁺	C ₁₃ H ₁₅ NO ₂
Pyraclostrobin	6.60	388.1059	[M+H] ⁺	C ₁₉ H ₁₈ ClN ₃ O ₄
Pyranocoumarin	6.47	323.1278	[M+H] ⁺	C ₂₀ H ₁₈ O ₄
Pyrazophos	6.51	374.0934	[M+H] ⁺	C ₁₄ H ₂₀ N ₃ O ₅ PS
Pyridaben	7.61	365.1449	[M+H] ⁺	C ₁₉ H ₂₅ ClN ₂ OS
Pyridaphenthion	5.86	341.0719	[M+H] ⁺	C ₁₄ H ₁₇ N ₂ O ₄ PS
PyrifenoX Isomero 1	4.57	295.0399	[M+H] ⁺	C ₁₄ H ₁₂ Cl ₂ N ₂ O
PyrifenoX Isomero 2	4.65	295.0399	[M+H] ⁺	C ₁₄ H ₁₂ Cl ₂ N ₂ O
Pyrimethanil	4.54	200.1182	[M+H] ⁺	C ₁₂ H ₁₃ N ₃
Pyriproxifen	7.10	322.1438	[M+H] ⁺	C ₂₀ H ₁₉ NO ₃
Pyroquilon	4.28	174.0913	[M+H] ⁺	C ₁₁ H ₁₁ NO
Quinalphos	6.35	299.0614	[M+H] ⁺	C ₁₂ H ₁₅ N ₂ O ₃ PS
Quinmerac	3.67	204.0211	C ₁₁ H ₇ ClNO ⁺	C ₁₁ H ₈ ClNO ₂
Quinoclamine	4.59	208.0160	[M+H] ⁺	C ₁₀ H ₆ ClNO ₂
Quinoxifen	6.75	308.0040	[M+H] ⁺	C ₁₅ H ₈ Cl ₂ FNO
Quizalofop-P-Ethyl	6.85	373.095	[M+H] ⁺	C ₁₉ H ₁₇ ClN ₂ O ₄
Resmethrin (R+S stereoisomers)	7.73	339.1955	[M+H] ⁺	C ₂₂ H ₂₆ O ₃
Rimsulfuron	4.96	432.0642	[M+H] ⁺	C ₁₄ H ₁₇ N ₅ O ₇ S ₂
Rotenone	6.15	395.1489	[M+H] ⁺	C ₂₃ H ₂₂ O ₆
Sebume-ton	4.05	226.1662	[M+H] ⁺	C ₁₀ H ₁₉ N ₅ O
Sethoxydim	7.13	328.1941	[M+H] ⁺	C ₁₇ H ₂₉ NO ₃ S
Siduron	5.51	233.1648	[M+H] ⁺	C ₁₄ H ₂₀ N ₂ O
Simazine	4.44	202.0854	[M+H] ⁺	C ₇ H ₁₂ ClN ₅
Spinosyn A	5.37	732.4681	[M+H] ⁺	C ₄₁ H ₆₅ NO ₁₀
Spinosyn D	5.54	746.4838	[M+H] ⁺	C ₄₂ H ₆₇ NO ₁₀
Spiromesifen	7.62	273.1485	C ₁₇ H ₂₂ O ₃ ⁺	C ₂₃ H ₃₀ O ₄
Spirotetramat	5.60	374.1962	[M+H] ⁺	C ₂₁ H ₂₇ NO ₅
Spiroxamine	4.91	298.2741	[M+H] ⁺	C ₁₈ H ₃₅ NO ₂
Sulcotrione	4.86	329.0245	[M+H] ⁺	C ₁₄ H ₁₃ ClO ₅ S
Sulfaquinoxaline	4.38	301.0754	[M+H] ⁺	C ₁₄ H ₁₂ N ₄ O ₂ S
Sulfometuron Methyl	4.87	365.0914	[M+H] ⁺	C ₁₅ H ₁₆ N ₄ O ₅ S
Sulfotep	6.65	323.0300	[M+H] ⁺	C ₈ H ₂₀ O ₅ P ₂ S ₂
Sulprofos	7.31	323.0358	[M+H] ⁺	C ₁₂ H ₁₉ O ₂ PS ₃
Tcpp	5.65	174.9923	C ₄ H ₉ Cl ₂ O ₃ ⁺	C ₉ H ₁₈ Cl ₃ O ₄ P
Tebuconazole	5.86	308.1524	[M+H] ⁺	C ₁₆ H ₂₂ ClN ₃ O
Tebufenpyrad	6.85	334.1681	[M+H] ⁺	C ₁₈ H ₂₄ ClN ₃ O
Tebutam	6.05	234.1852	[M+H] ⁺	C ₁₅ H ₂₃ NO
Tebuthiuron	4.27	229.1118	[M+H] ⁺	C ₉ H ₁₆ N ₄ OS

Teflubenzuron	6.68	378.9670	[M-H] ⁻	C ₁₄ H ₆ Cl ₂ F ₄ N ₂ O ₂
Tembotrione	5.76	341.0245	C ₁₅ H ₁₄ ClO ₅ S ⁺	C ₁₇ H ₁₆ ClF ₃ O ₆ S
Temephos	7.18	466.9970	[M+H] ⁺	C ₁₆ H ₂₀ O ₆ P ₂ S ₃
Tepraloxdim Isomer 1	5.84	342.1467	[M+H] ⁺	C ₁₇ H ₂₄ ClNO ₄
Tepraloxdim Isomer 2	4.65	342.1467	[M+H] ⁺	C ₁₇ H ₂₄ ClNO ₄
Terbacil	4.50	215.0593	[M-H] ⁻	C ₉ H ₁₃ ClN ₂ O ₂
Terbufos	7.13	187.0011	C ₄ H ₁₃ O ₂ PS ₂ ⁺	C ₉ H ₂₁ O ₂ PS ₃
Terbumeton	4.10	226.1662	[M+H] ⁺	C ₁₀ H ₁₉ N ₅ O
Terbutylazine	5.54	230.1167	[M+H] ⁺	C ₉ H ₁₆ ClN ₅
Terbutryn	4.79	242.1434	[M+H] ⁺	C ₁₀ H ₁₉ N ₅ S
Tetrachoviphos	6.08	127.0155	C ₈ H ₃ Cl ₄ ⁺	C ₁₀ H ₉ Cl ₄ O ₄ P
Thiabendazole	2.98	202.0433	[M+H] ⁺	C ₁₀ H ₇ N ₃ S
Thiacloprid	4.30	253.0309	[M+H] ⁺	C ₁₀ H ₉ ClN ₄ S
Thiamethoxam	3.43	211.0648	C ₈ H ₁₁ N ₄ OS ⁺	C ₈ H ₁₀ ClN ₅ O ₃ S
Thidiazuron	4.50	221.0492	[M+H] ⁺	C ₉ H ₈ N ₄ OS
Thifensulfuron methyl	4.68	388.038	[M+H] ⁺	C ₁₂ H ₁₃ N ₅ O ₆ S ₂
Thiocyclam	0.78	136.9548	C ₅ H ₅ S ₃ ⁺	C ₅ H ₁₁ NS ₃
Thiodicarb	4.77	377.0382	[M+Na] ⁺	C ₁₀ H ₁₈ N ₄ O ₄ S ₃
Thiofanox	4.99	241.0981	[M+Na] ⁺	C ₉ H ₁₈ N ₂ O ₂ S
Thiophanate Methyl	4.72	343.0529	[M+H] ⁺	C ₁₂ H ₁₄ N ₄ O ₄ S ₂
Tolclofos Methyl	6.67	300.9616	[M+H] ⁺	C ₉ H ₁₁ Cl ₂ O ₃ PS
Tralkoxidym	7.24	330.2064	[M+H] ⁺	C ₂₀ H ₂₇ NO ₃
Transfluthrin	7.36	163.0165	C ₇ H ₃ F ₄ ⁺	C ₁₅ H ₁₂ Cl ₂ F ₄ O ₂
Triadimefon	5.8	294.1004	[M+H] ⁺	C ₁₄ H ₁₆ ClN ₃ O ₂
Triadimenol isomer 1	5.43	70.0399	C ₂ H ₄ N ₃ ⁺	C ₁₄ H ₁₈ ClN ₃ O ₂
Triadimenol isomer 2	5.53	70.0399	C ₂ H ₄ N ₃ ⁺	C ₁₄ H ₁₈ ClN ₃ O ₂
Triallat	7.41	304.0091	[M+H] ⁺	C ₁₀ H ₁₆ Cl ₃ NOS
Triasulfuron	4.91	402.0633	[M+H] ⁺	C ₁₄ H ₁₆ ClN ₅ O ₅ S
Triazophos	6.11	314.0723	[M+H] ⁺	C ₁₂ H ₁₆ N ₃ O ₃ PS
Triazoxide	4.14	248.0334	[M+H] ⁺	C ₁₀ H ₆ ClN ₅ O
Trichlorfon	3.52	256.9299	[M+H] ⁺	C ₄ H ₈ Cl ₃ O ₄ P
Triclocarban	6.63	314.9853	[M+H] ⁺	C ₁₃ H ₉ Cl ₃ ON ₂
Tridemorph	5.44	298.3105	[M+H] ⁺	C ₁₉ H ₃₉ NO
Trietazine	5.95	230.1167	[M+H] ⁺	C ₉ H ₁₆ ClN ₅
Triethanolamine	0.28	150.1125	[M+H] ⁺	C ₆ H ₁₅ NO ₃
Trifloxystrobin	6.81	409.1370	[M+H] ⁺	C ₂₀ H ₁₉ F ₃ N ₂ O ₄
Trifloxysulfuron	5.12	438.0690	[M+H] ⁺	C ₁₄ H ₁₃ F ₃ N ₅ O ₆ S
Triflumizole	5.88	278.0554	C ₁₂ H ₁₂ ClF ₃ NO ⁺	C ₁₅ H ₁₅ ClF ₃ N ₃ O
Triflumuron	6.38	357.0259	[M-H] ⁻	C ₁₅ H ₁₀ ClF ₃ N ₂ O ₃
Trifluralin	7.27	336.1166	[M+H] ⁺	C ₁₃ H ₁₆ F ₃ N ₃ O ₄
Triforine	5.16	387.9106	C ₉ H ₁₂ Cl ₆ N ₃ O ⁺	C ₁₀ H ₁₄ Cl ₆ N ₄ O ₂
Trimethylsulfonium	0.26	77.0425	[M+H] ⁺	C ₃ H ₈ S
Trinexapac-Ethyl	5.35	253.1071	[M+H] ⁺	C ₁₃ H ₁₆ O ₅
Triticonazole	5.53	318.1368	[M+H] ⁺	C ₁₇ H ₂₀ ClN ₃ O
Vamidotion	3.65	146.0634	C ₆ H ₁₂ NOS ⁺	C ₈ H ₁₈ NO ₄ PS ₂

Vinclozolin	6.27	242.0134	$C_{11}H_{10}Cl_2NO^+$	$C_{12}H_9Cl_2NO_3$
Zoxamide	6.51	336.0319	$[M+H]^+$	$C_{14}H_{16}Cl_3NO_2$
Veterinary drugs				
Albendazole sulfone	3.97	298.0856	$[M+H]^+$	$C_{12}H_{15}N_3O_4S$
Albendazole sulfoxide	3.51	282.0907	$[M+H]^+$	$C_{12}H_{15}N_3O_3S$
Amoxicillin	0.93	349.0853	$C_{16}H_{17}N_2O_5S^+$	$C_{16}H_{19}N_3O_5S$
Ampicillin	3.17	350.1169	$[M+H]^+$	$C_{16}H_{19}N_3O_4S$
Benzothiazole	4.35	136.0215	$[M+H]^+$	C_7H_5NS
Benzylamine	4.47	310.1914	$[M+H]^+$	$C_{19}H_{23}N_3O$
Caffeine	3.04	195.0877	$[M+H]^+$	$C_8H_{10}N_4O_2$
Carbadox	3.40	263.0775	$[M+H]^+$	$C_{11}H_{10}N_4O_4$
Carbamazepine	4.65	237.1022	$[M+H]^+$	$C_{15}H_{12}N_2O$
Chloramphenicol	4.14	321.0051	$[M-H]^-$	$C_{11}H_{12}O_5N_2Cl_2$
Chlortetracycline isomer 1	3.62	479.1216	$[M+H]^+$	$C_{22}H_{23}ClN_2O_8$
Chlortetracycline isomer 2	3.87	479.1216	$[M+H]^+$	$C_{22}H_{23}ClN_2O_8$
Ciprofloxacin	3.46	332.1405	$[M+H]^+$	$C_{17}H_{18}FN_3O_3$
Clarithromycin	4.67	748.4842	$[M+H]^+$	$C_{38}H_{69}NO_{13}$
Clenbuterol	3.61	277.0869	$[M+H]^+$	$C_{12}H_{18}Cl_2N_2O$
Clofibric Acid	5.24	126.9951	$C_6H_4ClO^-$	$C_{10}H_{11}O_3Cl$
Cloxacillin	5.17	468.0991	$[M+CH_4OH]^+$	$C_{19}H_{18}ClN_3O_5S$
Cotinine	0.41	177.1022	$[M+H]^+$	$C_{10}H_{12}N_2O$
Danofloxacin	3.48	358.1561	$[M+H]^+$	$C_{19}H_{20}FN_3O_3$
Demeclocycline isomer 1	3.64	465.1059	$[M+H]^+$	$C_{21}H_{21}ClN_2O_8$
Demeclocycline isomer 2	3.46	465.1059	$[M+H]^+$	$C_{21}H_{21}ClN_2O_8$
Diclofenac	5.89	250.0196	$C_{13}H_8Cl_2N^-$	$C_{14}H_{11}Cl_2NO_2$
Dicloxacillin isomer 1	5.34	502.0601	$[M+CH_4OH]^+$	$C_{19}H_{17}N_3Cl_2O_5S$
Dicloxacillin isomer 2	5.45	502.0601	$[M+CH_4OH]^+$	$C_{19}H_{17}N_3Cl_2O_5S$
Difloxacin	3.72	400.1467	$[M+H]^+$	$C_{21}H_{19}F_2N_3O_3$
Digoxin	4.45	651.3739	$C_{35}H_{55}O_{11}^+$	$C_{41}H_{64}O_{14}$
Dimetridazole	1.29	142.0611	$[M+H]^+$	$C_5H_7N_3O_2$
Diphenhydramine	4.30	167.0855	$C_{13}H_{11}^+$	$C_{17}H_{21}NO$
Doramectin	7.99	331.2268	$C_{21}H_{31}O_3^+$	$C_{50}H_{74}O_{14}$
Doxycycline	3.98	445.1605	$[M+H]^+$	$C_{22}H_{24}N_2O_8$
Enoxacin	3.33	321.1357	$[M+H]^+$	$C_{15}H_{17}FN_4O_3$
Enrofloxacin	3.54	360.1718	$[M+H]^+$	$C_{19}H_{22}FN_3O_3$
Eprinomectin B _{1a}	7.14	936.5080	$[M+Na]^+$	$C_{50}H_{75}NO_{14}$
Eprinomectin B _{1b}	7.14	922.4923	$[M+Na]^+$	$C_{49}H_{73}NO_{14}$
Erythromycin	4.32	734.4685	$[M+H]^+$	$C_{37}H_{67}NO_{13}$
Estrone	5.47	271.1693	$[M+H]^+$	$C_{18}H_{22}O_2$
Febantel 1	4.16	331.1223	$[M+H]^+$	$C_{16}H_{18}N_4O_2S$
Febantel 2	4.29	389.1278	$[M+H]^+$	$C_{18}H_{20}N_4O_4S$
Fleroxacin	3.31	370.1373	$[M+H]^+$	$C_{17}H_{18}F_3N_3O_3$
Flufenamic Acid	6.22	264.0631	$C_{14}H_9F_3NO^+$	$C_{14}H_{10}F_3NO_2$
Flumequine	4.75	262.0874	$[M+H]^+$	$C_{14}H_{12}FNO_3$

Fluoxetine	4.75	310.1413	[M+H] ⁺	C ₁₇ H ₁₈ F ₃ NO
Furosemide	4.70	329.0040	[M-H] ⁻	C ₁₂ H ₁₁ ClN ₂ O ₂ S
Gemfibrozil	6.33	129.0910	C ₇ H ₁₃ O ₂ ⁺	C ₁₅ H ₂₂ O ₃
Hydrochlorothiazide	2.64	295.9572	[M-H] ⁻	C ₇ H ₈ ClN ₃ O ₄ S ₂
Hydroflumethiazide	3.58	314.9716	C ₈ H ₆ F ₃ N ₂ O ₄ S ₂ ⁺	C ₈ H ₈ F ₃ N ₃ O ₄ S ₂
Ibuprofen	5.97	161.1325	C ₁₂ H ₁₇ ⁺	C ₁₃ H ₁₈ O ₂
Indomethacine	5.90	358.0841	[M+H] ⁺	C ₁₉ H ₁₆ ClNO ₄
Irgasan	6.69	160.9555	C ₆ H ₃ Cl ₂ O ⁺	C ₁₂ H ₇ Cl ₃ O ₂
Josamycin	4.93	828.4740	[M+H] ⁺	C ₄₂ H ₆₉ NO ₁₅
Ketoprofen	5.24	255.1016	[M+H] ⁺	C ₁₆ H ₁₄ O ₃
Leucomalachite Green	4.88	331.2169	[M+H] ⁺	C ₂₃ H ₂₆ N ₂
Levamisole	1.98	205.0794	[M+H] ⁺	C ₁₁ H ₁₂ N ₂ S
Lincomycin	2.944	407.2210	[M+H] ⁺	C ₁₈ H ₃₄ N ₂ O ₆ S
Lomefloxacin	3.47	352.1467	[M+H] ⁺	C ₁₇ H ₁₉ F ₂ N ₃ O ₃
Malachite Green	5.06	329.2012	[M+H] ⁺	C ₂₃ H ₂₄ N ₂
Marbofloxacin	3.30	363.1463	[M+H] ⁺	C ₁₇ H ₁₉ FN ₄ O ₄
Mebendazole	4.42	296.1030	[M+H] ⁺	C ₁₆ H ₁₃ N ₃ O ₃
Meclofenamic Acid	6.26	278.0134	C ₁₄ H ₁₀ Cl ₂ NO ⁺	C ₁₄ H ₁₁ Cl ₂ NO ₂
Mefenamic Acid	6.25	224.1070	C ₁₅ H ₁₄ NO ⁺	C ₁₅ H ₁₅ NO ₂
Menadione	3.16	253.0171	[M-H] ⁻	C ₁₁ H ₁₀ O ₅ S
Metformin	0.27	130.1087	[M+H] ⁺	C ₄ H ₁₁ N ₅
Metronidazole	1.06	128.0456	C ₄ H ₆ N ₃ O ₂ ⁺	C ₆ H ₉ N ₃ O ₃
Miconazole	5.35	414.9933	[M+H] ⁺	C ₁₈ H ₁₄ Cl ₄ N ₂ O
Minocycline	3.06	458.1922	[M+H] ⁺	C ₂₃ H ₂₇ N ₃ O ₇
Monensin	8.94	693.4184	[M+Na] ⁺	C ₃₆ H ₆₂ O ₁₁
Naproxen	5.27	185.0961	C ₁₃ H ₁₃ O ⁺	C ₁₄ H ₁₄ O ₃
Natamycin	4.37	666.3120	[M+H] ⁺	C ₃₃ H ₄₇ NO ₁₃
Nicotine isomer 1	0.40	163.1230	[M+H] ⁺	C ₁₀ H ₁₄ N ₂
Nicotine isomer 2	0.29	163.1230	[M+H] ⁺	C ₁₀ H ₁₄ N ₂
Nifuroxazide	4.20	276.0615	[M+H] ⁺	C ₁₂ H ₉ N ₃ O ₅
Norfloxacin	3.381	320.1405	[M+H] ⁺	C ₁₆ H ₁₈ FN ₃ O ₃
Orbifloxacin	3.58	396.1530	[M+H] ⁺	C ₁₉ H ₂₀ F ₃ N ₃ O ₃
Oxacillin isomer 1	4.96	434.1380	[M+CH ₄ OH] ⁺	C ₁₉ H ₁₉ N ₃ O ₅ S
Oxacillin isomer 2	5.04	434.1380	[M+CH ₄ OH] ⁺	C ₁₉ H ₁₉ N ₃ O ₅ S
Oxolinic Acid	4.19	262.071	[M+H] ⁺	C ₁₃ H ₁₁ NO ₅
Oxybendazole	3.99	250.1186	[M+H] ⁺	C ₁₂ H ₁₅ N ₃ O ₃
Oxytetracycline	3.361	461.1555	[M+H] ⁺	C ₂₂ H ₂₄ N ₂ O ₉
Penicillin G isomer 1	4.50	335.1060	[M+H] ⁺	C ₁₆ H ₁₈ N ₂ O ₄ S
Penicillin G isomer 2	4.56	335.1060	[M+H] ⁺	C ₁₆ H ₁₈ N ₂ O ₄ S
Penicillin V Isomer 1	4.73	383.1271	[M+CH ₄ OH] ⁺	C ₁₇ H ₂₂ N ₂ O ₆ S
Penicillin V Isomer 2	4.87	383.1271	[M+CH ₄ OH] ⁺	C ₁₆ H ₁₈ N ₂ O ₅ S
Pentylentetrazole	2.43	139.0978	[M+H] ⁺	C ₆ H ₁₀ N ₄
Phenylbutazone	6.12	309.1598	[M+H] ⁺	C ₁₉ H ₂₀ N ₂ O ₂
Pravastatin	4.54	423.2388	[M-H] ⁻	C ₂₃ H ₃₆ O ₇
Prednisolone	4.36	361.201	[M+H] ⁺	C ₂₁ H ₂₈ O ₅

Promethazine	4.45	285.142	[M+H] ⁺	C ₁₇ H ₂₀ N ₂ S
Propranolol	4.15	260.1645	[M+H] ⁺	C ₁₆ H ₂₁ O ₂ N
Ranitidine	1.44	315.1485	[M+H] ⁺	C ₁₃ H ₂₂ N ₄ O ₃ S
Robenidine	3.43	302.1751	[M+H] ⁺	C ₁₈ H ₂₃ NO ₃
Ronidazole	1.55	140.0455	C ₅ H ₆ N ₃ O ₂ ⁺	C ₆ H ₈ N ₄ O ₄
Roxithromycin	4.74	837.5318	[M+H] ⁺	C ₄₁ H ₇₆ N ₂ O ₁₅
Salbutamol	1.01	240.1594	[M+H] ⁺	C ₁₃ H ₂₁ NO ₃
Sarafloxacin	3.694	386.1311	[M+H] ⁺	C ₂₀ H ₁₇ F ₂ N ₃ O ₃
Spiramycin	3.79	843.5213	[M+H] ⁺	C ₄₃ H ₇₄ N ₂ O ₁₄
Streptomycin	0.24	263.1462	C ₈ H ₁₉ N ₆ O ₄ ⁺	C ₂₁ H ₃₉ N ₇ O ₁₂
Sulfabenzamide	4.30	156.0114	C ₆ H ₆ NO ₂ S ⁺	C ₁₃ H ₁₂ N ₂ O ₃ S
Sulfacetamide	1.33	156.0114	C ₆ H ₆ NO ₂ S ⁺	C ₈ H ₁₀ N ₂ O ₃ S
Sulfachloropyridazine	3.80	285.0208	[M+H] ⁺	C ₁₀ H ₉ ClN ₄ O ₂ S
Sulfadiazine	1.63	251.0597	[M+H] ⁺	C ₁₀ H ₁₀ N ₄ O ₂ S
Sulfadimethoxyn	4.39	311.0809	[M+H] ⁺	C ₁₂ H ₁₄ N ₄ O ₄ S
Sulfadoxine	3.94	311.0809	[M+H] ⁺	C ₁₂ H ₁₄ N ₄ O ₄ S
Sulfaguanidine	0.47	215.0597	[M+H] ⁺	C ₇ H ₁₀ N ₄ O ₂ S
Sulfamerazine	2.90	265.0754	[M+H] ⁺	C ₁₁ H ₁₂ N ₄ O ₂ S
Sulfameter	3.51	281.0703	[M+H] ⁺	C ₁₁ H ₁₂ N ₄ O ₃ S
Sulfamethazine	3.32	279.0910	[M+H] ⁺	C ₁₂ H ₁₄ N ₄ O ₂ S
Sulfamethizole	3.49	271.0318	[M+H] ⁺	C ₉ H ₁₀ N ₄ O ₂ S ₂
Sulfamethoxazole	3.97	254.0594	[M+H] ⁺	C ₁₀ H ₁₁ N ₃ O ₃ S
Sulfamethoxypyridazine	3.53	281.0703	[M+H] ⁺	C ₁₁ H ₁₂ N ₄ O ₃ S
Sulfamonomethoxine	3.74	281.0703	[M+H] ⁺	C ₁₁ H ₁₂ N ₄ O ₃ S
Sulfanilamide	0.54	173.0379	[M+H] ⁺	C ₆ H ₈ N ₂ O ₂ S
Sulfapyridine	2.68	250.0645	[M+H] ⁺	C ₁₁ H ₁₁ N ₃ O ₂ S
Sulfathiazole	2.51	256.0209	[M+H] ⁺	C ₉ H ₉ N ₃ O ₂ S ₂
Sulfisoxazol	4.14	268.0750	[M+H] ⁺	C ₁₁ H ₁₃ N ₃ O ₃ S
Sulindac	4.93	357.0955	[M+H] ⁺	C ₂₀ H ₁₇ FO ₃ S
Tetracycline	3.46	445.1605	[M+H] ⁺	C ₂₂ H ₂₄ N ₂ O ₈
Theobromine	1.08	181.0720	[M+H] ⁺	C ₇ H ₈ N ₄ O ₂
Theophylline	1.87	181.0720	[M+H] ⁺	C ₇ H ₈ N ₄ O ₂
Thiamphenicol	3.32	353.9975	[M-H] ⁻	C ₁₂ H ₁₅ Cl ₂ NO ₅ S
Tilmicosin	4.02	435.2903	[M+2H] ²⁺	C ₄₆ H ₈₀ N ₂ O ₁₃
Tolfenamic Acid	6.39	262.0629	[M+H] ⁺	C ₁₄ H ₁₂ ClNO ₂
Tolmetin	5.13	258.1125	[M+H] ⁺	C ₁₅ H ₁₅ NO ₃
Trimethoprim	3.22	291.1452	[M+H] ⁺	C ₁₄ H ₁₈ N ₄ O ₃
Tylosin	4.43	916.5264	[M+H] ⁺	C ₄₆ H ₇₇ NO ₁₇
B-Estradiol	5.16	255.1743	C ₁₈ H ₂₃ O ⁺	C ₁₈ H ₂₄ O ₂
Food Packaging Contaminants				
1,3-Phenylenediamine	0.29	109.0760	[M+H] ⁺	C ₆ H ₈ N ₂
2-Ethylhexyl diphenyl phosphate	7.55	251.0468	C ₁₂ H ₁₂ O ₄ P ⁺	C ₂₀ H ₂₇ O ₄ P
2-Methoxy-5-methylalanine	1.70	138.0913	[M+H] ⁺	C ₈ H ₁₁ ON

2,4-Diaminoanisoole	0.41	139.0866	[M+H] ⁺	C ₇ H ₁₀ N ₂ O
2,4-Diaminotoluene	0.40	123.0917	[M+H] ⁺	C ₇ H ₁₀ N ₂
2,4-Dimethylaniline	1.72	122.0964	[M+H] ⁺	C ₈ H ₁₁ N
2,4,5-Trimethylaniline	3.27	136.1121	[M+H] ⁺	C ₉ H ₁₃ N
2,6-Diaminotoluene isomer 2	0.40	123.0917	[M+H] ⁺	C ₇ H ₁₀ N ₂
4-Aminobiphenyl	4.16	170.0964	[M+H] ⁺	C ₁₂ H ₁₁ N
4-Chloroaniline	1.60	128.0262	[M+H] ⁺	C ₆ H ₆ ClN
4-Hexylresorcinol	5.77	195.1380	[M+H] ⁺	C ₁₂ H ₁₈ O ₂
Aniline	0.44	94.0651	[M+H] ⁺	C ₆ H ₅ NH ₂
Benzyl butyl phthalate	6.88	91.0542	C ₇ H ₇ ⁺	C ₁₉ H ₂₀ O ₄
Bisphenol A	5.10	227.1078	[M-H] ⁻	C ₁₅ H ₁₆ O ₂
¹ BA(2,3-DHP)GE	5.25	376.2118	[M+NH ₄] ⁺	C ₂₁ H ₂₆ O ₅
² BA(3-Cl-2-HP)(2,3-DHP)E	5.22	439.1529	[M+COOH] ⁻	C ₂₁ H ₂₇ ClO ₅
³ BA(3-Cl-2-HP)GE isomer 1	6.22	394.1780	[M+NH ₄] ⁺	C ₂₁ H ₂₅ ClO ₄
BA(3-Cl-2-HP)GE ether isomer 2	6.41	394.1780	[M+NH ₄] ⁺	C ₂₁ H ₂₅ ClO ₄
⁴ BAB(2,3-DHP)E	4.44	209.1172	C ₁₂ H ₁₇ O ₃ ⁺	C ₂₁ H ₂₈ O ₆
Bisphenol A diglycidyl ether	6.31	358.2013	[M+NH ₄] ⁺	C ₂₁ H ₂₄ O ₄
Butyl p-hydroxybenzoate	5.45	193.0870	[M-H] ⁻	C ₁₁ H ₁₄ O ₃
Di (2-ethylhexyl)adipate	8.77	393.2975	[M+Na] ⁺	C ₂₂ H ₄₂ O ₄
Dibutyl sebacate	7.95	315.2530	[M+H] ⁺	C ₁₈ H ₃₄ O ₄
Dicyclohexyl phthalate	7.64	149.0233	C ₈ H ₅ O ₃ ⁺	C ₂₀ H ₂₆ O ₄
Diethyl phthalate	5.50	149.0233	C ₈ H ₅ O ₃ ⁺	C ₁₂ H ₁₄ O ₄
Diisodecyl phthalate	9.65	447.3469	[M+H] ⁺	C ₂₈ H ₄₆ O ₄
Diisononyl phthalate	8.96	419.3156	[M+H] ⁺	C ₂₆ H ₄₂ O ₄
Dimethyl phthalate	4.71	163.0390	C ₉ H ₇ O ₃ ⁺	C ₁₀ H ₁₀ O ₄
Di-N-butyl phthalate	6.97	149.0233	C ₈ H ₅ O ₃ ⁺	C ₁₆ H ₂₂ O ₄
Di N-octyl phthalate isomer 1	8.88	391.2843	[M+H] ⁺	C ₂₄ H ₃₈ O ₄
Di N-octyl phthalate isomer 2	8.94	391.2843	[M+H] ⁺	C ₂₄ H ₃₈ O ₄
Dipropyl phthalate	6.29	149.0233	C ₈ H ₅ O ₃ ⁺	C ₁₄ H ₁₈ O ₄
Ethyl 4-hydroxybenzoate	4.58	165.0557	[M-H] ⁻	C ₉ H ₁₀ O ₃
Melamine	0.26	127.0727	[M+H] ⁺	C ₃ H ₆ N ₆
Methyl paraben	4.08	151.0401	[M-H] ⁻	C ₈ H ₈ O ₃
N,N-diethylhydroxylamine isomer 1	0.30	90.0913	[M+H] ⁺	C ₄ H ₁₁ NO
N,N-diethylhydroxylamine isomer 2	0.41	90.0913	[M+H] ⁺	C ₄ H ₁₁ NO
Nordihydroguaiaretic acid	5.17	301.1445	[M-H] ⁻	C ₁₈ H ₂₂ O ₄
o-Anisidine	0.65	109.0522	C ₆ H ₇ NO ⁺	C ₇ H ₉ ON
o-Toluidine	0.79	108.0808	[M+H] ⁺	C ₇ H ₉ N
Propyl 4-hydroxybenzoate	5.06	179.0714	[M-H] ⁻	C ₁₀ H ₁₂ O ₃
Tributyl o-acetylacrylate	7.38	403.2326	[M+H] ⁺	C ₂₀ H ₃₄ O ₈

¹ BA(2,3-DHP)GE: Bisphenol A (2,3-dihydroxypropyl) glycidyl ether

² BA(3-Cl-2-HP)(2,3-DHP)E: Bisphenol A (3-chloro-2-hydroxypropyl) (2,3-dihydroxypropyl) ether

³ BA(3-Cl-2-HP)GE: Bisphenol A 3-chloro-2-hydroxypropyl glycidyl ether

⁴ BA(3Cl-2HP)GE: Bisphenol A bis(2,3-dihydroxypropyl) ether

Tributyl phosphate	6.43	98.9842	$H_4PO_4^+$	$C_{12}H_{27}PO_4$
Triethyl phosphate	4.03	98.9842	$H_4PO_4^+$	$C_6H_{15}O_4P$
Mycotoxins				
3-Acetyldeoxynivalenol	3.84	339.1438	$[M+H]^+$	$C_{17}H_{22}O_7$
Aflatoxin B ₁	4.66	313.0707	$[M+H]^+$	$C_{17}H_{12}O_6$
Aflatoxin B ₂	4.49	315.0863	$[M+H]^+$	$C_{17}H_{14}O_6$
Aflatoxin G ₁	4.51	329.0656	$[M+H]^+$	$C_{17}H_{12}O_7$
Aflatoxin G ₂	4.32	331.0812	$[M+H]^+$	$C_{17}H_{14}O_7$
Aflatoxin M ₁	4.18	329.0656	$[M+H]^+$	$C_{17}H_{12}O_7$
Alfa zearalenol	5.22	303.1591	$C_{18}H_{23}O_4^+$	$C_{18}H_{24}O_5$
Citrinin	5.03	251.0914	$[M+H]^+$	$C_{13}H_{14}O_5$
Cyclopiazonic acid	6.11	337.1547	$[M+H]^+$	$C_{20}H_{20}N_2O_3$
Deoxynivalenol	2.37	297.1333	$[M+H]^+$	$C_{15}H_{20}O_6$
Diacetoxyscirpenol	4.56	389.1571	$[M+Na]^+$	$C_{19}H_{26}O_7$
Ergocornine isomer 1	4.3	562.3024	$[M+H]^+$	$C_{31}H_{39}N_5O_5$
Ergocornine isomer 2	4.4	562.3024	$[M+H]^+$	$C_{31}H_{39}N_5O_5$
Fumonisin B ₁	4.41	722.3957	$[M+H]^+$	$C_{34}H_{59}NO_{15}$
Fumonisin B ₂	4.78	706.4008	$[M+H]^+$	$C_{34}H_{59}NO_{14}$
Glitoxin	4.45	263.1026	$C_{13}H_{15}N_2O_4^+$	$C_{13}H_{14}N_2O_4S_2$
HT-2 toxin	4.77	425.2170	$[M+H]^+$	$C_{22}H_{32}O_8$
Ochratoxin A	5.63	404.0895	$[M+H]^+$	$C_{20}H_{18}ClNO_6$
Patulin	1.09	155.0339	$[M+H]^+$	$C_7H_6O_4$
Sterigmatocystin	5.81	325.0707	$[M+H]^+$	$C_{18}H_{12}O_6$
T2-Toxin	5.4	489.2095	$[M+Na]^+$	$C_{24}H_{34}O_9$
Zearalenone	5.66	319.1540	$[M+H]^+$	$C_{18}H_{22}O_5$
Perfluorinated Compounds				
C ₃ Pentafluoropropionic acid	0.81	118.9926	$C_2F_5^-$	$C_3F_5HO_2$
C ₄ Perfluorobutyric acid	2.96	168.9894	$C_3F_7^-$	$C_4F_7HO_2$
C ₅ Perfluoropentanoic acid	4.09	218.9862	$C_4F_9^-$	$C_5HO_2F_9$
C ₇ Perfluoroheptanoic acid	5.05	318.9798	$C_6F_{13}^-$	$C_7HO_2F_{13}$
C ₈ Perfluorooctanoic acid	5.47	368.9766	$C_7F_{15}^-$	$C_8F_{15}O_2H$
C ₉ Perfluorononanoic acid	5.89	418.9734	$C_8F_{17}^-$	$C_9F_{17}O_2H$
C ₁₀ Perfluorodecanoic acid	6.33	468.9702	$C_9F_{19}^-$	$C_{10}F_{19}O_2H$
C ₁₁ Perfluoroundecanoic acid	6.81	518.967	$C_{10}F_{21}^-$	$C_{11}F_{21}O_2H$
C ₁₂ Perfluorododecanoic acid	7.35	568.9638	$C_{11}F_{23}^-$	$C_{12}F_{23}O_2H$
Heptadecafluorooctanesulfonic acid	6.66	498.9302	$[M-H]^-$	$C_8HSO_3F_{17}$
Nitrosamines				
N-nitrosodiethylamine	2.24	103.0866	$[M+H]^+$	$C_4H_{10}N_2O$
N-nitrosodimethylamine	0.51	75.0553	$[M+H]^+$	$C_2N_2H_6O$
N-nitrosodi-n-dibutylamine	5.75	159.1492	$[M+H]^+$	$C_8H_{18}N_2O$
N-nitrosodi-n-dipropylamine	4.62	131.1174	$[M+H]^+$	$C_6H_{14}N_2O$

N-nitrosomethylethylamine	0.89	89.0709	[M+H] ⁺	C ₃ H ₈ N ₂ O
N-nitrosomorpholine	0.75	117.0659	[M+H] ⁺	C ₄ H ₈ N ₂ O ₂
N-nitroso-n-diphenylamine	5.94	169.0886	C ₉ H ₁₁ N ⁺	C ₁₂ H ₁₀ N ₂ O
N-nitrosopiperidine	2.96	115.0866	[M+H] ⁺	C ₅ H ₁₀ N ₂ O
N-nitrosopyrrolidine	0.96	101.0709	[M+H] ⁺	C ₄ H ₈ N ₂ O
Sweeteners				
Aspartame	3.38	293.1143	[M-H] ⁻	C ₁₄ H ₁₈ N ₂ O ₅
Acesulfame	0.63	161.9867	[M-H] ⁻	C ₄ H ₅ NO ₄ S
Saccharin	1.25	181.9917	[M-H] ⁻	C ₇ H ₅ NO ₃ S
Sucralose	3.4	395.0073	[M-H] ⁻	C ₁₂ H ₁₉ Cl ₃ O ₈
Cyclamate	1.45	178.0538	[M-H] ⁻	C ₆ H ₁₂ NO ₃ S

Table S2. Relative abundance (%) of fragments for each compound using CID Fragmentation in source (160, 190, 220 and 250V) and MS/MS fragmentation (0,10, 20 and 30V)

Compound	Elemental Composition M	Ion Detected	Theoretical m/z	In-source CID fragmentation				All ion mode MS/MS fragmentation			
				160V	190V	220V	250V	0V	10V	20V	30V
Pesticides											
1-Naphtalene-acetamide	C ₁₂ H ₁₁ NO	[M+H] ⁺	186.0913	100	87	10	-	100	75	-	-
1-Naphtalene-acetamide F ₁		C ₁₂ H ₉ O	169.0648	-	-	-	-	-	6	2	-
1-Naphtalene-acetamide F ₂		C ₁₄ H ₉	141.0699	20	100	100	100	1	100	100	100
1-Naphtalene-acetamide	C ₁₂ H ₁₁ NO	[M+Na] ⁺	208.0733	-	-	-	-	-	6	2	1
1-Naphtalene-acetamide	C ₁₂ H ₁₁ NO	[2M+H] ⁺	371.1754	-	-	-	-	8	-	-	-
1-Naphtyl-N-methyl/carbamate	C ₁₂ H ₁₅ NO ₃	[M+H] ⁺	222.1125	100	25	2	-	100	8	1	-
1-Naphtyl-N-methyl/carbamate F ₁		C ₁₀ H ₁₃ O ₂	165.0910	36	100	56	6	9	100	22	17
1-Naphtyl-N-methyl/carbamate F ₂		C ₈ H ₉ O ₂	137.0597	-	-	-	-	-	1	6	4
1-Naphtyl-N-methyl/carbamate F ₃		C ₇ H ₇ O ₂	123.0441	8	31	100	100	-	20	100	100
1-Naphtyl-N-methyl/carbamate F ₄		C ₄ H ₇	55.0542	-	-	-	-	-	-	10	19
1-Naphtyl-N-methyl/carbamate	C ₁₂ H ₁₅ NO ₃	[M+Na] ⁺	244.0944	5	9	10	5	1	3	2	-
2,4-Dichlorophenoxyacetic acid	C ₈ H ₆ Cl ₂ O ₃	[M-H] ⁻	218.9621	100	100	3	3	100	100	23	-
2,4-Dichlorophenoxyacetic acid F ₁		C ₆ H ₃ Cl ₂ O	160.9566	46	19	100	100	5	65	100	100
2,4-Dichlorophenoxyacetic acid F ₂		C ₆ H ₂ ClO	124.0980	-	2	5	10	-	-	2	5
2,4-Dichlorophenoxyacetic acid	C ₈ H ₆ Cl ₂ O ₃	[2M-H] ⁻	438.9231	-	-	-	-	33	-	-	-
2,4-Dinitrophenol	C ₆ H ₄ N ₂ O ₅	[M-H] ⁻	183.0047	100	100	100	100	100	100	100	70
2,4-Dinitrophenol F ₁		C ₆ H ₃ NO ₃	137.0118	1	5	16	17	-	1	51	45
2,4-Dinitrophenol F ₂		C ₆ H ₃ O ₃	123.0077	-	-	-	-	-	2	72	65
2,4-Dinitrophenol F ₃		C ₅ H ₃ O ₂	95.0128	-	-	-	-	-	-	24	100
3,3-Dichlorobenzidine	C ₁₂ H ₁₀ Cl ₂ N ₂	[M+H] ⁺	253.0294	100	100	100	58	100	100	100	20
3,3-Dichlorobenzidine F ₁		C ₁₂ H ₁₀ ClN ₂	217.0527	1	4	30	100	-	-	61	100

Alachlor F ₄	C ₃ H ₅ CIN	90.0105	-	-	-	-	-	-	-	6	16	31
Alachlor	[M+Na] ⁺	292.1075	-	-	-	-	-	-	4	10	9	11
Albendazole	[M+H] ⁺	266.0958	100	100	100	27	100	100	100	100	21	16
Albendazole F ₁	C ₁₁ H ₁₂ N ₃ OS	234.0696	2	9	64	100	-	-	-	25	100	100
Albendazole F ₂	C ₈ H ₆ N ₃ OS	192.0226	-	-	-	-	-	-	-	-	5	57
Albendazole F ₃	C ₁₀ H ₇ O ₂ S	191.0161	-	-	-	-	-	-	-	-	3	65
Albendazole F ₄	C ₁₀ H ₇ O ₂	159.0441	-	-	-	-	-	-	-	-	-	19
Aldicarb	[M+H] ⁺	191.0849	-	-	-	-	-	5	-	-	-	-
Aldicarb F ₁	C ₅ H ₁₀ NS	116.0528	100	58	5	-	100	71	100	71	10	5
Aldicarb F ₂	C ₄ H ₆ NS	100.0213	3	33	100	100	-	-	-	-	8	17
Aldicarb F ₃	C ₄ H ₆ S	89.0419	43	100	47	14	11	100	100	100	100	100
Aldicarb F ₄	C ₆ H ₈ N	70.0654	3	10	4	-	8	51	34	51	34	24
Aldicarb	[M+Na] ⁺	213.0667	14	59	51	7	8	20	11	-	-	-
Aldicarb sulfone	[M+H] ⁺	223.0747	100	36	1	-	100	35	-	-	-	-
Aldicarb sulfone F ₁	C ₅ H ₁₂ NSO ₃	166.0532	-	-	-	-	4	48	-	-	-	-
Aldicarb sulfone F ₂	C ₅ H ₉ NSO ₂	148.0247	-	-	-	-	3	86	13	-	-	-
Aldicarb sulfone F ₃	C ₄ H ₈ NO	86.0600	14	100	54	63	-	64	100	100	100	100
Aldicarb sulfone F ₄	CH ₅ O ₂ S	81.0005	-	-	-	-	-	29	47	31	-	-
Aldicarb sulfone F ₅	C ₂ H ₆ NO ₂	76.0393	8	35	20	1	6	100	45	38	-	-
Aldicarb sulfone F ₆	CH ₃ OS	62.9899	-	-	-	-	-	-	-	1	42	-
Aldicarb sulfone F ₇	C ₃ H ₇ O	59.0491	-	-	-	-	-	-	-	28	47	-
Aldicarb sulfone	[M+Na] ⁺	245.0566	17	49	100	100	21	50	18	18	-	-
Aldicarb sulfoxide	[M+H] ⁺	207.0798	60	-	-	-	100	-	-	-	-	-
Aldicarb sulfoxide F ₁	C ₉ H ₁₂ NS	166.0685	-	-	-	-	-	4	7	8	-	-
Aldicarb sulfoxide F ₂	C ₅ H ₁₀ NOS	132.0478	100	19	-	-	71	84	3	-	-	-
Aldicarb sulfoxide F ₃	C ₄ H ₉ OS	105.0369	-	-	-	-	-	13	5	-	-	-
Aldicarb sulfoxide F ₄	C ₄ H ₉ S	89.0419	58	100	100	100	4	100	100	100	100	100
Aldicarb sulfoxide F ₅	C ₂ H ₆ NO ₂	76.0393	5	10	9	-	2	6	9	13	-	-
Aldicarb sulfoxide	[M+H ₂ O] ⁺	224.1063	-	-	-	-	9	-	-	-	-	-
Aldicarb sulfoxide	[M+Na] ⁺	229.0617	10	19	9	-	10	13	-	-	-	-
Allethrin	[M+H] ⁺	303.1955	100	55	4	-	100	13	13	13	9	-

Allethrin F ₁	C ₉ H ₁₁ O	135.0804	13	100	100	100	100	100	36	100	76	10
Allethrin F ₂	C ₉ H ₁₅	123.1168	6	46	78	47	11	51	11	51	92	44
Allethrin F ₃	C ₈ H ₁₁	107.0844	9	59	89	71	2	29	2	29	80	55
Allethrin	[M+Na] ⁺	325.1774	-	-	-	-	6	45	6	45	100	100
Ametryn	C ₁₉ H ₂₆ O ₃											
Ametryn F ₁	C ₉ H ₁₇ N ₅ S	228.1277	100	100	100	62	100	100	100	100	28	5
Ametryn F ₂	C ₆ H ₁₂ N ₅ S	186.0807	-	9	42	100	-	11	-	11	100	73
Ametryn F ₃	C ₄ H ₈ N ₅ S	158.0495	-	-	-	-	-	6	-	-	6	22
Ametryn F ₄	C ₅ H ₁₀ N ₃ S	144.0590	-	-	-	-	-	-	-	-	-	18
Ametryn F ₅	C ₅ H ₈ N ₅	138.0774	-	-	-	-	-	6	-	-	6	25
Ametryn F ₆	C ₃ H ₆ N ₃ S	116.0277	-	-	4	19	-	-	-	-	5	46
Ametryn F ₇	C ₄ H ₆ N ₃	96.0556	-	-	-	-	-	-	-	-	15	100
Ametryn F ₈	C ₂ H ₇ N ₂ S	91.0324	-	-	-	-	-	-	-	-	10	70
Ametryn F ₉	C ₃ H ₄ NS	74.0059	-	-	-	-	-	-	-	-	-	18
Aminocarb	C ₃ H ₇ N ₂	71.0604	-	-	-	-	-	-	-	-	6	69
Aminocarb F ₁	[M+H] ⁺	209.1285	100	60	8	4	100	25	4	100	1	-
Aminocarb F ₂	C ₉ H ₁₃ NO	152.1070	16	100	100	100	1	100	1	100	37	3
Aminocarb F ₃	C ₈ H ₁₁ NO	137.0835	-	-	-	-	-	11	-	11	100	100
Aminocarb F ₃	C ₇ H ₈ NO	122.0600	-	-	-	-	-	-	-	-	1	16
Amitraz	C ₁₉ H ₂₃ N ₃											
Amitraz F ₁	[M+H] ⁺	294.1965	100	50	2	-	-	-	-	-	-	-
Amitraz F ₂	C ₁₇ H ₂₁ N ₂	253.1699	2	6	6	9	-	-	-	-	-	-
Amitraz F ₃	C ₁₀ H ₁₅ N ₂	163.1230	19	100	100	100	-	-	-	-	-	-
Amitrol	C ₂ H ₄ N ₄	85.0509	100	100	100	100	100	100	100	100	100	100
Amitrol F ₁	C ₂ H ₅ N ₂	57.0447	-	-	-	-	-	-	-	-	9	35
Ampa	CH ₆ NPO ₃	110.0013	100	100	100	100	100	100	100	100	100	100
Anilazine	C ₉ H ₅ Cl ₃ N ₄	272.9507	100	100	100	100	100	100	100	100	100	100
Anilofos	C ₁₃ H ₁₉ ClNO ₃ PS ₂											
Anilofos F ₁	[M+H] ⁺	368.0305	100	100	24	-	100	16	-	100	-	-
Anilofos F ₂	C ₄ H ₈ O ₃ PS ₂	198.9647	5	38	61	6	3	100	3	100	40	-
Anilofos F ₃	C ₃ H ₈ O ₂ PS ₂	170.9698	2	13	50	13	-	16	-	16	100	25
Anilofos F ₄	C ₂ H ₆ O ₂ PS ₂	156.9541	-	-	15	10	-	-	-	-	6	8
Anilofos F ₄	C ₂ H ₆ O ₂ PS	124.9821	3	21	100	100	-	-	-	-	55	100

Anilofos	$C_{13}H_{19}ClNO_3PS_2$	$[M+Na]^+$	390.0125	-	-	-	-	3	16	26	14
Antimycín A	$C_{28}H_{40}N_2O_9$	$[M+H]^+$	549.2807	100	100	67	10	100	3	-	-
Antimycín A F ₁		$C_{12}H_{13}N_2O_5$	265.0819	7	22	100	100	24	100	100	83
Antimycín A F ₂		$C_{11}H_{13}N_2O_4$	237.0870	-	-	-	13	-	-	22	100
Antimycín A F ₃		$C_8H_6NO_3$	164.0342	1	3	43	31	-	-	8	60
Antimycín A	$C_{28}H_{40}N_2O_9$	$[M+Na]^+$	571.2626	21	26	13	45	3	2	-	-
Asulam	$C_8H_{10}N_2O_4S$	$[M+H]^+$	231.0434	100	16	3	-	100	19	3	-
Asulam F ₁		$C_6H_6NO_2S$	156.0114	78	100	26	10	9	100	100	13
Asulam F ₂		C_6H_6NO	108.0444	16	45	90	96	-	5	81	69
Asulam F ₃		C_6H_6N	92.0495	14	41	100	100	-	3	82	100
Asulam	$C_8H_{10}N_2O_4S$	$[M+Na]^+$	248.0700	-	-	-	-	15	-	-	-
Asulam	$C_8H_{10}N_2O_4S$	$[M+NH_4]^+$	253.0253	-	-	-	-	25	45	66	14
Atrazine	$C_8H_{14}ClN_5$	$[M+H]^+$	216.1010	100	100	100	49	100	100	100	100
Atrazine F ₁		$C_5H_9ClN_5$	174.0541	2	11	62	100	-	16	96	55
Atrazine F ₂		$C_3H_5ClN_5$	146.0228	-	-	-	-	-	-	11	15
Atrazine F ₃		$C_3H_5ClN_5$	138.0780	-	-	-	-	-	-	5	8
Atrazine F ₄		$C_4H_7ClN_3$	132.0323	-	-	-	-	-	-	14	23
Atrazine F ₅		$C_2H_3ClN_3$	104.0001	-	-	-	-	-	-	11	48
Atrazine F ₆		$C_4H_6N_3$	96.0556	-	-	-	-	-	-	26	58
Atrazine F ₇		CH_4ClN_2	79.0058	-	-	-	-	-	-	13	33
Atrazine desethyl	$C_6H_{10}ClN_5$	$[M+H]^+$	188.0697	100	100	47	16	100	100	34	22
Atrazine desethyl F ₁		$C_3H_5ClN_5$	146.0228	5	39	100	100	-	31	100	100
Atrazine desethyl F ₂		$C_2H_9ClN_3$	110.0480	-	-	-	-	-	-	19	42
Atrazine desethyl F ₃		$C_2H_3ClN_3$	104.0010	1	4	22	72	-	-	17	85
Atrazine desethyl F ₄		CH_4ClN_2	79.0058	-	-	-	-	-	-	15	94
Atrazine desisopropyl	$C_5H_8ClN_5$	$[M+H]^+$	174.0541	100	100	100	60	100	100	100	68
Atrazine desisopropyl F ₁		$C_3H_5ClN_5$	146.0228	1	4	16	25	-	3	22	13
Atrazine desisopropyl F ₂		$C_4H_7ClN_3$	132.0323	-	-	-	-	-	4	42	21
Atrazine desisopropyl F ₃		$C_2H_3ClN_3$	104.0010	1	4	33	100	-	-	37	100
Atrazine desisopropyl F ₄		$C_4H_6N_3$	96.0556	-	-	-	-	-	5	70	68
Atrazine desisopropyl F ₅		CH_4ClN_2	79.0058	-	-	-	-	-	3	41	62

Azaconazole	$C_{12}H_{11}Cl_2N_3O_2$	[M+H] ⁺	300.0301	100	100	100	100	100	11	100	100	39	5
Azaconazole F ₁	$C_{10}H_9Cl_2O_2$		230.9974	2	10	66	26	-	26	-	20	10	9
Azaconazole F ₂	$C_7H_5Cl_2$		158.9763	1	5	58	100	-	100	-	1	100	100
Azamethiphos	$C_9H_{10}ClN_2O_5PS$	[M+H] ⁺	324.9809	100	72	5	-	100	-	100	73	-	-
Azamethiphos F ₁	$C_4H_9ClN_2PS$		182.9956	12	100	65	6	-	100	100	100	100	32
Azamethiphos F ₂	$C_6H_4ClN_2$		139.0058	5	40	100	39	-	-	-	-	44	100
Azamethiphos F ₃	C_5H_3ClN		111.9949	3	25	76	100	-	-	-	-	-	66
Azamethiphos	$C_9H_{10}ClN_2O_5PS$	[M+Na] ⁺	346.9629	-	-	-	-	7	-	8	3	3	7
Azinphos-ethyl	$C_{12}H_{16}N_3O_3PS_2$	[M+H] ⁺	346.0444	42	1	-	-	77	-	-	-	-	-
Azinphos-ethyl F ₁	$C_{12}H_{17}NO_3PS_2$		318.0382	4	-	-	-	3	-	-	-	-	-
Azinphos-ethyl F ₂	$C_{12}H_9N_3O_2PS$		290.0148	6	-	-	-	-	-	-	-	-	-
Azinphos-ethyl F ₃	$C_{11}H_{14}O_3PS_2$		289.0117	35	12	-	-	100	4	-	-	-	-
Azinphos-ethyl F ₄	$C_2H_{12}O_2PS_2$		199.0011	7	-	-	-	-	-	-	-	-	-
Azinphos-ethyl F ₅	$C_3H_8O_2PS_2$		170.9698	2	2	-	-	14	17	1	-	-	-
Azinphos-ethyl F ₆	$C_8H_6N_3O$		160.0505	43	6	7	17	63	24	20	25	-	-
Azinphos-ethyl F ₇	$C_6H_5N_2OS$		153.0117	8	3	-	-	11	10	-	-	-	-
Azinphos-ethyl F ₈	C_8H_6NO		132.0440	100	100	100	100	70	100	100	100	100	100
Azinphos-ethyl F ₉	$C_2H_6O_2PS$		124.9821	4	4	2	-	-	16	14	4	-	-
Azinphos-ethyl F ₁₀	C_7H_6N		104.0495	6	10	22	13	2	11	24	37	-	-
Azinphos-ethyl F ₁₁	H_2O_2PS		96.9508	10	24	77	38	-	9	34	57	-	-
Azinphos-ethyl	$C_{12}H_{16}N_3O_3PS_2$	[M+Na] ⁺	368.0263	30	37	84	54	61	69	6	16	-	-
Azinphos-methyl	$C_{10}H_{12}N_3O_3PS_2$	[M+H] ⁺	318.0130	-	-	-	-	47	-	-	-	-	-
Azinphos-methyl F ₁	$C_9H_{10}O_3PS_2$		260.9803	-	-	-	-	96	11	-	-	-	-
Azinphos-methyl F ₂	$C_8H_6N_3O$		160.0505	31	7	18	14	100	16	17	20	-	-
Azinphos-methyl F ₃	C_3H_6NO		132.0443	100	100	100	100	91	100	100	100	100	100
Azinphos-methyl F ₄	$C_2H_6O_2PS$		124.9821	10	25	41	5	6	32	56	71	-	-
Azinphos-methyl	$C_{10}H_{12}N_3O_3PS_2$	[M+Na] ⁺	339.9950	21	37	82	12	38	23	15	-	-	-
Azobenzene	$C_{12}H_{10}N_2$	[M+H] ⁺	183.0917	100	100	27	-	100	-	-	-	-	-
Azobenzene F ₁	$C_6H_5N_2$		105.0447	7	53	100	100	-	-	-	-	-	-
Azocyclotin F ₁	$C_{20}H_{35}N_3Sn$	[M-C ₂ H ₂ N ₃] ⁺	369.1604	100	100	61	13	100	35	-	-	-	-
Azocyclotin F ₂	$C_{12}H_{25}Sn$		287.0822	13	21	91	24	2	100	16	2	100	2

Azocyclotin F ₃	C ₆ H ₁₃ Sn	205.0034	6	14	100	100	100	-	22	100	23
Azocyclotin F ₄	C ₆ H ₉	81.0699	-	-	-	-	-	-	-	32	100
Azoxystrobin	[M+H] ⁺	404.1241	100	100	10	-	100	4	100	1	3
Azoxystrobin F ₁	C ₂₁ H ₁₅ N ₃ O ₄	372.0979	8	71	100	100	100	8	100	100	63
Azoxystrobin F ₂	C ₁₂ H ₉ NO ₃	216.0655	-	-	-	-	-	-	-	-	28
Azoxystrobin	[M+Na] ⁺	426.1060	-	-	-	-	-	2	9	18	100
Barban	[M+H] ⁺	258.0083	100	34	-	-	100	-	-	-	-
Barban F ₁	C ₁₀ H ₉ CIN	178.0418	28	100	100	100	100	22	100	100	-
Benalaxyl	[M+H] ⁺	326.1751	100	100	17	2	100	28	-	-	-
Benalaxyl F ₁	C ₁₉ H ₂₀ NO ₂	294.1489	4	22	11	-	7	93	2	1	-
Benalaxyl F ₂	C ₁₈ H ₂₀ NO	266.1539	-	-	-	-	-	58	2	-	-
Benalaxyl F ₃	C ₁₂ H ₁₈ NO ₂	208.1332	6	45	73	13	-	100	25	3	-
Benalaxyl F ₄	C ₁₀ H ₁₄ N	148.1121	4	27	100	100	-	95	100	100	-
Benalaxyl F ₅	C ₅ H ₁₃ O ₃	121.0859	-	-	-	-	-	-	-	13	37
Benalaxyl	[M+Na] ⁺	348.1570	-	-	-	-	-	2	26	12	14
Bendiocarb	[M+H] ⁺	224.0917	88	6	-	-	100	5	-	-	-
Bendiocarb F ₁	C ₉ H ₁₁ O ₃	167.0703	100	100	19	1	47	100	11	-	-
Bendiocarb F ₂	C ₆ H ₅ O ₂	109.0284	21	66	100	30	-	56	100	100	-
Bendiocarb F ₃	C ₅ H ₅ O	81.0335	5	18	73	100	-	-	11	76	-
Bendiocarb	[M+Na] ⁺	246.0737	4	6	5	1	-	-	-	-	-
Benfluralin	[M+H] ⁺	336.1166	100	100	100	3	100	100	-	-	-
Benfluralin F ₁	C ₁₀ H ₄ F ₂ N ₃ O ₂	236.0266	-	4	34	-	-	-	-	-	-
Benfuracarb	[M+H] ⁺	411.1948	100	100	20	1	100	23	-	-	-
Benfuracarb F ₁	C ₁₂ H ₁₄ NSO ₃	252.0689	2	21	68	7	-	100	13	-	-
Benfuracarb F ₂	C ₁₀ H ₁₁ O ₂ S	195.0474	2	19	100	100	-	30	100	100	-
Benfuracarb F ₃	C ₈ H ₁₆ NO ₂ S	190.0896	11	49	76	10	12	49	10	-	-
Benfuracarb F ₄	C ₈ H ₁₆ NO ₂	158.1176	-	-	-	-	2	72	20	8	-
Benfuracarb F ₅	C ₆ H ₁₀ NOS	144.0478	-	-	-	-	-	10	12	7	-
Benfuracarb F ₆	C ₃ H ₄ NOS	102.0008	-	-	-	-	-	6	10	22	-
Benfuracarb	[M+Na] ⁺	433.1768	18	38	70	90	7	58	45	36	-
Bensulfuron methyl	[M+H] ⁺	411.0969	100	100	100	3	100	97	-	-	-

Bensulfuron methyl F ₁	C ₁₅ H ₄ NO ₅	278.0084	-	-	-	-	-	-	-	-	-	-	-	2	8
Bensulfuron methyl F ₂	C ₇ H ₈ N ₃ O ₃	182.0560	-	-	-	-	-	-	-	-	-	-	-	53	45
Bensulfuron methyl F ₃	C ₈ H ₈ N ₃ O ₂	178.0611	-	-	-	-	-	-	-	-	-	-	-	7	31
Bensulfuron methyl F ₄	C ₉ H ₉ O ₂	149.0597	1	8	77	100	-	-	-	-	-	-	-	91	100
Bensulfuron methyl F ₅	C ₈ H ₇ O	119.0491	-	-	-	-	-	-	-	-	-	-	-	1	12
Bensulfuron methyl	[M+Na] ⁺	433.0788	-	-	-	-	-	-	-	-	-	-	-	100	30
Bensulide	[M+H] ⁺	398.0678	100	22	3	-	-	-	-	-	-	-	-	90	1
Bensulide F ₁	C ₁₁ H ₁₉ NO ₄ PS ₃	356.0208	-	-	-	-	-	-	-	-	-	-	-	100	25
Bensulide F ₂	C ₈ H ₁₃ NO ₄ PS ₃	313.9739	37	100	82	8	29	100	9	-	-	-	-	100	9
Bensulide F ₃	C ₈ H ₁₂ NO ₂ S ₂	218.0304	-	-	-	-	-	-	-	-	-	-	-	62	48
Bensulide F ₄	C ₈ H ₁₀ NOS ₂	200.0198	-	-	-	-	-	-	-	-	-	-	-	16	15
Bensulide F ₅	C ₂ H ₈ NO ₂ S	158.0270	7	21	100	100	-	-	-	-	-	-	-	15	100
Bensulide F ₆	C ₆ H ₅ O ₂ S	141.0005	-	-	-	-	-	-	-	-	-	-	-	15	76
Bensulide F ₇	C ₂ H ₅ S	61.0106	-	-	-	-	-	-	-	-	-	-	-	5	20
Bensulide	[M+Na] ⁺	420.0497	13	16	58	83	13	18	14	14	13	18	14	14	13
Bentazone	[M-H] ⁻	239.0496	100	100	100	100	100	100	100	100	100	100	100	100	74
Bentazone F ₁	C ₇ H ₅ N ₂ O ₃ S	197.0026	-	-	9	42	-	1	41	100	-	-	-	1	100
Bentazone F ₂	C ₁₀ H ₁₁ N ₂ O	175.0877	-	4	21	38	-	1	39	48	-	-	-	1	48
Benzidine	[M+H] ⁺	185.1073	100	100	100	60	100	100	100	82	-	-	-	100	82
Benzidine F ₁	C ₁₂ H ₁₀ N	168.0808	4	10	58	100	-	6	67	100	-	-	-	6	100
Benzidine F ₂	C ₁₂ H ₈ N	166.0651	-	-	-	-	-	-	-	9	-	-	-	-	9
Benzidine F ₃	C ₁₁ H ₁₀ N	156.0808	-	-	-	-	-	-	-	12	-	-	-	-	12
Bifenazate	[M+H] ⁺	301.1547	100	33	42	5	97	18	2	-	-	-	-	18	2
Bifenazate F ₁	C ₁₄ H ₁₅ N ₂ O ₃	259.1077	16	14	11	6	6	3	2	-	-	-	-	3	2
Bifenazate F ₂	C ₁₃ H ₁₂ NO	198.0913	50	100	100	100	100	100	100	81	-	-	-	100	81
Bifenazate F ₃	C ₁₂ H ₁₀ NO	184.0757	-	-	-	-	-	-	4	17	-	-	-	-	17
Bifenazate F ₄	C ₁₂ H ₁₂ N	170.0964	-	-	52	70	-	29	97	100	-	-	-	29	100
Bifenazate F ₅	C ₁₂ H ₈	153.0699	-	-	-	-	-	-	10	36	-	-	-	-	36
Bifenazate	[M+Na] ⁺	323.1366	10	24	59	84	5	16	24	20	-	-	-	16	20
Bifenox	[M+H] ⁺	341.9930	51	5	1	-	97	-	-	-	-	-	-	-	-
	C ₁₄ H ₉ Cl ₂ NO ₅														

Bupirimate	$C_{13}H_{24}N_4O_3S$	[M+H] ⁺	317.1642	100	100	100	100	100	100	100	100	95	4
Bupirimate F ₁		$C_{11}H_{18}N_3O_3S$	272.1063	-	-	5	9	-	1	51	5	51	5
Bupirimate F ₂		$C_{11}H_{20}N_3O$	210.1601	-	1	13	49	-	1	55	54	55	54
Bupirimate F ₃		$C_8H_{12}N_3O$	166.0975	-	1	7	24	-	-	100	100	100	100
Bupirimate F ₄		$C_8H_{12}N_3$	150.1026	-	-	-	-	-	-	26	23	26	23
Bupirimate F ₅		$C_2H_6NO_2S$	108.0114	-	-	-	-	-	-	33	66	33	66
Bupropfezin	$C_{16}H_{23}N_3OS$	[M+H] ⁺	306.1635	100	100	57	25	100	18	-	-	-	-
Bupropfezin F ₁		$C_9H_{17}N_2OS$	201.1056	5	39	100	100	6	100	23	-	23	-
Bupropfezin F ₂		$C_5H_9N_2OS$	145.0430	-	-	-	-	-	-	26	3	26	3
Bupropfezin F ₃		$C_5H_{10}NS$	116.0527	-	-	-	-	-	47	100	2	100	2
Bupropfezin F ₄		C_7H_8N	106.0650	-	-	-	-	-	5	87	100	87	100
Butachlor	$C_{17}H_{26}ClNO_2$	[M+H] ⁺	312.1725	100	100	100	100	90	9	3	-	3	-
Butachlor F ₁		$C_{13}H_{17}ClNO$	238.0993	-	-	-	-	100	100	35	19	35	19
Butachlor F ₂		$C_{12}H_{15}ClNO$	224.0837	-	4	40	54	-	-	-	-	-	-
Butachlor F ₃		$C_{11}H_{16}N$	162.1277	-	-	-	-	2	40	100	81	100	81
Butachlor F ₄		$C_7H_{15}O_3$	147.1016	-	-	-	-	-	-	24	100	24	100
Butachlor F ₅		$C_9H_{10}N$	132.0808	-	-	-	-	-	-	3	37	3	37
Butachlor F ₆		C_3H_5ClN	90.0105	-	-	-	-	-	-	18	22	18	22
Butocarbexim F ₁		C_3H_9NS	116.0528	-	-	-	-	38	10	10	10	10	10
Butocarbexim F ₂		C_3H_7S	75.0262	72	18	83	100	17	41	100	100	41	100
Butocarbexim	$C_7H_{14}N_2O_2S$	[M+Na] ⁺	213.0668	100	100	100	19	100	100	54	11	54	11
Butoxycarbexim	$C_7H_{14}N_2O_4S$	[M+H] ⁺	223.0747	100	12	-	-	100	5	-	-	-	-
Butoxycarbexim F ₁		$C_5H_{12}NO_3S$	166.0532	-	-	-	-	5	50	15	2	15	2
Butoxycarbexim F ₂		$C_5H_{10}NO_2S$	148.0432	2	3	-	-	-	-	-	-	-	-
Butoxycarbexim F ₃		C_3H_8NOS	106.0321	-	-	-	-	4	100	78	10	78	10
Butoxycarbexim F ₄		C_4H_8NO	86.0606	8	57	69	47	-	-	46	100	46	100
Butoxycarbexim F ₅		CH_5O_2S	81.0010	-	3	4	5	-	-	-	9	-	9
Butoxycarbexim F ₆		C_3H_6NO	72.0449	-	2	3	-	-	-	-	-	-	-
Butoxycarbexim F ₇		CH_5OS	65.0056	-	-	-	-	-	-	19	100	19	100
Butoxycarbexim	[M+Na] ⁺		245.0564	26	100	100	100	15	26	82	55	82	55
Butralin	$C_{14}H_{21}N_3O_4$	[M+H] ⁺	296.1605	100	27	-	-	100	5	-	-	-	-

Butralin F ₁	C ₁₀ H ₁₄ N ₃ O ₄	240.0979	31	100	100	100	100	100	100	100	100	100	20
Butralin F ₂	C ₁₀ H ₁₂ N ₃ O ₃	222.0873	2	6	22	95	-	2	90	100	100	100	100
Butralin F ₃	C ₉ H ₁₀ N ₃ O ₃	208.0717	-	-	-	-	-	-	1	54	-	-	54
Butralin F ₄	C ₈ H ₁₀ N	132.0808	-	-	-	-	-	-	2	22	-	-	22
Buturon	C ₁₂ H ₁₃ ClN ₂ O	237.0789	100	100	100	100	100	100	100	100	100	100	19
Buturon F ₁	[M+H] ⁺	185.0476	-	2	5	8	-	-	-	-	-	-	-
Buturon F ₂	C ₈ H ₁₀ ClN ₂ O	167.0371	-	-	4	24	-	-	9	6	-	-	6
Buturon F ₃	C ₈ H ₈ N ₂ Cl	126.0105	-	1	6	61	-	-	16	62	-	-	62
Buturon F ₄	C ₆ H ₅ ClN	84.0808	1	5	18	77	-	32	100	56	-	-	56
Buturon F ₅	C ₅ H ₁₀ N	68.0495	-	-	-	-	-	-	9	28	-	-	28
Buturon F ₆	C ₄ H ₆ N	58.0651	-	-	-	-	-	-	18	38	-	-	38
Buturon F ₇	C ₃ H ₈ N	53.0386	-	-	-	-	-	-	28	100	-	-	100
Cadusafos	C ₁₀ H ₂₃ O ₂ PS ₂	271.0948	100	36	55	6	100	21	4	-	-	-	-
Cadusafos F ₁	[M+H] ⁺	215.0324	25	33	23	9	23	28	16	4	-	-	4
Cadusafos F ₂	C ₈ H ₁₆ O ₂ PS ₂	158.9698	23	100	100	100	100	3	100	69	-	-	39
Cadusafos F ₃	C ₂ H ₈ O ₂ PS ₂	130.9385	-	-	-	-	-	-	11	100	-	-	100
Cadusafos F ₄	H ₄ O ₂ PS ₂	96.9508	-	-	-	-	-	-	14	88	-	-	88
Carbaryl	H ₂ O ₂ PS	202.0863	26	-	-	-	100	1	-	-	-	-	-
Carbaryl F ₁	[M+H] ⁺	145.0648	100	100	100	70	53	100	100	67	-	-	67
Carbaryl F ₂	C ₁₀ H ₉ O	127.0542	-	-	10	100	-	-	13	100	-	-	100
Carbendazim	C ₉ H ₆ N ₃ O ₂	192.0768	100	100	14	3	100	100	11	7	-	-	7
Carbendazim F ₁	[M+H] ⁺	160.0505	13	96	100	100	-	93	100	100	-	-	100
Carbendazim F ₂	C ₈ H ₆ N ₃ O	132.0553	-	-	-	-	-	-	2	25	-	-	25
Carbofuran	C ₆ H ₅ N ₂	222.1125	100	75	2	-	100	8	-	-	-	-	-
Carbofuran F ₁	[M+H] ⁺	165.0910	4	30	6	1	9	100	22	2	-	-	2
Carbofuran F ₂	C ₁₀ H ₁₃ O ₂	123.0441	7	100	100	100	-	20	100	100	-	-	100
Carbofuran F ₃	C ₇ H ₇ O ₂	95.0491	-	-	-	-	-	-	-	6	-	-	6
Carbofuran F ₄	C ₆ H ₇ O	55.0542	-	-	-	-	-	-	9	18	-	-	18
Carbofuran	C ₄ H ₇	244.0944	-	-	-	-	-	3	3	2	-	-	2
Carbofuran 3-hydroxy	[M+Na] ⁺	238.1074	100	22	1	-	100	7	-	-	-	-	-
Carbofuran 3-hydroxy F ₁	[M+H] ⁺	181.0859	18	48	26	11	1	51	19	3	-	-	3

Carbofuran 3-hydroxy F ₂	C ₁₀ H ₁₁ O ₂	163.0754	42	100	100	100	6	100	100	100	55
Carbofuran 3-hydroxy F ₃	C ₁₀ H ₉ O	145.0648	-	-	-	-	-	-	-	-	26
Carbofuran 3-hydroxy F ₄	C ₉ H ₁₁ O	135.0804	-	-	-	-	-	-	-	-	100
Carbosulfan	[M+H] ⁺	381.2206	100	100	100	14	100	72	1	1	-
Carbosulfan F ₁	C ₁₀ H ₁₃ O ₂	165.0910	-	-	-	-	-	7	21	19	-
Carbosulfan F ₂	C ₈ H ₁₈ NS	160.1154	1	5	44	59	2	100	46	29	-
Carbosulfan F ₃	C ₈ H ₁₈ N	128.1434	-	-	-	-	-	30	37	49	-
Carbosulfan F ₄	C ₅ H ₁₂ NS	118.0685	1	4	47	100	-	84	100	100	-
Carbosulfan F ₅	C ₄ H ₁₀ NS	104.0528	-	-	-	-	-	-	5	19	-
Carbosulfan F ₆	C ₂ H ₆ NS	76.0215	-	-	-	-	-	-	18	92	-
Carbosulfan	[M+Na] ⁺	403.2018	-	-	-	-	2	20	18	23	-
Carboxine	[M+H] ⁺	236.0740	100	100	36	12	100	39	2	-	-
Carboxine F ₁	C ₆ H ₇ O ₂ S	143.0161	6	45	100	100	2	100	100	91	-
Carboxine F ₂	C ₈ H ₆ NO	132.0444	-	-	-	-	-	-	-	14	-
Carboxine F ₃	C ₆ H ₆ NS	124.0215	-	-	-	-	-	1	8	29	-
Carboxine F ₄	C ₃ H ₃ OS	86.9899	-	-	-	-	-	1	27	100	-
Carfentazone-ethyl	[M+H] ⁺	412.0437	100	100	100	30	100	100	55	-	-
Carfentazone-ethyl F ₁	C ₁₃ H ₉ Cl ₂ F ₃ N ₃ O ₂	366.0018	-	8	43	100	-	-	55	23	-
Carfentazone-ethyl F ₂	C ₁₃ H ₈ Cl ₂ F ₂ N ₃ O ₂	345.9956	-	-	-	21	-	-	100	100	-
Carfentazone-ethyl F ₃	C ₁₀ H ₅ Cl ₂ F ₂ N ₂ O	276.9742	-	-	-	-	-	-	-	13	-
Carfentazone-ethyl F ₄	[M+NH ₄] ⁺	429.0703	-	-	-	-	100	-	-	-	-
Carfentazone-ethyl F ₅	[M+Na] ⁺	434.0257	-	-	-	-	41	18	47	14	-
Chlorbromuron	[M+H] ⁺	292.9687	10	100	37	7	100	100	8	-	-
Chlorbromuron F ₁	C ₈ H ₇ BrClN ₂ O	260.9425	-	2	9	16	-	-	8	-	-
Chlorbromuron F ₂	C ₆ H ₄ BrClN	203.9210	4	30	100	100	-	23	100	100	-
Chlordimeform	[M+H] ⁺	197.0840	100	100	100	100	100	100	100	-	-
Chlordimeform F ₁	C ₈ H ₇ ClN	152.0262	-	1	5	17	-	-	11	-	-
Chlordimeform F ₂	C ₇ H ₆ Cl	125.0153	-	-	4	48	-	-	-	15	-
Chlordimeform F ₃	C ₈ H ₇ N	117.0573	-	1	7	58	-	-	40	100	-
Chlorfenvinfos	[M+H] ⁺	358.9768	100	100	10	2	100	18	4	-	-
Chlorfenvinfos F ₁	C ₁₀ H ₁₁ Cl ₃ O ₄ P	330.9455	1	7	2	-	-	2	-	-	-

Chlorfeninfos F ₂	C ₇ H ₄ Cl ₂ OP	204.9371	-	-	-	-	-	-	-	-	4	27	15
Chlorfeninfos F ₃	C ₈ H ₄ Cl ₂	169.9863	-	-	-	-	-	-	-	1	1	4	15
Chlorfeninfos F ₄	C ₄ H ₁₂ O ₄ P	155.0468	5	65	29	6	5	100	65	100	65	10	10
Chlorfeninfos F ₅	C ₂ H ₈ O ₄ P	127.0155	3	28	29	6	-	31	100	26	31	100	26
Chlorfeninfos F ₆	H ₄ O ₄ P	98.9842	7	61	100	100	-	4	85	100	4	85	100
Chlorfeninfos	[M+Na] ⁺	380.9587	-	-	-	-	-	2	5	7	5	7	3
Chlorfluazuron	C ₁₂ H ₁₄ Cl ₃ O ₄ P	539.9702	100	100	100	44	100	100	100	13	100	13	4
Chlorfluazuron F ₁	C ₂₀ H ₉ Cl ₃ F ₅ N ₃ O ₃	382.9363	-	4	20	58	-	26	89	99	26	89	99
Chlorfluazuron F ₂	C ₁₃ H ₅ Cl ₃ F ₃ N ₂ O ₂	158.0412	-	3	29	100	-	27	100	100	27	100	100
Chlorfluazuron F ₃	C ₇ H ₆ F ₂ NO	141.0146	-	4	15	36	-	-	9	23	-	9	23
Chlorfluazuron	C ₃ H ₃ F ₂ O	561.9522	8	13	20	30	5	16	19	20	5	16	20
Chloridazon	[M+H] ⁺	222.0429	100	100	100	100	100	100	100	100	100	100	54
Chloridazon F ₁	C ₄ H ₅ ClN ₃ O	146.0116	-	-	1	10	-	-	2	15	-	2	15
Chloridazon F ₂	C ₄ H ₂ ClN ₂ O	128.9850	-	-	2	7	-	-	4	14	-	4	14
Chloridazon F ₃	C ₆ H ₇ N	104.0495	-	-	-	-	-	-	35	87	-	35	87
Chloridazon F ₄	C ₃ H ₂ ClN ₂	100.9901	-	-	-	-	-	-	-	12	-	-	12
Chloridazon F ₅	C ₆ H ₆ N	92.0495	-	-	-	-	-	-	-	16	-	16	100
Chloridazon F ₆	C ₂ H ₃ N ₂	55.0291	-	-	-	-	-	-	-	12	-	-	12
Chloridazon	[M+Na] ⁺	244.0248	-	-	-	-	-	-	5	6	-	5	6
Chlormequat chloride	C ₁₀ H ₈ ClN ₃ O	122.0737	100	100	100	100	100	100	100	100	100	100	4
Chlormequat chloride F ₁	C ₅ H ₁₂ CIN	59.0730	-	-	-	-	-	-	3	39	-	3	39
Chlormequat chloride F ₂	C ₃ H ₇ N	58.0651	-	1	3	23	-	2	83	100	-	2	83
Chlorotoluron	[M+H] ⁺	213.0789	100	100	100	73	100	100	37	11	100	37	11
Chlorotoluron F ₁	C ₈ H ₇ CINO	168.0211	-	-	5	14	-	-	-	-	-	-	-
Chlorotoluron F ₂	C ₇ H ₇ ClN	140.0262	-	-	-	-	-	-	3	4	-	3	4
Chlorotoluron F ₃	C ₃ H ₆ NO	72.0444	-	7	33	100	-	54	100	100	-	54	100
Chloroxuron	[M+H] ⁺	291.0895	100	100	100	100	100	100	100	22	100	22	9
Chloroxuron F ₁	C ₃ H ₆ NO	72.0444	-	1	10	63	-	29	100	100	-	29	100
Chlorpropham	[M+H] ⁺	214.0629	-	-	-	-	-	40	-	-	-	-	-
Chlorpropham F ₁	C ₇ H ₇ CINO ₂	172.0160	100	100	62	9	100	100	33	-	100	33	-
Chlorpropham F ₂	C ₇ H ₅ CINO	154.0054	10	34	95	29	-	27	100	56	-	27	100

Chlorpropham F ₃	C ₆ H ₅ ClN	126.0105	3	13	100	100	100	100	3	33	100
Chlorpropham	[M+Na] ⁺	236.0449	3	2	1	-	-	-	-	-	-
Chlorpyrifos	C ₁₀ H ₁₂ ClNO ₂	349.9336	100	100	4	-	100	48	-	-	-
Chlorpyrifos F ₁	[M+H] ⁺	321.9023	8	48	7	-	-	74	-	-	-
Chlorpyrifos F ₂	C ₇ H ₈ Cl ₃ NO ₃ PS	295.8681	2	27	16	4	-	41	11	-	-
Chlorpyrifos F ₃	C ₄ H ₂ Cl ₃ NO ₆ P	197.9273	5	84	100	100	-	100	100	100	100
Chlorpyrifos methyl F ₁	C ₄ H ₃ Cl ₂ NO ₂ P	321.9023	100	100	100	100	100	100	2	-	-
Chlorpyrifos methyl F ₂	[M+H] ⁺	289.8760	-	-	-	-	-	27	15	4	-
Chlorpyrifos methyl F ₃	C ₆ H ₄ Cl ₃ NO ₂ PS	124.9822	-	-	-	-	-	100	100	100	100
Chlorpyrifos methyl F ₃	C ₃ H ₆ ClOS	78.9943	-	-	-	-	-	-	-	5	35
Chlorpyrifos methyl F ₃	CH ₄ PO ₂	358.0371	100	100	25	3	100	53	-	-	-
Chlorpropham	[M+H] ⁺	167.0564	-	-	-	-	-	77	77	74	-
Chlorpropham F ₁	C ₆ H ₆ N ₄ O ₂	163.0576	-	-	-	-	-	-	31	36	-
Chlorpropham F ₂	C ₁₀ H ₁₁ S	141.0770	5	45	100	100	-	100	100	100	100
Chlorpropham F ₃	C ₅ H ₉ N ₄ O	110.9923	-	-	-	-	-	-	-	-	8
Chlorpropham F ₄	C ₆ H ₄ Cl	56.0495	-	-	-	-	-	-	-	-	23
Chlorpropham F ₅	C ₃ H ₆ N	380.0191	-	-	-	-	-	5	57	20	5
Chlorpropham	[M+Na] ⁺	414.1077	100	100	100	14	100	32	1	1	1
Cinosulfuron	[M+H] ⁺	280.0234	-	-	-	-	-	12	25	77	-
Cinosulfuron F ₁	C ₇ H ₉ N ₃ O ₇ S	183.0513	2	7	47	63	-	100	100	100	100
Cinosulfuron F ₂	C ₆ H ₇ N ₄ O ₃	179.0550	-	-	-	-	-	-	7	22	-
Cinosulfuron F ₃	C ₈ H ₁₁ O ₆	157.0720	-	3	32	53	-	6	19	31	-
Cinosulfuron F ₄	C ₅ H ₉ N ₄ O ₂	141.0005	-	-	-	-	-	-	3	13	-
Cinosulfuron F ₅	C ₆ H ₅ O ₂ S	125.0056	-	-	-	-	-	-	4	15	-
Cinosulfuron F ₆	C ₆ H ₅ OS	83.0240	-	-	-	-	-	-	-	1	21
Cinosulfuron F ₇	C ₃ H ₃ N ₂ O	436.0897	12	14	35	100	17	49	44	15	15
Cinosulfuron	[M+Na] ⁺	360.1395	100	100	75	45	100	100	3	3	3
Clethodim	[M+H] ⁺	268.1366	9	47	100	93	-	68	8	2	-
Clethodim F ₁	C ₁₄ H ₂₂ NO ₂ S	240.1053	-	-	-	-	-	14	18	7	-
Clethodim F ₂	C ₁₂ H ₁₈ NO ₂ S	206.1176	1	5	33	100	2	24	19	4	-
Clethodim F ₃	C ₁₂ H ₁₆ NO ₂	178.1226	-	-	-	-	-	-	-	6	3
Clethodim F ₄	C ₁₁ H ₁₆ NO	-	-	-	-	-	-	-	-	-	-

Clethodim F ₅	C ₉ H ₁₀ NO ₂	164.0706	-	-	-	-	-	-	-	-	-	24	100	100
Clethodim F ₆	C ₈ H ₉ NO	136.0684	-	-	-	-	-	-	-	-	-	-	5	36
Clodinafop-propargyl	[M+H] ⁺	350.0590	100	100	100	26	100	93	19	5				
Clodinafop-propargyl F ₁	C ₁₇ H ₁₃ ClFNO ₄	266.0367	2	10	68	100	-	100	100	30				
Clodinafop-propargyl F ₂	C ₁₂ H ₁₀ ClFNO	238.0429	-	-	-	-	-	-	-	3				
Clodinafop-propargyl F ₃	C ₉ H ₈ FO	91.0554	-	-	-	-	-	-	-	100				
Clofentezine	[M+H] ⁺	303.0198	100	19	-	-	100	-	-	-				
Clofentezine F ₁	C ₁₃ H ₁₃ CIN ₄	261.0902	-	-	-	-	-	-	42	9				
Clofentezine F ₂	C ₇ H ₅ CIN	138.0105	41	100	100	100	19	100	83	8				
Clofentezine F ₃	C ₅ H ₁₀ CIN ₂	133.0527	-	-	-	-	-	-	100	100				
Clomazone	[M+H] ⁺	240.0786	100	99	10	1	100	100	10	3				
Clomazone F ₁	C ₇ H ₆ Cl	125.0153	15	100	100	100	-	67	100	100				
Clopyralid	[M+H] ⁺	191.9614	66	5	-	-	100	10	-	-				
Clopyralid F ₁	C ₆ H ₂ Cl ₂ NO	173.9508	100	42	5	-	17	100	18	-				
Clopyralid F ₂	C ₅ H ₂ CIN	145.9559	48	100	100	36	-	22	100	100				
Clopyralid F ₃	C ₅ H ₃ CIN	109.9792	5	17	50	100	-	-	-	76				
Clothianidin	[M+H] ⁺	250.0160	100	32	9	3	100	25	9	4				
Clothianidin F ₁	C ₆ H ₉ CIN ₃ OS	206.0149	5	7	3	1	-	-	-	-				
Clothianidin F ₂	C ₆ H ₉ CIN ₄ S	204.0231	5	6	3	2	-	-	-	-				
Clothianidin F ₃	C ₆ H ₉ N ₄ S	169.0542	1	100	100	77	11	100	100	82				
Clothianidin F ₄	C ₄ H ₃ CINS	131.9669	23	58	85	100	2	36	67	100				
Clothianidin F ₅	C ₄ H ₅ N ₂ S	113.0168	-	-	-	-	-	-	31	81				
Clothianidin F ₆	C ₅ H ₈ N ₃	110.0713	-	-	-	-	-	-	24	7				
Clothianidin F ₇	C ₃ H ₃ S	70.9950	-	-	-	-	-	-	-	14				
Clothianidin	[M+Na] ⁺	271.9979	-	-	-	-	7	24	21	25				
Coumaphos	[M+H] ⁺	363.0217	100	100	100	100	100	100	38	11				
Coumaphos F ₁	C ₁₂ H ₁₃ ClO ₅ PS	334.9904	1	3	14	34	-	14	29	-				
Coumaphos F ₂	C ₁₀ H ₉ ClO ₅ PS	306.9591	-	2	8	27	-	16	57	8				
Coumaphos F ₃	C ₁₀ H ₇ ClO ₄ PS	288.9486	-	2	2	13	-	-	20	19				
Coumaphos F ₄	C ₁₄ H ₈ ClO ₂ S	226.9928	-	1	5	34	-	3	100	100				
Coumaphos F ₅	C ₉ H ₈ O ₄ P	211.0155	-	-	-	-	-	-	-	8				

Coumaphos	$C_{14}H_{16}ClO_5PS$	$[M+Na]^+$	385.0037	-	-	-	-	-	-	3	25	47	19
Cyanazine	$C_9H_{13}ClN_6$	$[M+H]^+$	241.0963	100	100	100	59	100	100	100	100	33	50
Cyanazine F ₁		$C_8H_{13}ClN_5$	214.0854	2	11	48	100	-	-	-	41	100	100
Cyanazine F ₂		$C_4H_7ClN_3$	132.0323	-	-	-	-	-	-	-	-	9	70
Cyanazine F ₃		$C_2H_3ClN_3$	104.0010	-	1	4	28	-	-	-	-	6	98
Cyanazine F ₄		$C_4H_6N_3$	96.0556	-	-	-	-	-	-	-	-	16	97
Cyanazine F ₅		$C_3H_7N_2$	71.0604	-	-	-	-	-	-	-	-	-	94
Cyanazine		$[M+Na]^+$	263.0782	-	-	-	-	-	-	-	-	-	9
Cyazofamid	$C_{13}H_{13}ClN_4O_2S$	$[M+H]^+$	325.0521	100	34	-	-	100	12	7	7	7	7
Cyazofamid F ₁		$C_{13}H_{10}ClO$	217.0415	-	-	73	100	-	-	-	-	-	7
Cyazofamid F ₂		$C_2H_6NO_2S$	108.0114	14	100	100	28	7	100	100	100	100	100
Cyazofamid	$C_{13}H_{13}ClN_4O_2S$	$[M+Na]^+$	347.0340	-	-	-	-	-	4	6	13	6	13
Cycloate	$C_{11}H_{21}NOS$	$[M+H]^+$	216.1416	100	100	47	6	100	100	100	4	4	-
Cycloate F ₁		$C_{11}H_{10}N$	156.0808	-	1	100	38	-	-	-	-	-	-
Cycloate F ₂		$C_9H_{10}NO$	154.1226	-	-	-	-	1	86	20	-	20	-
Cycloate F ₃		$C_5H_{12}NOS$	134.0634	5	32	11	100	2	41	15	-	15	-
Cycloate F ₄		C_6H_{11}	83.0855	-	-	-	-	2	86	100	62	100	62
Cycloate F ₅		C_3H_6NO	72.0444	-	-	-	-	-	28	52	33	52	33
Cycloate F ₆		C_2H_7S	63.0263	-	-	-	-	-	21	53	33	53	33
Cycloate F ₇		C_4H_7	55.0542	-	-	-	-	-	-	-	61	61	100
Cycloheximid	$C_{15}H_{23}NO_4$	$[M+H]^+$	282.1700	100	100	43	41	100	94	19	9	19	9
Cycloheximid F ₁		$C_{15}H_{22}NO_3$	264.1594	17	73	100	100	4	100	-	-	-	-
Cycloheximid F ₂		$C_{15}H_{20}NO_2$	246.1483	2	9	32	56	-	51	50	11	50	11
Cycloheximid		$[M+NH_4]^+$	299.1965	-	-	-	-	36	-	-	-	-	-
Cycloheximid		$[M+Na]^+$	304.1519	-	-	-	-	14	67	100	100	100	100
Cycloxiidim	$C_{17}H_{27}NO_3S$	$[M+H]^+$	326.1784	100	100	81	19	100	54	19	19	19	19
Cycloxiidim F ₁		$C_{15}H_{22}NO_2S$	280.1366	4	19	100	100	2	100	58	14	58	14
Cycloxiidim F ₂		$C_{10}H_{14}NO_2$	180.1019	-	4	30	62	-	16	100	100	100	100
Cycloxiidim F ₃		C_6H_8NO	110.0600	-	-	-	-	-	1	24	45	24	45
Cycloxiidim F ₄		C_5H_9S	101.0419	-	-	-	-	-	8	55	55	55	55
Cymoxanil	$C_7H_{10}N_4O_3$	$[M+H]^+$	199.0826	100	100	100	100	100	100	100	100	25	28

Cymoxanil F ₁	C ₅ H ₇ N ₄ O ₃	171.0513	-	24	78	-	-	29	33	-
Cymoxanil F ₂	C ₆ H ₁₀ N ₃ O ₂	156.0768	-	16	24	-	-	10	-	-
Cymoxanil F ₃	C ₄ H ₆ N ₃ O ₂	128.0455	-	19	97	-	-	21	100	13
Cymoxanil F ₄	C ₄ H ₃ N ₂ O ₂	111.0189	-	-	-	-	-	-	60	58
Cymoxanil F ₅	C ₃ H ₃ N ₂ O	83.0240	-	-	-	-	-	-	26	100
Cyphenothrin	C ₂₄ H ₂₅ NO ₃	376.1907	36	28	6	1	100	5	-	-
Cyphenothrin F ₁	C ₁₄ H ₉ NO	208.0757	-	-	-	-	8	17	14	10
Cyphenothrin F ₂	C ₁₃ H ₉ O	181.0648	-	-	-	-	-	1	29	39
Cyphenothrin F ₃	C ₁₀ H ₁₅ O	151.1117	7	26	37	10	22	100	59	24
Cyphenothrin F ₄	C ₉ H ₁₄	123.1168	6	14	23	22	4	33	100	100
Cyphenothrin	[M+NH ₄] ⁺	393.2173	61	17	1	-	25	-	-	-
Cyphenothrin	[M+Na] ⁺	398.1727	82	100	100	100	4	6	3	6
Cyphenothrin	[M+K] ⁺	414.1466	100	54	10	3	3	-	-	-
Cyproconazole	[M+H] ⁺	292.1211	100	100	100	38	100	100	13	5
Cyproconazole F ₁	C ₇ H ₆ Cl	125.0153	-	3	23	91	-	3	14	23
Cyproconazole F ₂	C ₂ H ₄ N ₃	70.0401	9	29	34	100	-	39	100	100
Cyprodinil	[M+H] ⁺	226.1339	100	100	100	100	100	100	100	100
Cyprodinil F ₁	C ₃ H ₁₂ N ₃	210.1026	-	-	-	-	-	-	2	18
Cyprodinil F ₂	C ₁₀ H ₁₀ N	144.0808	-	-	-	-	-	-	1	13
Cyprodinil F ₃	C ₈ H ₉ N ₂	133.0760	-	-	1	6	-	-	2	19
Cyprodinil F ₄	C ₇ H ₇ N ₂	119.0604	-	-	-	-	-	-	1	22
Cyprodinil F ₅	C ₈ H ₆ N	116.0495	-	-	-	-	-	-	-	11
Cyprodinil F ₆	C ₇ H ₁₀ N	108.0808	-	-	-	-	-	-	3	42
Cyprodinil F ₇	C ₆ H ₇ N	93.0573	-	-	-	-	-	-	1	51
Cyprodinil F ₈	C ₆ H ₅	77.0386	-	-	-	-	-	-	-	7
Cyromacine	[M+H] ⁺	167.1040	100	100	100	100	100	100	100	100
Cyromacine F ₁	C ₅ H ₉ N ₄	125.0822	1	5	19	32	-	2	31	11
Cyromacine F ₂	C ₆ H ₆ N ₃	108.0556	-	2	9	22	-	-	22	27
Cyromacine F ₃	C ₂ H ₅ N ₄	85.0509	1	4	20	55	-	-	53	64
Cyromacine F ₄	CH ₆ N ₃	60.0556	-	-	-	-	-	2	55	70
Daminozide	[M+H] ⁺	161.0920	100	24	27	100	100	10	20	73
	C ₆ H ₁₂ N ₂ O ₃									

Daminozide F ₁	C ₆ H ₁₁ N ₂ O ₂	143.0815	52	100	100	100	44	13	100	100	100	100
Daminozide F ₁	C ₂ H ₉ N ₂	61.0716	-	-	-	-	-	-	15	76	73	73
Daminozide	[M+Na] ⁺	183.0740	-	-	-	-	-	-	5	23	15	15
Dazomet	[M+H] ⁺	163.0358	100	19	-	-	-	100	70	-	-	-
Dazomet F ₁	C ₃ H ₆ NS ₂	119.9936	70	100	-	-	-	-	100	-	-	-
DEET	[M+H] ⁺	192.1383	100	100	100	100	58	100	100	63	41	41
DEET F ₁	C ₈ H ₇ O	119.0491	13	13	58	93	-	-	33	100	74	74
DEET F ₂	C ₇ H ₇	91.0542	3	3	24	100	-	-	-	22	100	100
Demeton-S-methyl	[M+H] ⁺	231.0273	-	-	-	-	-	6	-	-	-	-
Demeton-S-methyl F ₁	C ₄ H ₉ S	89.0419	100	100	96	100	100	100	100	100	100	100
Demeton-S-methyl F ₂	C ₂ H ₅ S	61.0106	-	-	-	-	-	-	2	17	73	73
Demeton-S-methyl	[M+Na] ⁺	253.0092	13	60	100	19	-	-	5	3	4	4
Desethyl-terbutylazine	[M+H] ⁺	202.0854	100	69	10	3	100	100	76	9	7	7
Desethyl-terbutylazine F ₁	C ₃ H ₅ ClN ₅	146.0227	20	100	100	100	-	-	100	100	100	100
Desethyl-terbutylazine F ₂	C ₂ H ₉ ClN ₃	110.0480	-	-	-	-	-	-	-	8	34	34
Desethyl-terbutylazine F ₃	C ₂ H ₃ ClN ₃	104.0010	-	-	-	-	-	-	-	-	53	53
Desethyl-terbutylazine F ₄	CH ₄ ClN ₂	79.0058	-	-	-	-	-	-	-	6	55	55
Desmedipham	[M+H] ⁺	301.1183	80	31	5	-	-	81	-	-	-	-
Desmedipham F ₁	C ₉ H ₁₂ NO ₃	182.0812	46	100	100	100	100	9	100	10	-	-
Desmedipham F ₂	C ₈ H ₇ NO	153.0546	-	-	-	-	-	-	-	100	100	100
Desmedipham F ₃	C ₇ H ₆ NO ₂	136.0393	-	-	-	-	-	-	6	49	20	20
Desmedipham	[M+NH ₄] ⁺	318.1448	100	5	-	-	-	100	-	-	-	-
Desmetryn	[M+H] ⁺	214.1121	100	100	100	59	100	100	100	19	-	-
Desmetryn F ₁	C ₅ H ₁₀ N ₅ S	172.0651	2	11	56	100	-	24	100	40	40	40
Desmetryn F ₂	C ₄ H ₈ N ₃ S	130.0433	-	-	-	-	-	-	-	-	11	11
Desmetryn F ₃	C ₄ H ₆ N ₅	124.0618	-	-	-	-	-	-	-	9	20	20
Desmetryn F ₄	C ₃ H ₆ N ₃ S	116.0277	-	-	-	-	-	-	-	-	12	12
Desmetryn F ₅	C ₂ H ₇ N ₂ S	91.0324	-	-	-	-	-	-	-	-	12	41
Desmetryn F ₆	C ₃ H ₄ N ₃	82.0400	-	1	8	50	-	-	-	15	100	100
Desmetryn F ₇	C ₂ H ₅ N ₂	57.0447	-	-	-	-	-	-	-	7	65	65
Diafenthiuron	[M+H] ⁺	385.2308	100	100	100	35	100	100	100	12	13	13

Diafenthion F ₁	C ₂₃ H ₃₀ N ₂ O	351.2431	-	-	-	-	-	-	-	-	-	-	3	18
Diafenthion F ₂	C ₂₀ H ₂₅ N ₂ OS	341.1682	-	-	-	-	-	-	-	-	-	-	4	41
Diafenthion F ₃	C ₁₉ H ₂₅ N ₂ OS	329.1682	-	6	35	100	-	19	100	-	-	-	7	25
Diafenthion F ₄	C ₁₉ H ₂₂ NOS	312.1417	-	-	-	-	-	-	-	-	-	-	8	75
Diafenthion F ₅	C ₁₆ H ₁₉ N ₂ OS	287.1213	-	-	-	-	-	-	-	-	-	-	4	100
Diafenthion F ₆	C ₁₉ H ₂₀ NO	278.1539	-	-	-	-	2	-	-	-	-	-	11	41
Diafenthion F ₇	C ₁₈ H ₂₄ NO	270.1852	-	-	-	-	-	-	-	-	-	-	5	43
Diafenthion F ₈	C ₁₈ H ₂₁ O	253.1587	-	-	-	-	-	-	-	-	-	-	-	22
Diafenthion F ₉	C ₁₃ H ₁₃ N ₂ OS	245.0743	-	-	-	-	-	-	-	-	-	-	-	23
Diafenthion F ₁₀	C ₁₅ H ₁₄ O	211.1117	-	-	-	-	-	-	-	-	-	-	-	20
Diafenthion F ₁₁	C ₁₂ H ₁₂ NO	186.0913	-	-	-	-	-	-	-	-	-	-	-	-
Diazinon	C ₁₂ H ₂₁ N ₂ O ₃ PS	305.1083	100	100	100	100	33	-	-	-	-	-	-	-
Diazinon F ₁	C ₈ H ₁₃ N ₂ S	169.0794	1	5	36	100	-	-	-	-	-	-	-	-
Diazinon F ₂	C ₈ H ₁₃ N ₂ O	153.1021	-	3	19	54	100	100	100	100	59	32	10	100
Diazinon F ₃	C ₄ H ₆ NO	84.0444	-	-	-	-	-	-	-	-	10	100	100	100
Dibrom	[M+H] ⁺	378.7899	38	10	-	-	-	100	10	-	-	-	-	-
Dibrom F ₁	C ₂ H ₈ O ₄ P	127.0178	100	100	100	100	100	-	100	100	100	100	100	100
Dibrom F ₂	C ₂ H ₆ O ₃ P	109.0049	12	10	16	68	-	-	-	-	3	10	-	-
Dibrom	[M+Na] ⁺	395.8164	-	-	-	-	-	-	55	-	-	-	-	-
Dicamba	[M-H] ⁻	218.9621	34	7	-	-	-	18	7	9	8	-	-	-
Dicamba F ₁	C ₇ H ₆ Cl ₂ O	174.9723	100	100	100	100	100	100	100	100	100	100	100	100
Dichlofenthion	[M+H] ⁺	314.9773	100	49	2	-	-	100	100	-	-	-	-	-
Dichlofenthion F ₁	C ₆ H ₈ Cl ₂ O ₃ PS	258.9147	13	100	100	100	100	-	50	100	100	100	-	-
Dichlofluamid F ₁	C ₇ H ₅ Cl ₂ FNS	223.9498	100	100	15	1	-	-	-	-	-	-	-	-
Dichlofluamid F ₂	C ₈ H ₅ NS	123.0137	47	100	100	100	-	-	-	-	-	-	-	-
Dichlofluamid	[M+NH ₄] ⁺	349.9958	-	-	-	-	-	100	100	-	-	-	-	-
Dichlofluamid	[M+Na] ⁺	354.9515	12	8	3	1	-	-	-	-	-	-	-	-
Dichlorprop	[M-H] ⁻	232.9778	39	29	3	1	100	85	12	2	-	-	-	-
Dichlorprop F ₁	C ₆ H ₃ Cl ₂ O	160.9566	100	100	100	100	100	13	100	100	100	100	100	100
Dichlorprop F ₂	C ₆ H ₂ ClO	124.9800	-	2	5	9	-	-	-	-	2	8	-	-
Dichlorvos	[M+H] ⁺	220.9532	100	100	46	10	-	-	-	-	-	-	-	-

Dichlorvos F ₁	C ₂ H ₆ O ₃ P	109.0049	6	33	100	100	100	100	100	100	100	100	100
Dicloran	[M-H] ⁻	204.9577	100	100	100	100	100	100	100	100	100	100	100
Dicrotophos	[M+H] ⁺	238.0839	100	65	6	1	100	30	30	100	100	100	100
Dicrotophos F ₁	C ₆ H ₁₀ O ₅ P	193.0260	4	14	3	-	7	71	8	8	1	8	1
Dicrotophos F ₂	C ₂ H ₈ O ₄ P	127.0155	4	41	83	100	-	35	98	50	50	98	50
Dicrotophos F ₃	C ₆ H ₁₀ NO	112.0757	10	100	100	56	3	100	100	25	25	100	25
Dicrotophos F ₄	C ₂ H ₆ O ₃ P	109.0049	-	-	-	-	-	-	2	13	13	2	13
Dicrotophos F ₅	C ₃ H ₆ NO	72.0444	-	-	-	-	-	12	88	100	100	12	88
Diethanolamine	[M+H] ⁺	106.0863	100	69	28	-	25	26	8	14	14	26	8
Diethanolamine F ₁	C ₄ H ₁₀ NO	88.0757	29	100	100	100	18	100	100	100	100	18	100
Diethanolamine F ₂	C ₄ H ₈ N	70.0651	-	1	67	-	-	26	40	24	24	26	40
Diethanolamine F ₃	C ₄ H ₂ N	64.0182	-	-	-	-	100	38	-	-	-	100	38
Diethanolamine	[M+Na] ⁺	128.0682	-	-	-	-	-	-	-	-	-	-	-
Diethofencarb	[M+H] ⁺	268.1543	62	4	2	-	95	2	-	-	-	95	2
Diethofencarb F ₁	C ₁₁ H ₁₆ NO ₄	226.1074	100	100	100	79	100	100	18	-	-	100	18
Diethofencarb F ₂	C ₉ H ₁₂ NO ₄	198.0761	5	12	61	100	2	10	8	-	-	10	8
Diethofencarb F ₃	C ₁₀ H ₁₄ NO ₂	180.1019	-	-	-	-	-	28	66	5	5	28	66
Diethofencarb F ₄	C ₈ H ₁₀ NO ₂	152.0706	-	-	-	-	-	1	100	35	35	1	100
Diethofencarb F ₅	C ₆ H ₆ NO ₂	124.0393	-	-	-	-	-	-	34	100	100	-	34
Difenacoum	[M+H] ⁺	445.1798	100	100	100	100	100	100	100	100	100	100	100
Difenacoum F ₁	C ₁₉ H ₁₅ O ₃	291.1012	-	4	15	10	-	4	15	11	11	4	15
Difenacoum F ₂	C ₂₁ H ₁₆	257.1325	-	-	-	-	-	7	64	42	42	7	64
Difenacoum F ₃	C ₁₁ H ₉ O ₃	189.0546	-	-	-	-	-	2	11	13	13	2	11
Difenacoum F ₄	C ₁₄ H ₁₁	179.0855	-	-	-	-	-	-	21	100	100	-	21
Difenacoum F ₅	C ₁₀ H ₇ O ₃	175.0390	-	-	-	-	-	-	10	26	26	-	10
Difenacoum F ₆	C ₁₃ H ₉	165.0699	-	-	-	-	-	-	-	11	11	-	-
Difenacoum	[M+Na] ⁺	467.1618	-	-	-	-	-	12	32	56	56	12	32
Difenoconazole	[M+H] ⁺	406.0720	100	100	100	66	100	100	26	5	5	100	26
Difenoconazole F ₁	C ₁₇ H ₁₅ Cl ₂ O ₃	337.0392	-	-	-	-	-	10	21	2	2	-	10
Difenoconazole F ₂	C ₁₃ H ₉ Cl ₂ O	251.0025	-	2	14	100	-	3	100	100	100	3	100
Difenoxuron	[M+H] ⁺	287.1390	100	100	100	100	100	100	100	100	100	100	100

Difenoxuron F ₁	C ₇ H ₇ O ₂	123.0441	-	2	17	48	-	9	55	52
Difenoxuron F ₂	C ₃ H ₆ NO	72.0444	-	1	5	20	-	13	82	100
Difenoxuron	[M+Na] ⁺	309.1210	-	-	-	-	-	6	14	11
Difenoquat	[M] ⁺	249.1392	100	100	100	100	100	100	100	100
Difenoquat F ₁	C ₁₆ H ₁₄ N ₂	234.1151	-	1	2	10	-	-	1	21
Difenoquat F ₂	C ₁₆ H ₁₃ N ₂	233.1073	-	-	-	-	-	-	1	25
Difenoquat F ₃	C ₁₅ H ₁₄ N	208.1121	-	-	-	-	-	-	2	12
Difenoquat F ₄	C ₁₄ H ₁₁ N	193.0886	-	-	-	-	-	-	4	79
Difenoquat F ₅	C ₁₀ H ₁₂ N	146.0964	-	-	-	-	-	-	2	12
Difenoquat F ₆	C ₉ H ₉ N	131.0730	-	-	-	-	-	-	2	64
Difenoquat F ₇	C ₉ H ₈ N	130.0651	-	-	-	-	-	-	1	35
Difenoquat F ₈	C ₈ H ₈ N	118.0651	-	-	-	-	-	-	3	60
Diflubenzuron	[M-H] ⁻	309.0248	100	100	90	32	100	-	-	-
Diflubenzuron F ₁	C ₄ H ₅ ClFN ₂ O	151.0080	-	7	90	44	-	-	-	-
Diflubenzuron F ₂	C ₆ H ₃ F ₂	113.0208	-	7	100	25	-	-	-	-
Diflubenzuron F ₃	C ₆ H ₂ F	93.0146	-	3	92	100	-	-	-	-
Diflufenican	[M+H] ⁺	395.0813	100	100	100	100	100	100	37	2
Diflufenican F ₁	C ₁₃ H ₇ F ₃ NO ₂	266.0423	-	-	8	52	-	7	100	100
Diflufenican F ₂	C ₁₆ H ₄ FNO	246.0350	-	-	-	-	-	-	5	10
Dimethametryn	[M+H] ⁺	256.1590	100	100	100	75	100	100	35	-
Dimethametryn F ₁	C ₁₁ H ₂₁ N ₅ S	186.0808	1	4	25	100	-	8	100	100
Dimethametryn F ₂	C ₄ H ₈ N ₅ S	158.0495	-	-	-	-	-	-	3	16
Dimethametryn F ₃	C ₅ H ₈ N ₅	138.0770	-	-	-	-	-	-	2	15
Dimethametryn F ₄	C ₄ H ₆ N ₃	96.0056	-	-	-	-	-	-	5	36
Dimethametryn F ₅	C ₂ H ₇ N ₂ S	91.0324	-	-	-	-	-	-	4	44
Dimethametryn F ₆	C ₃ H ₇ N ₂	71.0604	-	-	-	-	-	-	2	31
Dimethenamid	[M+H] ⁺	276.0820	100	49	4	-	100	7	-	-
Dimethenamid F ₁	C ₁₁ H ₁₅ ClNOS	244.0557	23	100	100	100	8	100	100	23
Dimethenamid F ₂	C ₉ H ₁₄ NS	168.0841	1	6	19	73	-	2	58	100
Dimethenamid F ₃	C ₆ H ₇ S	111.0263	-	-	-	-	-	-	5	43
Dimethoate	[M+H] ⁺	230.0069	100	20	-	-	100	15	1	-
	C ₅ H ₁₂ NO ₃ PS ₂									

Dimethoate F ₁	C ₄ H ₈ O ₃ PS ₂	198.9647	64	28	4	-	44	100	13	6
Dimethoate F ₂	C ₃ H ₈ O ₂ PS ₂	170.9698	18	32	8	3	-	69	16	5
Dimethoate F ₃	C ₂ H ₆ O ₂ PS ₂	156.9541	4	13	8	6	-	3	7	4
Dimethoate F ₄	C ₂ H ₆ O ₂ PS	124.9821	27	100	100	100	-	40	100	100
Dimethoate F ₅	C ₃ H ₆ NS	88.0215	-	-	-	-	3	36	15	9
Dimethoate F ₆	CH ₄ O ₂ P	78.0943	-	-	-	-	-	-	7	28
Dimethomorph	[M+H] ⁺	388.1310	100	100	100	100	100	100	21	12
Dimethomorph F ₁	C ₁₇ H ₁₄ ClO ₃	301.0626	-	2	12	60	-	19	100	71
Dimethomorph F ₂	C ₁₆ H ₁₄ ClO ₂	273.0677	-	-	-	-	-	-	-	13
Dimethomorph F ₃	C ₉ H ₉ O ₃	165.0546	-	-	-	-	-	-	8	100
Dimethomorph F ₄	C ₇ H ₆ ClO ₂	138.9945	-	-	-	-	-	-	-	11
Dimethomorph	[M+Na] ⁺	410.1113	-	-	-	-	1	6	8	15
Diniconazole	[M+H] ⁺	326.0821	100	100	53	43	100	100	23	2
Diniconazole F ₁	C ₈ H ₈ N ₃ O	162.0662	6	29	100	80	-	87	100	100
Diniconazole F ₂	C ₇ H ₅ Cl ₂	158.9763	-	7	51	100	-	-	11	28
Diniconazole F ₃	C ₂ H ₄ N ₃	70.0400	-	-	8	23	-	-	38	81
Diphenylamine	[M+H] ⁺	170.0964	100	100	100	25	100	100	100	14
Diphenylamine F ₂	C ₆ H ₇ N	93.0573	-	5	47	100	-	-	60	100
Diquat dibromide	[M-Br ₂ -H] ⁺	183.0917	100	100	100	100	100	100	100	30
Diquat dibromide F ₁	C ₁₁ H ₉ N ₂	169.0760	-	11	22	36	-	8	21	100
Diuron	[M+H] ⁺	233.0243	100	100	100	29	100	100	63	16
Diuron F ₁	C ₆ H ₄ Cl ₂ N	159.9715	-	-	6	22	-	-	4	5
Diuron F ₂	C ₃ H ₆ NO	72.0444	-	6	80	100	-	50	100	100
Diuron	[M+Na] ⁺	255.0062	-	-	-	-	1	3	3	1
Dmst	[M+H] ⁺	215.0849	100	8	1	-	100	14	2	-
Dmst F ₁	C ₉ H ₁₅ N ₂	151.1230	20	8	3	-	17	24	4	2
Dmst F ₂	C ₇ H ₉ N	106.0651	85	100	100	100	10	100	100	100
Dmst F ₃	C ₆ H ₇	79.0542	6	9	31	34	-	-	-	71
DNOC	[M-H] ⁻	197.0204	100	100	100	100	100	100	100	100
DNOC F ₁	C ₇ H ₅ O ₃	137.0244	-	4	16	19	-	2	46	17
DNOC F ₂	C ₆ H ₅ O ₂	109.029	-	3	19	62	-	-	26	45

Edifenphos	$C_{14}H_{15}O_2PS_2$	$[M+H]^+$	311.0324	100	100	51	33	100	73	42	6
Edifenphos F ₁	$C_{12}H_{12}O_2PS_2$	$[M+H]^+$	283.0010	9	59	100	100	-	100	68	14
Edifenphos F ₂	$C_6H_6O_2PS$	$[M+H]^+$	172.9821	-	-	-	-	-	20	100	13
Edifenphos F ₃	$C_6H_5S_2$	$[M+H]^+$	140.9827	-	-	-	-	-	-	16	18
Edifenphos F ₄	C_6H_5S	$[M+H]^+$	109.0106	-	-	-	-	-	-	90	100
Edifenphos F ₅	$C_{14}H_{15}O_2PS_2$	$[M+Na]^+$	333.0143	-	-	-	-	-	9	22	7
Emamectin	$C_{49}H_{75}NO_{13}$	$[M+H]^+$	886.5311	100	100	100	100	100	100	100	22
Emamectin F ₁	$C_{15}H_{28}NO_5$	$[M+H]^+$	302.1962	-	-	-	-	-	-	-	6
Emamectin F ₂	$C_8H_{16}NO_2$	$[M+H]^+$	158.1176	-	-	1	1	-	1	14	100
Emamectin F ₃	$C_7H_{12}NO$	$[M+H]^+$	126.0913	-	-	-	-	-	-	-	5
Endosulfan sulfate	$C_9H_6Cl_6O_4S$	$[M-H]^-$	418.8045	100	100	10	1	100	28	-	-
Endosulfan sulfate F ₁	HSO_4	$[M-H]^-$	96.9605	16	89	100	100	-	100	100	100
EPN	$C_{14}H_{14}NO_4PS$	$[M+H]^+$	324.0454	100	100	20	2	100	37	-	-
EPN F ₁	$C_{12}H_{11}NO_4PS$	$[M+H]^+$	296.0141	9	65	100	45	-	100	24	-
EPN F ₂	C_6H_6OPS	$[M+H]^+$	156.9871	2	9	40	100	-	-	100	100
Epoxiconazole	$C_{17}H_{13}ClFN_3O$	$[M+H]^+$	330.0804	100	100	100	100	100	100	100	100
Eptc	$C_9H_{19}NOS$	$[M+H]^+$	190.1260	100	100	100	-	100	53	-	-
Eptc F ₁	$C_7H_{14}NO$	$[M+H]^+$	128.1070	6	20	38	-	5	100	100	-
Eptc F ₂	C_4H_8NO	$[M+H]^+$	86.0600	1	6	19	-	-	82	20	-
Etaconazol	$C_{14}H_{15}Cl_2N_3O_2$	$[M+H]^+$	328.0614	100	100	100	31	100	100	52	15
Etaconazol F ₁	$C_8H_7Cl_2O_2$	$[M+H]^+$	204.9818	-	-	-	-	-	4	18	3
Etaconazol F ₂	$C_7H_5Cl_2$	$[M+H]^+$	158.9763	-	4	29	100	-	3	75	92
Etaconazol F ₃	C_4H_7	$[M+H]^+$	55.0542	-	-	-	-	-	6	100	100
Ethephon	$C_2H_6ClO_3P$	$[M-H]^-$	142.9670	23	8	4	-	76	36	37	15
Ethephon F ₁	$C_2H_4O_3P$	$[M-H]^-$	106.9904	74	20	12	2	100	100	70	59
Ethephon F ₂	PO_3	$[M-H]^-$	78.9591	100	100	100	100	3	56	100	100
Ethidimuron	$C_7H_{12}N_4O_3S_2$	$[M+H]^+$	265.0424	100	60	9	7	100	32	8	5
Ethidimuron F ₁	$C_5H_{10}N_3O_2S_2$	$[M+H]^+$	208.0209	19	100	100	100	2	100	100	100
Ethidimuron F ₂	$C_3H_4N_3OS_2$	$[M+H]^+$	161.9790	-	2	11	45	-	-	34	32
Ethidimuron F ₃	$C_3H_5N_3S$	$[M+H]^+$	116.0277	-	-	-	-	-	-	10	21
Ethidimuron F ₄	$C_3H_4N_3S$	$[M+H]^+$	114.0120	1	10	16	25	-	13	72	29

Ethidimuron F ₅	C ₃ H ₄ NS	74.0059	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	25
Ethidimuron F ₆	C ₂ H ₅ N ₂	57.0447	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	49
Ethidimuron	[M+Na] ⁺	287.0243	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	26
Ethiofencarb	[M+H] ⁺	226.0896	25	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	100
Ethiofencarb F ₁	C ₉ H ₁₃ OS	169.0982	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	52
Ethiofencarb F ₂	C ₉ H ₁₀ NO ₂	164.0706	49	5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	21
Ethiofencarb F ₃	C ₇ H ₇ O	107.0491	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100
Ethiofencarb sulfone	[M+H] ⁺	258.0795	94	5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	100
Ethiofencarb sulfone F ₁	C ₉ H ₁₃ O ₃ S	201.0580	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	28
Ethiofencarb sulfone F ₂	C ₁₀ H ₁₃ O ₃	181.0859	17	42	24	3	-	-	-	-	-	-	-	-	-	-	-	-	-	35
Ethiofencarb sulfone F ₃	C ₁₀ H ₁₁ O ₂	163.0754	40	91	100	30-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ethiofencarb sulfone F ₄	C ₉ H ₁₁ O	135.0804	5	13	38	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ethiofencarb sulfone F ₅	C ₇ H ₇ O	107.0492	100	100	97	100	-	-	-	-	-	-	-	-	-	-	-	-	-	100
Ethiofencarb sulfone	[M+NH ₄] ⁺	275.1060	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	30
Ethiofencarb sulfone	[M+Na] ⁺	280.0611	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6
Ethiofencarb sulfoxide	[M+H] ⁺	242.0845	92	5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	100
Ethiofencarb sulfoxide F ₁	C ₉ H ₁₃ O ₂ S	185.0631	45	5	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	77
Ethiofencarb sulfoxide F ₂	C ₉ H ₁₀ NO ₂	164.0706	34	6	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2
Ethiofencarb sulfoxide F ₃	C ₇ H ₇ O	107.0492	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100
Ethiofencarb sulfoxide F ₄	C ₆ H ₇	79.0542	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	11
Ethiofencarb sulfoxide	[M+Na] ⁺	264.0665	6	8	6	6	-	-	-	-	-	-	-	-	-	-	-	-	-	5
Ethion	[M+H] ⁺	384.9949	100	22	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	100
Ethion F ₁	C ₅ H ₁₂ O ₂ PS ₃	230.9732	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4
Ethion F ₂	C ₆ H ₁₆ O ₂ PS ₂	215.0324	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6
Ethion F ₃	C ₃ H ₁₂ O ₂ PS ₂	199.0011	33	100	100	-	-	-	-	-	-	-	-	-	-	-	-	-	-	96
Ethion F ₄	C ₃ H ₈ O ₂ PS ₂	170.9698	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2
Ethion F ₅	C ₄ H ₁₀ O ₂ PS	153.0134	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	68
Ethion F ₆	CH ₄ O ₂ PS ₂	142.9384	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	17
Ethion F ₇	C ₂ H ₆ O ₂ PS	124.9821	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	23
Ethiprofe	[M+H] ⁺	396.9899	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	61
Ethiprofe F ₁	C ₁₁ HCl ₂ F ₃ N ₄ S	350.9480	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6

Fenamidone	$C_{17}H_{17}N_3OS$	$[M+H]^+$	312.1165	100	100	53	4	100	19	-	-
Fenamidone F ₁		$C_{15}H_{14}N_3$	236.1182	2	9	54	73	-	100	76	16
Fenamidone F ₂		$C_8H_9N_2S$	165.0481	-	-	-	-	-	14	13	4
Fenamidone F ₃		$C_7H_8N_3$	134.0713	-	-	-	-	-	-	6	15
Fenamidone F ₄		C_6H_6N	92.0495	2	17	100	100	-	18	100	100
Fenamiphos	$C_{13}H_{22}NO_3PS$	$[M+H]^+$	304.1131	100	100	100	100	100	100	100	43
Fenamiphos F ₁		$C_{11}H_{19}NO_3PS$	276.0818	3	17	45	47	-	14	13	25
Fenamiphos F ₂		$C_{10}H_{17}NO_3PS$	262.0661	1	2	3	3	-	11	11	20
Fenamiphos F ₃		$C_8H_{13}NO_3PS$	234.0348	1	4	20	37	-	12	29	28
Fenamiphos F ₄		$C_8H_{10}O_3PS$	217.0083	1	4	21	69	-	5	91	100
Fenamiphos F ₅		$C_{10}H_5NPS$	201.9875	-	-	-	-	-	-	-	26
Fenamiphos F ₆		$C_3H_{10}N$	60.0808	-	-	-	-	-	2	11	9
Fenamiphos sulfone	$C_{13}H_{22}NO_5PS$	$[M+H]^+$	336.1029	100	100	100	99	100	100	100	83
Fenamiphos sulfone F ₁		$C_{11}H_{19}NO_5PS$	308.0716	3	11	52	100	-	16	90	45
Fenamiphos sulfone F ₂		$C_8H_{13}NO_5PS$	266.0247	1	3	15	77	-	3	94	100
Fenamiphos sulfone F ₃		$C_8H_{10}O_5PS$	248.9982	-	-	-	-	-	-	5	13
Fenamiphos sulfone F ₄		$C_7H_8O_4PS$	218.9875	-	-	-	-	-	-	-	13
Fenamiphos sulfone F ₅		$C_7H_{11}NO_3P$	188.0471	-	-	3	17	-	-	12	92
Fenamiphos sulfone F ₆		$C_3H_{11}O_4PS$	108.0573	-	-	-	-	-	-	-	10
Fenamiphos sulfoxide	$C_{13}H_{22}NO_4PS$	$[M+H]^+$	320.1080	100	100	100	100	100	100	100	100
Fenamiphos sulfoxide F ₁		$C_{11}H_{19}NO_4PS$	292.0767	1	6	24	36	-	18	55	42
Fenamiphos sulfoxide F ₂		$C_{14}H_{12}O_4S$	277.0529	-	1	7	31	-	-	20	25
Fenamiphos sulfoxide F ₃		$C_8H_{10}O_4PS$	233.0032	-	-	-	-	-	-	5	26
Fenamiphos sulfoxide	$C_{13}H_{22}NO_4PS$	$[M+Na]^+$	342.0899	2	4	8	17	-	6	25	83
Fenarimol	$C_{17}H_{12}Cl_2N_2O$	$[M+H]^+$	331.0399	100	100	100	100	100	100	100	31
Fenarimol F ₁		C_7H_4ClO	138.9945	-	-	1	6	-	-	3	34
Fenarimol F ₂		$C_4H_5N_2$	81.0447	-	-	2	17	-	-	21	100
Fenzaquin	$C_{20}H_{22}N_2O$	$[M+H]^+$	307.1805	100	100	100	50	100	100	36	13
Fenzaquin F ₁		$C_{12}H_{17}$	161.1324	3	32	69	100	-	32	100	100
Fenzaquin F ₂		$C_8H_7N_2O$	147.0552	-	7	16	35	-	3	25	48
Fenbendazole	$C_{15}H_{13}N_3O_2S$	$[M+H]^+$	300.0801	100	100	100	86	100	100	78	48

Fenbendazole F ₁	C ₁₄ H ₁₀ N ₃ O ₅	268.0539	1	5	25	100	-	100	-	10	100	100
Fenbendazole F ₂	C ₈ H ₄ N ₃ O ₅	190.0070	-	-	-	-	-	-	-	-	-	7
Fenbendazole F ₃	C ₁₀ H ₇ O ₂	159.0441	-	-	-	-	-	-	-	-	-	37
Fenhexamid	[M+H] ⁺	302.0709	100	100	100	100	100	100	100	100	100	85
Fenhexamid F ₁	C ₇ H ₁₃	97.1011	-	2	8	61	-	4	100	4	100	100
Fenhexamid 4-o-glucoside	[M+H] ⁺	464.1237	100	100	100	36	100	13	-	-	-	-
Fenhexamid 4-o-glucoside F ₁	C ₁₄ H ₁₈ Cl ₂ NO ₂	302.0709	16	24	61	100	60	100	100	100	100	100
Fenhexamid 4-o-glucoside F ₂	C ₇ H ₁₃	97.1012	-	-	-	-	-	-	-	-	7	35
Fenhexamid 4-o-glucoside	[M+Na] ⁺	486.1057	3	3	7	13	8	8	11	16	-	-
Fenhexamid 4-o-glucoside	[M+NH ₄] ⁺	481.1503	44	8	1	1	43	-	-	-	-	-
Fenitrothion	[M+H] ⁺	278.0247	100	100	100	58	100	100	100	100	100	100
Fenobucarb	[M+H] ⁺	208.1332	100	19	1	-	100	15	-	-	-	-
Fenobucarb F ₁	C ₈ H ₁₀ NO ₂	152.0706	11	13	1	-	9	45	-	-	-	-
Fenobucarb F ₂	C ₆ H ₇ O	95.0491	31	100	100	100	2	100	100	100	100	100
Fenoxaprop-P-ethyl	[M+H] ⁺	362.0790	100	100	100	100	100	100	100	100	34	22
Fenoxaprop-P-ethyl F ₁	C ₁₅ H ₁₀ ClNO ₃	288.0422	1	2	10	41	-	17	100	100	100	100
Fenoxaprop-P-ethyl F ₂	C ₁₅ H ₉ ClNO ₂	270.0316	-	-	-	-	-	-	-	-	3	15
Fenoxaprop-P-ethyl F ₃	C ₁₄ H ₁₁ ClNO ₂	260.0473	-	-	-	-	-	-	-	-	4	30
Fenoxaprop-P-ethyl F ₄	C ₁₁ H ₁₂ O ₄	209.0808	-	-	-	-	-	-	-	-	3	15
Fenoxaprop-P-ethyl F ₅	C ₈ H ₈ O	121.0647	-	-	-	10	-	-	-	-	-	-
Fenoxycarb	[M+H] ⁺	302.1387	100	100	31	17	100	13	2	-	-	-
Fenoxycarb F ₁	C ₁₅ H ₁₄ NO ₃	256.0968	5	45	100	100	1	32	6	-	-	-
Fenoxycarb F ₂	C ₅ H ₉ NO ₂	116.0706	4	42	36	20	8	100	14	-	-	-
Fenoxycarb F ₃	C ₃ H ₆ NO ₂	88.0393	-	-	-	-	-	-	96	100	100	100
Fenpiclonil	[M+H] ⁺	236.9981	100	100	100	38	100	100	100	100	100	14
Fenpiclonil F ₁	C ₁₁ H ₇ ClN ₂	202.0292	-	8	41	100	-	-	-	-	76	100
Fenpropathrin	[M+H] ⁺	350.1750	97	38	4	2	100	7	1	2	-	-
Fenpropathrin F ₁	C ₁₃ H ₉ O	181.0648	-	-	-	-	-	4	8	14	-	-
Fenpropathrin F ₂	C ₈ H ₁₃ O	125.0960	47	100	100	96	20	100	100	100	100	100
Fenpropathrin	[M+NH ₄] ⁺	367.2016	-	-	-	-	22	-	-	-	-	-
Fenpropathrin	[M+Na] ⁺	372.1570	100	78	60	100	9	9	8	12	-	-

Fipronil	$C_{12}H_4Cl_2F_6N_4OS$	$[M+H]^+$	436.9460	100	100	100	100	63	100	100	100	-
Fipronil F ₁	$C_{11}H_5Cl_2F_3N_4OS$		367.9508	-	-	-	-	-	-	-	46	100
Fipronil F ₂	$C_{11}H_5ClF_3N_4OS$		332.9819	-	-	-	-	-	-	-	-	26
Fipronil F ₃	$[M+NH_4]^+$		453.9725	-	-	-	-	100	-	-	-	-
Fipronil F ₄	$[M+Na]^+$		458.9279	-	-	-	-	5	-	-	-	-
Fluzifop	$C_{15}H_{12}F_3NO_4$	$[M+H]^+$	328.0791	100	100	100	100	-	-	-	-	-
Fluzifop F ₁	$C_{14}H_{11}F_3NO_2$		282.0736	-	2	10	-	-	-	-	-	-
Fluzifop-butyl	$C_{19}H_{20}F_3NO_4$	$[M+H]^+$	384.1417	100	100	100	100	100	100	100	15	4
Fluzifop-butyl F ₁	$C_{15}H_{13}F_3NO_4$		328.0791	1	3	13	66	-	22	51	13	-
Fluzifop-butyl F ₂	$C_{14}H_{11}F_3NO_2$		282.0736	1	2	11	68	-	16	100	100	-
Fluzifop-butyl F ₃	$C_{13}H_{11}F_3NO$		254.0787	-	-	-	-	-	-	6	31	-
Fluzifop-butyl F ₄	C_4H_8FO		91.0554	-	-	-	-	-	-	3	32	-
Fluzinam	$C_{13}H_4Cl_2F_6N_4O_4$	$[M+H]^+$	464.9587	100	100	100	100	-	-	-	-	-
Fluzinam F ₁	$C_{13}H_2Cl_2F_6N_3O_2$		415.9725	-	-	-	-	100	-	-	-	-
Fluzinam F ₂	$C_{13}H_3ClF_6N_3O_3$		397.9773	-	-	-	-	38	90	99	93	-
Fluzinam F ₃	$C_{13}H_5Cl_2F_6N_2$		372.9728	-	1	7	43	-	-	-	-	-
Fluchloralin	$C_{12}H_{13}ClF_3N_3O_4$	$[M+H]^+$	356.0619	100	100	100	100	-	100	100	-	-
Fluchloralin F ₁	$C_9H_8ClF_3N_3O_4$		314.0150	-	24	100	-	-	-	-	-	-
Flucythrinate	$C_{26}H_{23}F_2NO_4$	$[M+H]^+$	452.1668	-	-	-	-	-	-	-	-	-
Flucythrinate F ₁	$C_{26}H_{22}NO_4$		412.1543	12	20	20	25	7	100	56	12	-
Flucythrinate F ₂	$C_{14}H_{10}NO$		208.0757	12	23	28	54	4	35	43	26	-
Flucythrinate F ₃	$C_{11}H_{13}F_2O$		199.0929	3	5	10	14	-	29	50	33	-
Flucythrinate F ₄	$C_{13}H_9O$		181.0648	4	13	26	63	1	26	81	100	-
Flucythrinate	$C_{26}H_{23}F_2NO_4$	$[M+NH_4]^+$	469.1933	100	100	18	2	100	43	43	26	-
Flucythrinate	$C_{26}H_{23}F_2NO_4$	$[M+Na]^+$	474.1487	51	91	100	100	5	53	100	98	-
Flucythrinate	$C_{26}H_{23}F_2NO_4$	$[M+K]^+$	490.1227	73	78	22	14	3	9	25	25	-
Fludioxonil	$C_{12}H_6F_2N_2O_2$	$[M-H]^-$	247.0325	100	100	100	100	100	100	100	100	100
Fludioxonil F ₁	$C_{11}H_5N_2O$		181.0407	-	1	7	25	-	-	18	55	-
Fludioxonil F ₂	C_9H_4N		126.0349	-	-	2	16	-	-	19	98	-
Flufenacet	$C_{14}H_{13}F_4N_3O_2S$	$[M+H]^+$	364.0737	100	4	1	-	100	-	-	-	-
Flufenacet F ₁	$C_{11}H_{13}FNO$		194.0976	28	100	31	4	35	100	10	-	-

Flufenacet F ₂	C ₈ H ₇ FNO	152.0506	14	48	100	100	100	100	34	100	100	100
Flufenacet F ₃	C ₇ H ₇ FN	124.0557	-	-	-	-	-	-	-	15	86	
Flufenacet F ₄	C ₇ H ₆ F	109.0448	-	-	-	-	-	-	-	7	24	
Flufenacet	[M+Na] ⁺	386.0556	-	-	-	-	5	21	19	25		
Flufenoxuron	C ₂₁ H ₁₃ F ₄ N ₃ O ₂ S	489.0441	100	100	69	6	100	65	-	-	-	
Flufenoxuron F ₁	[M+H] ⁺	331.0013	-	-	-	-	-	8	7	6		
Flufenoxuron F ₂	C ₁₇ H ₃ F ₄ O ₃	158.0412	2	15	100	100	-	100	100	100	100	
Flufenoxuron F ₃	C ₇ H ₆ F ₂ NO	141.0135	-	-	-	-	-	-	8	28		
Flufenoxuron	C ₁₀ H ₂ F	511.0255	-	-	-	-	24	53	28	31		
Fluometuron	[M+Na] ⁺	233.0896	100	100	100	54	100	100	27	8		
Fluometuron F ₁	C ₁₀ H ₁₁ F ₃ N ₂ O	160.0369	-	-	2	17	-	-	2	1		
Fluometuron F ₂	C ₇ H ₅ F ₃ N	72.0444	1	4	29	100	-	35	100	100		
Fluquinconazole	C ₁₆ H ₈ Cl ₂ FN ₃ O	376.0163	100	100	100	42	100	100	49	-		
Fluquinconazole F ₁	C ₁₅ H ₈ Cl ₂ FN ₄ O	349.0054	1	3	28	89	-	-	100	86		
Fluquinconazole F ₂	C ₁₄ H ₆ Cl ₂ FN ₂ O	306.9836	1	2	26	100	-	-	30	100		
Fluroxypr	[M-H] ⁻	252.9588	37	9	3	2	100	30	6	3		
Fluroxypr F ₁	C ₅ C ₃ FN ₂ O	194.9534	100	100	100	100	18	100	100	100		
Flusilazole	[M+H] ⁺	316.1076	100	100	100	50	100	100	43	65		
Flusilazole F ₁	C ₁₄ H ₁₃ F ₂ Si	247.0749	1	4	30	100	-	13	100	80		
Flusilazole F ₂	C ₁₂ H ₉ SiF ₂	219.0436	-	-	-	-	-	-	6	100		
Flusilazole F ₃	C ₁₃ H ₁₀ F	185.0761	-	-	-	-	-	-	5	65		
Flusilazole F ₄	C ₇ H ₇ F ₂ Si	157.0280	-	-	-	-	-	-	3	85		
Flusilazole F ₅	CH ₃ F ₂ Si	80.9967	-	-	-	-	-	-	8	90		
Flutolanil	[M+H] ⁺	324.1206	100	100	71	9	100	100	19	6		
Flutolanil F ₁	C ₁₄ H ₁₁ F ₃ NO ₂	282.0736	-	-	-	-	-	70	12	8		
Flutolanil F ₂	C ₁₇ H ₉ FNO	262.0663	2	12	100	100	-	48	100	24		
Flutolanil F ₃	C ₁₄ H ₉ FNO ₂	242.0612	-	3	25	66	-	1	56	100		
Flutolanil F ₄	C ₈ H ₄ F ₃ O	173.0209	-	-	-	-	-	-	2	6		
Flutolanil F ₅	C ₈ H ₄ NO	130.0287	-	-	-	-	-	-	-	8		
Flutolanil F ₆	C ₃ H ₅ FO ₂	93.0346	-	-	-	-	-	-	1	21		
Flutolanil	[M+Na] ⁺	346.1025	-	-	-	-	-	8	6	4		
	C ₁₇ H ₁₆ F ₃ NO ₂											

Flutriafol	C ₁₆ H ₁₃ F ₂ N ₃ O	[M+H] ⁺	302.1099	100	100	100	28	100	100	11	4
Flutriafol F ₁	C ₁₄ H ₁₁ F ₂ O		233.0772	-	6	46	24	-	8	6	-
Flutriafol F ₂	C ₇ H ₄ FO		123.0241	-	-	-	-	-	-	17	34
Flutriafol F ₃	C ₇ H ₅ F		109.0448	-	1	22	100	-	-	7	13
Flutriafol F ₄	C ₂ H ₄ N ₃		70.0400	-	-	-	-	-	76	100	100
Fomesafen	C ₁₅ H ₁₀ ClF ₃ N ₂ O ₆ S	[M+H] ⁺	438.9973	1	3	4	3	1	-	-	-
Fomesafen F ₁	C ₁₄ H ₆ ClF ₃ NO ₄		343.9932	27	51	100	100	19	66	40	15
Fomesafen F ₂	C ₁₃ H ₆ ClF ₃ NO ₂		300.0034	-	-	-	-	-	5	8	18
Fomesafen F ₃	C ₈ H ₃ ClF ₃ O ₂		222.9768	-	-	7	34	-	-	14	31
Fomesafen	C ₁₅ H ₁₀ ClF ₃ N ₂ O ₆ S	[M+NH ₄] ⁺	456.0238	100	100	24	-	100	9	-	-
Fomesafen	C ₁₅ H ₁₀ ClF ₃ N ₂ O ₆ S	[M+Na] ⁺	460.9792	-	-	-	-	21	100	100	100
Fonofos	C ₁₂ H ₆ F ₂ N ₂ O ₂	[M-H]	247.0325	100	100	100	100	100	12	-	-
Fonofos F ₁	C ₈ H ₁₂ OPS ₂		219.0062	-	-	-	-	4	6	-	-
Fonofos F ₂	C ₁₁ H ₅ N ₂ O		181.0407	-	1	7	25	-	-	-	-
Fonofos F ₃	C ₄ H ₁₀ OPS		137.0184	-	-	-	-	8	100	7	-
Fonofos F ₄	C ₉ H ₄ N		126.0349	-	-	2	16	-	-	-	-
Fonofos F ₅	C ₂ H ₆ OPS		108.9871	-	-	-	-	6	74	100	100
Foramsulfuron	C ₁₇ H ₂₀ N ₆ O ₇ S	[M+H] ⁺	453.1187	100	100	79	82	100	83	1	1
Foramsulfuron F ₁	C ₁₅ H ₁₃ N ₆ O ₅ S		408.0608	-	-	-	-	-	36	1	-
Foramsulfuron F ₂	C ₁₀ H ₁₄ N ₃ O ₄ S		272.0700	-	3	18	96	-	53	8	1
Foramsulfuron F ₃	C ₁₀ H ₁₁ N ₂ O ₄ S		255.0434	-	-	-	-	-	9	14	14
Foramsulfuron F ₄	C ₇ H ₈ N ₃ O ₃		182.0560	2	12	100	100	-	100	100	100
Foramsulfuron	C ₁₇ H ₂₀ N ₆ O ₇ S	[M+Na] ⁺	475.1006	-	-	-	-	-	9	6	4
Forchlofenuron	C ₁₂ H ₁₀ ClN ₃ O	[M+H] ⁺	248.0585	100	100	9	2	100	60	3	4
Forchlofenuron F ₁	C ₆ H ₄ ClN ₂ O		155.0007	1	11	12	12	-	26	14	12
Forchlofenuron F ₂	C ₅ H ₆ ClN ₂		129.0214	9	85	100	100	-	100	100	100
Forchlofenuron F ₃	C ₅ H ₅ N ₂		93.0447	1	8	16	62	-	-	9	79
Formetanate	C ₁₁ H ₁₅ N ₃ O ₂	[M+H] ⁺	222.1237	100	82	8	-	100	72	-	-
Formetanate F ₁	C ₉ H ₁₃ N ₂ O		165.1022	16	100	100	100	-	100	100	100
Formetanate F ₂	C ₇ H ₅ NO		120.0444	-	-	-	-	-	-	4	55
Fosetyl	C ₂ H ₇ O ₃ P	[M+H] ⁺	111.0206	26	1	-	-	100	24	-	-

Glufosinate-N-acetyl F ₁	C ₄ H ₁₁ NO ₂ P	136.0533	3	10	50	100	-	1	22	49
Glyphosate	[M-H] ⁻	168.0067	100	100	100	100	100	100	100	100
Glyphosate F ₁	C ₂ H ₇ NO ₃ P	124.0169	27	71	82	90	-	14	8	29
Griseofulvin	[M+H] ⁺	353.0786	100	100	100	100	100	100	100	85
Griseofulvin F ₁	C ₁₇ H ₁₇ ClO ₆	285.0524	-	2	7	16	-	9	44	34
Griseofulvin F ₂	C ₁₃ H ₁₄ ClO ₅	215.0119	-	2	11	31	-	9	48	66
Griseofulvin F ₃	C ₉ H ₇ ClO ₆	165.0546	1	4	19	53	-	13	70	100
Griseofulvin F ₄	C ₉ H ₉ O ₃	69.0335	-	-	-	-	-	-	47	90
Griseofulvin	C ₄ H ₅ O	375.0606	5	8	23	67	3	10	30	42
Haloxypol	[M+Na] ⁺	362.0401	100	100	100	100	100	100	28	8
Haloxypol F ₁	C ₁₅ H ₁₁ ClF ₃ NO ₄	316.0347	1	4	19	94	-	19	100	63
Haloxypol F ₂	C ₁₄ H ₁₀ ClF ₃ NO ₂	288.0398	-	-	-	-	-	-	11	39
Haloxypol F ₃	C ₁₃ H ₁₀ ClF ₃ NO	272.0073	-	1	2	21	-	-	-	18
Haloxypol F ₄	C ₁₅ H ₅ ClF ₂ N	91.00554	-	-	-	-	-	-	7	100
Hexaflumuron	C ₄ H ₇ FO	460.9894	100	100	25	3	100	18	-	-
Hexaflumuron F ₁	[M+H] ⁺	158.0412	5	35	100	100	-	100	100	100
Hexaflumuron	C ₇ H ₆ F ₂ NO	482.9708	-	-	-	-	20	10	16	11
Hexazinone	[M+Na] ⁺	253.1659	100	96	16	4	100	48	6	5
Hexazinone F ₁	C ₁₂ H ₂₀ N ₄ O ₂	171.0877	15	100	100	100	-	100	100	62
Hexazinone F ₂	C ₆ H ₁₁ N ₄ O ₂	85.0760	-	-	-	-	-	-	12	63
Hexazinone F ₃	C ₄ H ₈ N ₂	71.0604	-	2	5	21	-	-	15	100
Hexazinone	C ₃ H ₇ N ₂	275.1478	-	-	-	-	-	5	5	8
Hexythiazox	[M+Na] ⁺	353.1085	100	100	10	-	100	21	-	-
Hexythiazox F ₁	C ₁₇ H ₂₁ ClN ₂ O ₂ S	271.0303	4	30	25	3	-	39	12	-
Hexythiazox F ₂	C ₁₁ H ₁₂ ClN ₂ O ₂ S	228.0244	54	75	100	33	-	100	100	11
Hexythiazox F ₃	C ₁₀ H ₁₁ CINOS	194.0367	-	-	-	-	-	11	30	18
Hexythiazox F ₄	C ₁₀ H ₉ CINO	168.0575	-	15	51	100	-	-	98	100
Hexythiazox F ₅	C ₉ H ₁₁ CIN	151.0309	-	-	-	-	-	-	7	27
Hexythiazox F ₆	C ₉ H ₈ Cl	375.0904	-	-	-	-	14	28	33	24
Hydramethylnon	[M+Na] ⁺	495.1978	100	100	100	100	100	100	100	100
Hydramethylnon F ₁	C ₁₇ H ₂₁ ClN ₂ O ₂ S	368.0868	-	-	-	-	1	1	2	68
	C ₂₅ H ₂₄ F ₆ N ₄									

Imazamox F ₉	C ₃ H ₈ N ₃	86.0713	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	25	76
Imazamox F ₁₀	C ₅ H ₉	69.0999	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	11	88
Imazapyr	[M+H] ⁺	262.1186	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	38	-
Imazapyr F ₁	C ₁₂ H ₁₆ N ₃ O ₂	234.1237	-	4	24	69	-	-	-	-	-	-	-	-	-	-	-	-	-	4	16
Imazapyr F ₂	C ₁₀ H ₁₀ N ₃ O ₃	220.0717	-	-	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-	5	41
Imazapyr F ₃	C ₁₃ H ₁₅ N ₃ O ₃	217.0971	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3	100
Imazapyr F ₄	C ₁₀ H ₈ N ₃ O ₂	202.0611	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	38
Imazapyr F ₅	C ₅ H ₁₂ N	86.0964	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	25	100
Imazaquin	[M+H] ⁺	312.1343	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	-
Imazaquin F ₁	C ₁₆ H ₁₈ N ₃ O ₂	284.1394	-	-	6	20	-	-	-	-	-	-	-	-	-	-	-	-	-	1	15
Imazaquin F ₂	C ₁₄ H ₁₂ N ₃ O ₃	270.0873	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	41
Imazaquin F ₃	C ₁₆ H ₁₅ N ₂ O ₂	267.1128	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	82
Imazaquin F ₄	C ₁₄ H ₁₀ N ₃ O ₃	252.0768	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	31
Imazaquin F ₅	C ₁₃ H ₁₀ N ₃ O	224.0818	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2
Imazaquin F ₆	C ₁₁ H ₇ N ₂ O ₂	199.0502	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	22
Imazaquin F ₇	C ₁₁ H ₅ N ₂ O	181.0396	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	16
Imazaquin F ₈	C ₅ H ₁₂ N	86.0964	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	18
Imidacloprid	[M+H] ⁺	256.0596	100	100	36	100	3	100	100	100	100	100	100	100	100	100	100	100	100	82	17
Imidacloprid F ₁	C ₉ H ₁₀ ClN ₄	209.0589	6	27	54	63	-	-	-	-	-	-	-	-	-	-	-	-	-	27	67
Imidacloprid F ₂	C ₉ H ₁₁ N ₄	175.0978	9	46	100	100	-	-	-	-	-	-	-	-	-	-	-	-	-	24	100
Imidacloprid F ₃	C ₃ H ₆ N ₃	84.0564	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	5	24
Imidacloprid	[M+Na] ⁺	278.0415	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	32	21
Indoxacarb	[M+H] ⁺	528.0780	100	100	100	42	100	86	-	-	-	-	-	-	-	-	-	-	-	-	-
Indoxacarb F ₁	C ₁₇ H ₃ F ₃ N ₂	293.0321	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	46
Indoxacarb F ₂	C ₁₂ H ₁₀ ClN ₂ O ₂	249.0425	-	-	10	41	-	36	-	-	-	-	-	-	-	-	-	-	-	42	11
Indoxacarb F ₃	C ₁₁ H ₈ ClO ₃	223.0156	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	12
Indoxacarb F ₆	C ₉ H ₇ F ₃ NO ₂	218.0423	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	50
Indoxacarb F ₇	C ₇ H ₇ O ₇	203.0186	-	2	13	100	-	-	-	-	-	-	-	-	-	-	-	-	-	-	12
Indoxacarb F ₄	C ₁₀ H ₅ ClNO	190.0054	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	22
Indoxacarb F ₅	C ₈ H ₅ ClN	150.0105	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	50
Indoxacarb	[M+Na] ⁺	550.0599	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	17	100
	C ₂₂ H ₁₇ ClF ₃ N ₃ O ₇																				

Ivermectin F ₇	C ₄₈ H ₇₂ O ₁₄	[M+Na] ⁺	895.4818	-	-	-	-	-	74	100	100	100	100
Ivermectin	C ₄₈ H ₇₂ O ₁₄	[M+NH ₄] ⁺	892.5417	100	100	100	94	-	-	-	-	-	-
Karbutilate F ₁	C ₁₄ H ₂₁ N ₃ O ₃	[M+H] ⁺	280.1656	100	79	18	15	100	32	10	100	100	2
Karbutilate F ₂	C ₉ H ₁₃ N ₂ O ₂	C ₉ H ₁₃ N ₂ O ₂	181.0972	23	100	100	100	9	100	100	100	68	-
Karbutilate F ₃	C ₇ H ₆ NO ₂	C ₇ H ₆ NO ₂	136.0393	-	2	3	17	-	-	-	-	12	-
Karbutilate F ₃	C ₃ H ₆ NO	C ₃ H ₆ NO	72.0444	-	2	5	34	-	-	-	21	100	-
Karbutilate	C ₁₄ H ₂₁ N ₃ O ₃	[M+Na] ⁺	302.1471	4	8	12	31	-	-	-	10	17	-
Kresoxim-methyl	C ₁₈ H ₁₉ NO ₄	[M+H] ⁺	314.1387	100	19	-	-	41	-	-	-	-	-
Kresoxim-methyl F ₁	C ₁₇ H ₁₆ NO ₃	C ₁₇ H ₁₆ NO ₃	282.1125	35	100	18	4	40	20	-	-	-	-
Kresoxim-methyl F ₂	C ₁₇ H ₁₅ O ₃	C ₁₇ H ₁₅ O ₃	267.1016	23	52	7	-	100	47	-	-	-	-
Kresoxim-methyl F ₃	C ₁₆ H ₁₆ NO ₂	C ₁₆ H ₁₆ NO ₂	254.1176	5	52	36	15	-	12	5	-	-	-
Kresoxim-methyl F ₄	C ₁₆ H ₁₇ O ₂	C ₁₆ H ₁₇ O ₂	235.0754	-	-	-	-	2	78	41	12	-	-
Kresoxim-methyl F ₅	C ₁₅ H ₁₂ NO ₄	C ₁₅ H ₁₂ NO ₄	222.0917	9	85	100	100	12	100	55	24	-	-
Kresoxim-methyl F ₆	C ₁₁ H ₁₂ NO ₃	C ₁₁ H ₁₂ NO ₃	206.0812	98	47	-	-	95	23	-	-	-	-
Kresoxim-methyl F ₇	C ₁₄ H ₁₂ N	C ₁₄ H ₁₂ N	194.0964	-	-	-	-	-	3	12	21	-	-
Kresoxim-methyl F ₈	C ₆ H ₁₁ O ₃	C ₆ H ₁₁ O ₃	131.0703	-	-	-	-	3	83	100	100	-	-
Kresoxim-methyl	C ₁₈ H ₁₉ NO ₄	[M+Na] ⁺	336.1206	-	-	-	-	14	57	33	18	-	-
Lactofen	C ₁₉ H ₁₅ ClF ₃ NO ₇	[M+H] ⁺	462.0562	11	7	2	-	10	3	-	-	-	-
Lactofen F ₁	C ₁₇ H ₅ ClF ₂ NO ₃	C ₁₇ H ₅ ClF ₂ NO ₃	343.9921	29	80	100	54	30	100	100	41	-	-
Lactofen F ₂	C ₁₃ H ₆ ClF ₃ NO ₂	C ₁₃ H ₆ ClF ₃ NO ₂	300.0034	-	-	-	-	-	2	12	44	-	-
Lactofen F ₃	C ₈ H ₃ ClF ₃ O ₂	C ₈ H ₃ ClF ₃ O ₂	222.9768	-	-	-	-	-	2	11	56	-	-
Lactofen	C ₁₉ H ₁₅ ClF ₃ NO ₇	[M+NH ₄] ⁺	479.0827	100	100	14	-	100	3	-	-	-	-
Lactofen	C ₁₉ H ₁₅ ClF ₃ NO ₇	[M+Na] ⁺	484.0381	40	74	93	100	30	57	77	100	-	-
Lenacil	C ₁₃ H ₁₈ N ₂ O ₂	[M+H] ⁺	235.1441	100	23	8	-	100	23	3	2	-	-
Lenacil F ₁	C ₇ H ₉ N ₂ O ₂	C ₇ H ₉ N ₂ O ₂	153.0659	39	100	100	100	4	100	100	100	-	-
Lenacil F ₂	C ₇ H ₆ NO ₂	C ₇ H ₆ NO ₂	136.0393	-	-	-	-	-	-	2	23	-	-
Lenacil F ₃	C ₆ H ₈ NO ₂	C ₆ H ₈ NO ₂	110.0600	-	-	-	-	-	-	-	8	-	-
Lenacil F ₄	C ₅ H ₈ N	C ₅ H ₈ N	82.0651	-	-	-	-	-	-	-	8	-	-
Linuron	C ₉ H ₁₀ Cl ₂ N ₂ O ₂	[M+H] ⁺	249.0192	100	100	27	5	100	100	10	-	-	-
Linuron F ₁	C ₈ H ₇ ClN ₂ O	C ₈ H ₇ ClN ₂ O	182.0241	3	24	61	85	-	59	40	73	-	-
Linuron F ₂	C ₆ H ₅ Cl ₂ N	C ₆ H ₅ Cl ₂ N	159.9715	4	37	100	100	-	35	100	100	-	-

Mesotriione F ₁	C ₈ H ₆ NO ₅ S	227.9961	5	18	100	100	100	100	100	24	100	100	100
Mesotriione F ₂	C ₆ H ₂ NO	104.0131	-	-	-	-	-	-	-	-	-	-	19
Mesotriione	[M+N ₄ H ₄] ⁺	357.0751	-	-	-	-	-	27	3	3	-	-	-
Mesotriione	[M+Na] ⁺	362.0305	-	-	-	-	-	3	8	8	11	14	14
Metaflumizone	[M+H] ⁺	507.1250	100	100	100	100	100	100	100	100	100	100	5
Metaflumizone F ₁	C ₁₅ H ₁₂ FN ₂ O ₃	287.0791	-	-	2	16	-	1	1	42	95	95	95
Metaflumizone F ₂	C ₈ H ₈ F ₄ NO ₂	178.0486	-	-	2	12	-	1	1	59	100	100	100
Metaxyl	[M+H] ⁺	280.1543	100	100	29	22	100	16	7	2	2	2	2
Metaxyl F ₁	C ₁₄ H ₁₈ NO ₃	248.1281	5	21	8	6	6	27	3	5	5	5	5
Metaxyl F ₂	C ₁₃ H ₁₈ NO ₂	220.1332	7	61	88	85	1	100	29	11	11	11	11
Metaxyl F ₃	C ₁₂ H ₁₈ NO	192.1383	4	33	100	100	-	-	60	16	16	16	16
Metaxyl F ₄	C ₁₁ H ₁₆ N	162.1277	-	-	-	-	-	-	13	19	19	19	19
Metaxyl F ₅	C ₁₁ H ₁₄ N	160.1121	-	-	-	-	-	-	3	100	100	100	100
Metaxyl F ₆	C ₁₀ H ₁₄ N	148.1121	-	-	-	-	-	-	3	17	18	18	18
Metaxyl F ₇	C ₇ H ₁₃ O ₃	145.0859	-	-	-	-	-	-	-	-	-	-	16
Metaxyl F ₈	C ₉ H ₁₂ N	134.0964	-	-	-	-	-	-	-	-	-	-	12
Metaxyl F ₉	C ₉ H ₁₀ N	132.0808	-	-	-	-	-	-	-	-	-	-	6
Metaxyl	[M+Na] ⁺	302.1363	-	-	-	-	-	3	24	43	47	47	47
Metamitron	C ₁₅ H ₂₁ NO ₄	203.0927	100	100	100	100	34	100	100	15	5	5	5
Metamitron F ₁	C ₉ H ₁₁ N ₄	175.0978	4	24	89	68	-	9	100	27	27	27	27
Metamitron F ₂	C ₇ H ₆ N	104.0495	-	-	-	-	-	-	-	53	100	100	100
Metazachlor	[M+H] ⁺	278.1055	75	1	-	-	100	-	-	-	-	-	-
Metazachlor F ₁	C ₁₄ H ₁₆ N ₃ O	242.1288	-	-	-	-	-	2	4	9	9	9	9
Metazachlor F ₂	C ₁₁ H ₁₃ CINO	210.0680	100	38	2	-	33	96	2	-	-	-	-
Metazachlor F ₃	C ₉ H ₁₂ N	134.0964	65	100	100	100	100	1	100	100	100	100	100
Metazachlor	[M+Na] ⁺	300.0874	10	12	16	22	4	19	7	3	3	3	3
Methabenzthiazuron	[M+H] ⁺	222.0696	100	23	1	-	100	100	-	-	-	-	-
Methabenzthiazuron F ₁	C ₈ H ₉ N ₂ S	165.0481	33	100	100	100	-	10	100	100	100	100	100
Methabenzthiazuron F ₂	C ₇ H ₆ NS	150.0246	-	-	-	-	-	-	-	4	69	69	69
Methabenzthiazuron F ₃	C ₆ H ₆ NS	124.0215	-	-	-	-	-	-	-	4	31	31	31
Methabenzthiazuron F ₄	C ₆ H ₆ N	92.0495	-	-	-	-	-	-	-	-	-	-	9

Methacriphos	C ₇ H ₁₃ O ₅ PS	[M+H] ⁺	241.0294	95	8	-	-	74	1	-	-
Methacriphos F ₁	C ₆ H ₁₀ O ₄ PS	C ₆ H ₁₀ O ₄ PS	209.0032	100	100	21	40	100	100	100	36
Methacriphos F ₂	C ₂ H ₈ O ₃ PS	C ₂ H ₈ O ₃ PS	142.9926	-	2	3	-	-	-	-	-
Methacriphos F ₃	C ₂ H ₆ O ₂ PS	C ₂ H ₆ O ₂ PS	124.9821	16	48	100	100	-	13	75	100
Methamidophos	C ₂ H ₈ NO ₂ PS	[M+H] ⁺	142.0086	100	52	8	6	100	100	84	8
Methamidophos F ₁	C ₂ H ₆ O ₂ PS	C ₂ H ₆ O ₂ PS	124.9821	16	52	37	30	1	30	100	29
Methamidophos F ₂	CH ₅ NO ₂ P	CH ₅ NO ₂ P	94.0052	27	100	100	100	2	75	13	100
Methamidophos F ₃	CH ₄ O ₂ P	CH ₄ O ₂ P	78.9943	-	-	-	-	-	-	26	12
Methidathion	C ₆ H ₁₁ N ₂ O ₄ PS ₃	[M+H] ⁺	302.9691	-	-	-	-	100	1	-	-
Methidathion F ₁	C ₄ H ₅ N ₂ O ₂ S	C ₄ H ₅ N ₂ O ₂ S	145.0066	100	63	7	17	70	100	30	5
Methidathion F ₂	C ₃ H ₅ N ₂ O	C ₃ H ₅ N ₂ O	85.0396	33	100	26	42	-	35	100	100
Methidathion	C ₆ H ₁₁ N ₂ O ₄ PS ₃	[M+Na] ⁺	324.9511	32	98	100	100	8	7	5	-
Methiocarb	C ₁₁ H ₁₅ NO ₂ S	[M+H] ⁺	226.0896	100	7	-	-	100	6	1	-
Methiocarb F ₁	C ₉ H ₁₃ OS	C ₉ H ₁₃ OS	169.0682	89	100	34	3	25	100	100	100
Methiocarb F ₂	C ₈ H ₉ O	C ₈ H ₉ O	121.0648	-	-	100	100	-	-	-	-
Methiocarb sulfoxide	C ₁₁ H ₁₅ NO ₃ S	[M+H] ⁺	242.0845	100	52	17	6	100	69	26	9
Methiocarb sulfoxide F ₁	C ₉ H ₁₃ O ₂ S	C ₉ H ₁₃ O ₂ S	185.0631	31	100	100	100	5	100	100	100
Methiocarb sulfoxide F ₂	C ₈ H ₁₀ O ₂ S	C ₈ H ₁₀ O ₂ S	170.0396	3	9	32	93	-	1	21	36
Methiocarb sulfoxide	C ₁₁ H ₁₅ NO ₃ S	[M+Na] ⁺	264.0665	-	-	-	-	-	5	5	8
Methomyl	C ₅ H ₁₀ N ₂ O ₂ S	[M+H] ⁺	163.0536	-	-	-	-	83	-	-	-
Methomyl F ₁	C ₃ H ₇ NOSNa	C ₃ H ₇ NOSNa	128.0141	-	4	11	9	-	5	13	7
Methomyl F ₂	C ₃ H ₈ NOS	C ₃ H ₈ NOS	106.0321	42	30	15	8	48	75	54	30
Methomyl F ₃	C ₃ H ₆ NS	C ₃ H ₆ NS	88.0215	100	100	100	100	100	100	100	67
Methomyl F ₄	C ₂ H ₄ NO	C ₂ H ₄ NO	58.0287	-	-	-	-	-	16	85	100
Methomyl	C ₅ H ₁₀ N ₂ O ₂ S	[M+Na] ⁺	185.0355	7	18	13	30	10	8	2	-
Methoprotryne	C ₁₁ H ₂₁ N ₅ OS	[M+H] ⁺	272.1540	100	100	100	100	100	100	96	6
Methoprotryne F ₁	C ₁₀ H ₁₈ N ₅ S	C ₁₀ H ₁₈ N ₅ S	240.1277	-	1	5	18	-	6	100	12
Methoprotryne F ₂	C ₈ H ₁₄ N ₅ S	C ₈ H ₁₄ N ₅ S	212.0964	-	-	-	-	-	-	15	11
Methoprotryne F ₃	C ₇ H ₁₂ N ₅ S	C ₇ H ₁₂ N ₅ S	198.0808	-	1	3	24	-	-	94	65
Methoprotryne F ₄	C ₁₀ H ₁₈ N ₅ S	C ₁₀ H ₁₈ N ₅ S	170.0495	-	-	1	14	-	-	28	100
Methoprotryne F ₅	C ₅ H ₉ N ₄	C ₅ H ₉ N ₄	125.0822	-	-	-	-	-	-	8	31

Methoxyfenozide	$C_{22}H_{28}N_2O_3$	[M+H] ⁺	369.2173	100	13	10	23	28	10	-	-
Methoxyfenozide F ₁		$C_{18}H_{21}N_2O_3$	313.1546	68	80	10	36	100	47	23	5
Methoxyfenozide F ₂		$C_{18}H_{21}N_2O_3$	149.0597	28	100	100	100	7	100	100	100
Metobromuron	$C_9H_{11}BrN_2O_2$	[M+H] ⁺	259.0077	100	100	14	-	-	100	6	-
Metobromuron F ₁		$C_8H_8BrN_2O$	226.9815	-	5	11	23	-	-	-	-
Metobromuron F ₂		C_6H_5BrN	169.9600	7	60	100	97	-	-	100	100
Metobromuron F ₃		C_5H_4Br	142.9491	-	5	21	100	-	-	-	-
Metolachlor	$C_{15}H_{22}ClNO_2$	[M+H] ⁺	284.1412	100	92	7	-	100	12	-	-
Metolachlor F ₁		$C_{14}H_{19}ClNO$	252.1150	14	100	100	100	4	100	100	25
Metolachlor F ₂		$C_{12}H_{18}N$	176.1434	-	-	-	-	-	-	37	100
Metolachlor F ₃		$C_{11}H_{14}N$	160.1121	-	-	-	-	-	-	-	9
Metolachlor F ₄		$C_{10}H_{12}N$	146.0964	-	-	-	-	-	-	-	9
Metolachlor F ₅		$C_9H_{12}N$	134.0964	-	-	-	-	-	-	-	25
Metolachlor	$C_{15}H_{22}ClNO_2$	[M+Na] ⁺	306.1231	-	-	-	-	2	11	12	11
Metolcarb	$C_9H_{11}NO_2$	[M+H] ⁺	166.0863	32	1	-	-	100	4	-	-
Metolcarb F ₁		C_7H_9O	109.0647	100	100	100	100	34	100	100	100
Metolcarb F ₂		C_7H_7O	107.0491	-	-	-	-	-	-	2	20
Metolcarb F ₃		C_6H_9	81.0699	-	-	-	-	-	-	6	30
Metolcarb F ₄		C_6H_7	79.0542	-	-	-	-	-	-	1	11
Metolcarb	$C_9H_{11}NO_2$	[M+Na] ⁺	188.0681	2	1	-	-	1	1	-	-
Metoxuron	$C_{10}H_{13}ClN_2O_2$	[M+H] ⁺	229.0738	100	100	100	49	100	100	56	18
Metoxuron F ₁		C_3H_6NO	72.0444	1	6	37	100	-	40	100	100
Metribuzin	$C_8H_{14}N_4OS$	[M+H] ⁺	215.0961	100	100	100	29	100	100	93	100
Metribuzin F ₁		$C_7H_{15}N_4S$	187.1012	2	13	83	100	-	6	100	43
Metribuzin F ₂		$C_3H_7N_4S$	131.0386	-	-	-	-	-	-	17	35
Metsulfuron methyl	$C_{14}H_{15}N_5O_6S$	[M+H] ⁺	382.0816	100	100	29	2	100	11	-	-
Metsulfuron methyl F ₁		$C_8H_7O_6S$	199.0060	1	3	18	11	-	4	12	14
Metsulfuron methyl F ₂		$C_6H_7N_4O_2$	167.0564	5	30	100	-	3	100	100	100
Metsulfuron methyl F ₃		$C_5H_9N_4O$	141.0771	-	-	-	-	1	11	14	17
Metsulfuron methyl F ₄		$C_8H_7O_2$	135.0446	-	-	-	-	-	-	2	12
Metsulfuron methyl	$C_{14}H_{15}N_5O_6S$	[M+Na] ⁺	404.0635	-	-	-	-	7	36	16	3

Mevinphos	C ₇ H ₁₃ O ₆ P	[M+H] ⁺	225.0523	99	3	-	-	100	2	-	-
Mevinphos F ₁		C ₆ H ₁₀ O ₅ P	193.0260	68	8	-	-	88	63	2	-
Mevinphos F ₂		C ₂ H ₈ O ₄ P	127.0155	100	100	100	97	4	100	100	100
Mevinphos F ₃		C ₂ H ₆ O ₃ P	109.0049	5	6	25	100	-	-	4	37
Mevinphos F ₄		C ₅ H ₇ O ₂	99.0441	-	-	-	-	4	11	7	4
Mevinphos F ₅		C ₄ H ₃ O	67.0178	-	-	-	-	-	2	9	20
Mevinphos	C ₇ H ₁₃ O ₆ P	[M+NH ₄] ⁺	242.0788	-	-	-	-	20	-	-	-
Molinolate	C ₉ H ₁₇ NOS	[M+H] ⁺	188.1104	100	100	43	17	100	54	5	-
Molinolate F ₁		C ₇ H ₁₂ NO	126.0913	10	60	100	100	2	100	59	6
Molinolate F ₂		C ₆ H ₁₂ N	98.0964	-	-	-	-	-	9	29	10
Molinolate F ₃		C ₄ H ₇	55.0542	-	-	-	-	-	5	100	100
Monocrotophos	C ₇ H ₁₄ NO ₅ P	[M+H] ⁺	224.0682	100	15	1	-	26	9	-	-
Monocrotophos F ₁		C ₆ H ₁₀ O ₅ P	193.0260	23	13	1	-	100	100	4	-
Monocrotophos F ₂		C ₂ H ₈ O ₄ P	127.0155	28	100	100	100	-	80	100	100
Monocrotophos F ₃		C ₂ H ₆ O ₃ P	109.0049	1	5	21	86	-	-	3	32
Monocrotophos F ₄		C ₅ H ₈ NO	98.0600	17	46	17	7	-	50	32	20
Monocrotophos F ₅		C ₂ H ₄ NO	58.0287	-	-	-	-	-	5	30	76
Monocrotophos	C ₇ H ₁₄ NO ₅ P	[M+Na] ⁺	246.0502	-	-	-	-	14	4	4	6
Monolinuron	C ₉ H ₁₁ ClN ₂ O ₂	[M+H] ⁺	215.0582	100	100	9	1	100	100	-	-
Monolinuron F ₁		C ₈ H ₈ ClN ₂ O	183.0320	1	10	14	39	-	-	-	-
Monolinuron F ₂		C ₈ H ₅ ClN	126.0105	8	89	100	100	-	96	100	100
Monuron	C ₉ H ₁₁ ClON ₂	[M+H] ⁺	199.0633	100	100	71	10	100	87	9	2
Monuron F ₁		C ₇ H ₅ ClNO	154.0054	-	1	6	4	-	-	-	-
Monuron F ₂		C ₆ H ₅ ClN	126.0105	-	2	18	32	-	-	3	8
Monuron F ₃		C ₃ H ₆ NO	72.0444	2	17	100	100	-	100	100	100
Morpholin	C ₄ H ₉ NO	[M+H] ⁺	88.0757	100	100	100	100	100	24	11	5
Morpholin F ₁		C ₄ H ₈ N	70.0651	4	16	46	48	-	100	100	100
Myclobutanil	C ₁₅ H ₁₇ ClN ₄	[M+H] ⁺	289.1215	100	100	100	36	100	100	21	11
Myclobutanil F ₁		C ₇ H ₈ Cl	151.0309	-	-	-	-	-	-	3	6
Myclobutanil F ₂		C ₇ H ₆ Cl	125.0153	-	2	18	100	-	-	9	24
Myclobutanil F ₃		C ₂ H ₄ N ₃	70.0399	-	2	21	82	-	29	100	100

Naptalam	$C_{18}H_{13}NO_3$	[M+H] ⁺	292.0968	100	53	23	-	100	19	2	2
Naptalam F ₁	$C_{18}H_{14}NO_3$	$C_{18}H_{14}NO_3$	274.0863	10	37	50	70	1	9	11	8
Naptalam F ₂	$C_{18}H_{10}NO$	$C_{18}H_{10}NO$	256.0757	-	-	-	-	-	-	8	19
Naptalam F ₃	$C_8H_5O_3$	$C_8H_5O_3$	149.0233	-	-	-	-	-	26	53	70
Naptalam F ₄	$C_{10}H_{10}N$	$C_{10}H_{10}N$	144.0808	45	100	100	100	68	100	100	100
Naptalam	$C_{18}H_{13}NO_3$	[M+Na] ⁺	314.0788	-	-	-	-	5	14	7	2
Neburon	$C_{12}H_{16}Cl_2N_2O$	[M+H] ⁺	275.0715	100	100	100	100	100	100	67	30
Neburon F ₁	$C_6H_{12}NO$	$C_6H_{12}NO$	114.0913	-	1	5	10	-	15	15	10
Neburon F ₂	$C_5H_{14}N$	$C_5H_{14}N$	88.1121	-	3	16	41	-	33	93	41
Neburon	$C_{12}H_{16}Cl_2N_2O$	[M+Na] ⁺	57.0699	-	-	-	-	-	10	100	100
Nereistoxin	$C_5NH_{11}S_2$	[M+H] ⁺	150.0406	100	39	9	4	100	100	12	7
Nereistoxin F ₁	$C_3H_5S_2$	$C_3H_5S_2$	104.9827	28	100	100	100	-	73	100	75
Nereistoxin F ₂	C_2H_5S	C_2H_5S	61.0106	-	-	-	-	-	-	27	100
Nitenpyram	$C_{11}H_{15}ClN_4O_2$	[M+H] ⁺	271.0956	100	100	39	16	100	51	15	3
Nitenpyram F ₁	$C_{11}H_{16}ClN_3$	$C_{11}H_{16}ClN_3$	225.1027	-	-	-	-	3	100	13	5
Nitenpyram F ₂	$C_{11}H_{15}ClN_3$	$C_{11}H_{15}ClN_3$	224.0949	-	-	-	-	-	17	21	7
Nitenpyram F ₃	$C_{10}H_{13}ClN_3$	$C_{10}H_{13}ClN_3$	210.0793	-	-	-	-	-	5	10	1
Nitenpyram F ₄	$C_9H_{11}ClN_3$	$C_9H_{11}ClN_3$	196.0636	4	37	100	100	-	19	34	4
Nitenpyram F ₅	$C_{11}H_{16}N_5$	$C_{11}H_{16}N_5$	190.1339	-	-	-	-	-	9	13	2
Nitenpyram F ₆	$C_8H_{10}ClN_2$	$C_8H_{10}ClN_2$	169.0527	-	-	-	-	-	6	12	5
Nitenpyram F ₇	C_8H_5ClN	C_8H_5ClN	126.0105	-	-	-	-	-	-	8	7
Nitenpyram F ₈	$C_5H_{11}N_2$	$C_5H_{11}N_2$	99.0917	-	-	-	-	-	53	54	9
Nitenpyram F ₉	C_3H_6N	C_3H_6N	56.0495	-	-	-	-	-	9	100	100
N,N-Diethyl-2-naphtholoxpropamide	$C_{17}H_{21}NO_2$	[M+H] ⁺	272.1645	100	100	49	7	100	93	8	-
N,N-Diethyl-2-naphtholoxpropamide F ₁	$C_{13}H_{17}O_2$	$C_{13}H_{17}O_2$	199.0754	-	-	-	-	-	100	12	-
N,N-Diethyl-2-naphtholoxpropamide F ₂	$C_{12}H_{11}O$	$C_{12}H_{11}O$	171.0804	2	14	100	100	-	52	100	30
N,N-Diethyl-2-naphtholoxpropamide F ₃	$C_6H_{12}NO_2$	$C_6H_{12}NO_2$	114.0914	-	-	-	-	-	10	55	16
N,N-Diethyl-2-naphtholoxpropamide F ₄	$C_4H_{12}N$	$C_4H_{12}N$	74.0964	-	-	-	-	-	67	32	15
N,N-Diethyl-2-naphtholoxpropamide F ₅	$C_4H_{10}N$	$C_4H_{10}N$	72.0808	-	-	-	-	-	24	38	33
N,N-Diethyl-2-naphtholoxpropamide F ₆	C_3H_8N	C_3H_8N	58.0651	-	-	-	-	-	-	60	100
N,N-Diethyl-2-naphtholoxpropamide	$C_{17}H_{21}NO_2$	[M+Na] ⁺	294.1465	15	21	62	81	1	17	13	7

Omethoate	C ₅ H ₁₂ NO ₄ PS	[M+Na] ⁺	236.0117	-	-	-	-	-	-	-	7	24	12	9
Orbencarb	C ₁₂ H ₁₆ ClNOS	[M+H] ⁺	258.0714	100	95	5	-	100	42	-	100	42	-	-
Orbencarb F ₁	C ₇ H ₆ Cl		125.0153	11	100	100	100	100	2	70	2	70	100	100
Orbencarb F ₂	C ₅ H ₁₀ NO		100.0757	-	-	-	-	-	1	100	1	100	21	5
Orbencarb F ₃	C ₃ H ₆ NO		72.0444	-	-	-	-	-	-	11	-	11	21	14
Oryzalin	C ₁₂ H ₁₈ N ₄ O ₆ S	[M-H] ⁻	345.0874	100	100	100	100	100	100	100	100	100	100	100
Oryzalin F ₁	C ₁₀ H ₁₁ N ₄ O ₅ S		299.0456	-	-	-	-	-	-	-	-	-	20	21
Oryzalin F ₂	C ₁₂ H ₁₆ N ₃ O ₂		234.1248	-	-	-	-	-	-	-	-	-	39	18
Oryzalin F ₃	C ₉ H ₉ N ₄ O ₃		221.0680	-	-	-	-	-	-	-	-	-	8	11
Oxadiazon	C ₁₅ H ₁₈ Cl ₂ N ₂ O ₃	[M+H] ⁺	345.0757	100	100	100	57	100	100	100	100	100	31	10
Oxadiazon F ₁	C ₁₂ H ₁₃ Cl ₂ N ₂ O ₃		303.0298	-	-	-	-	-	-	58	-	58	100	26
Oxadiazon F ₂	C ₇ H ₄ Cl ₂ NO ₃		219.9563	2	6	34	100	-	3	69	-	3	69	100
Oxadiazon F ₃	C ₄ H ₇ Cl ₂ N ₂ O ₂		184.9879	-	-	-	-	-	-	-	-	-	7	64
Oxadiazon F ₄	C ₆ H ₃ Cl ₂ O ₂		176.9505	-	2	8	34	-	-	7	-	-	7	61
Oxadiazon	[M+NH ₄] ⁺		362.1033	-	-	-	-	-	60	2	-	-	-	-
Oxadiazon	[M+Na] ⁺		367.0587	-	-	-	-	-	5	16	-	24	24	24
Oxadixyl	C ₁₄ H ₁₈ N ₂ O ₄	[M+H] ⁺	279.1339	100	35	25	13	100	44	13	-	-	-	-
Oxadixyl F ₁	C ₁₂ H ₁₅ N ₂ O ₂		219.1128	36	100	100	100	8	100	100	8	100	100	38
Oxadixyl F ₂	C ₆ H ₁₃ O ₃		133.0859	-	-	-	-	-	8	69	-	8	69	88
Oxadixyl F ₃	C ₉ H ₁₀ N		132.0808	-	-	-	-	-	-	40	-	40	48	100
Oxadixyl F ₄	C ₅ H ₉ O ₃		117.0546	-	-	-	-	-	-	-	-	-	-	18
Oxadixyl F ₅	C ₄ H ₈ NO ₂		102.0550	4	13	13	16	3	42	31	3	42	31	23
Oxadixyl F ₆	C ₃ H ₆ NO ₂		88.0395	-	-	-	-	-	-	12	-	-	12	10
Oxadixyl	[M+NH ₄] ⁺		296.1605	-	-	-	-	-	-	-	10	-	-	-
Oxadixyl	[M+Na] ⁺		301.1159	-	-	-	-	-	3	78	-	47	47	44
Oxamyl	C ₇ H ₁₃ N ₃ O ₃ S	[M+H] ⁺	220.0750	-	-	-	-	-	35	-	-	-	-	-
Oxamyl F ₁	C ₃ H ₈ NO ₂		90.0550	88	53	22	-	79	28	14	-	28	14	6
Oxamyl F ₂	C ₃ H ₆ NO		72.0444	100	100	100	100	100	100	100	100	100	100	100
Oxamyl	[M+NH ₄] ⁺		237.1016	-	-	-	-	-	40	-	-	-	-	-
Oxamyl	[M+Na] ⁺		242.0570	16	30	48	78	6	-	-	-	-	-	-
Oxfendazole	C ₁₅ H ₁₃ N ₃ O ₃ S	[M+H] ⁺	316.0751	100	100	100	100	100	100	100	100	100	100	100

Oxfendazole F ₁	C ₁₄ H ₁₀ N ₃ O ₂ S	284.0488	-	1	9	24	-	6	73	29
Oxfendazole F ₂	C ₁₃ H ₇ N ₂ OS	239.0274	-	2	5	20	-	1	13	14
Oxyfluorfen	[M+H] ⁺	362.0401	100	100	76	15	100	100	11	-
Oxyfluorfen F ₁	C ₁₃ H ₈ ClF ₃ NO ₄	334.9983	-	-	-	-	-	15	-	-
Oxyfluorfen F ₂	C ₁₅ H ₃ F ₃ NO ₄	318.0009	-	-	-	-	-	22	11	-
Oxyfluorfen F ₃	C ₁₃ H ₆ ClF ₃ NO ₃	315.9983	-	15	100	100	-	46	55	11
Oxyfluorfen F ₄	C ₁₃ H ₅ ClNO ₄	273.9902	-	-	-	-	-	6	59	18
Oxyfluorfen F ₅	C ₉ H ₈ F ₃ O ₄	237.0369	-	-	-	-	2	2	100	100
Paclobutrazol	[M+H] ⁺	294.1368	100	100	100	48	100	100	8	3
Paclobutrazol F ₁	C ₇ H ₆ Cl	125.0153	-	-	6	21	-	-	-	6
Paclobutrazol F ₂	C ₂ H ₄ N ₃	70.0400	-	4	37	100	-	47	100	100
Paraoxon methyl	[M+H] ⁺	248.0319	100	100	100	42	100	100	100	52
Paraoxon methyl F ₁	C ₁₂ H ₇ O ₅	231.0288	-	-	-	-	-	-	12	18
Paraoxon methyl F ₂	C ₈ H ₁₁ O ₄ P	202.0389	1	6	43	100	-	-	38	100
Paraoxon methyl F ₃	C ₂ H ₆ O ₃ P	109.0049	1	2	9	42	-	-	15	65
Paraoxon methyl F ₄	C ₇ H ₇ O	107.0491	-	-	-	-	-	-	10	30
Paraoxon methyl F ₅	C ₄ H ₃ NP	95.9998	-	-	-	-	-	-	3	20
Paraoxon methyl F ₆	C ₃ H ₉ NP	90.0467	-	-	-	-	-	-	12	80
Paraoxon methyl	[M+Na] ⁺	270.0138	-	-	-	-	4	4	10	22
Parathion	[M+H] ⁺	292.0403	100	25	-	-	100	7	-	-
Parathion F ₁	C ₈ H ₁₁ NO ₅ PS	264.0090	18	30	4	-	8	23	-	-
Parathion F ₂	C ₆ H ₇ NO ₅ PS	235.9777	22	100	100	100	-	100	100	18
Parathion F ₃	C ₆ H ₅ NO ₄ PS	217.9599	-	-	-	-	-	-	16	17
Parathion F ₄	C ₆ H ₇ NPS	156.0031	-	-	-	-	-	-	21	41
Parathion F ₅	C ₆ H ₆ NO ₃	140.0338	-	-	-	-	-	-	30	78
Parathion F ₆	C ₂ H ₉ NPS	110.0188	-	-	-	-	-	-	9	93
Parathion F ₇	C ₂ H ₉ NOP	94.0416	-	-	-	-	-	1	6	100
Parathion-methyl	[M+H] ⁺	264.0090	100	100	85	30	100	100	13	-
Parathion-methyl F ₁	C ₇ H ₇ NO ₄ PS	231.9828	3	23	100	100	-	20	72	18
Parathion-methyl F ₂	C ₂ H ₆ O ₂ PS	124.9821	-	-	-	-	-	19	100	100
Parathion-methyl F ₃	C ₂ H ₆ O ₃ P	109.0053	-	-	-	-	-	11	42	55

Pebulate	$C_{10}H_{21}NOS$	$[M+H]^+$	204.1417	100	100	100	100	100	100	100	100	100	100	15	8
Pebulate F ₁		$C_3H_{22}NS$	176.1467	-	2	8	-	-	-	8	-	-	8	11	-
Pebulate F ₂		$C_7H_{16}NOS$	162.0947	-	8	86	79	-	-	-	-	-	-	28	13
Pebulate F ₃		$C_7H_{14}NO$	128.1070	3	12	19	-	1	94	100	100	100	100	100	100
Pebulate F ₄		C_3H_8NOS	106.0321	-	1	26	100	-	-	-	-	-	-	10	40
Penconazole	$C_{13}H_{15}Cl_2N_3$	$[M+H]^+$	284.0716	100	100	78	5	100	98	7	3				
Penconazole F ₁		$C_8H_7Cl_2$	172.9919	-	1	11	8	-	4	6	5				
Penconazole F ₂		$C_7H_5Cl_2$	158.9763	2	10	100	100	-	5	22	38				
Penconazole F ₃		$C_2H_4N_3$	70.0400	-	-	-	-	-	100	100	100				
Pencycuron	$C_{19}H_{21}ClN_2O$	$[M+H]^+$	329.1415	100	100	100	31	100	100	11	3				
Pencycuron F ₁		$C_{13}H_{13}ClN$	218.0731	-	-	-	-	-	10	6	-				
Pencycuron F ₂		C_7H_6Cl	125.0153	1	7	44	100	-	17	100	100				
Pencycuron	$C_{19}H_{21}ClN_2O$	$[M+Na]^+$	351.1235	-	-	-	-	-	6	7	5				
Pendimethalin	$C_{13}H_{19}N_3O_4$	$[M+H]^+$	282.1448	70	2	-	-	100	-	-	-				
Pendimethalin F ₁		$C_8H_{10}N_3O_4$	212.0666	100	100	100	42	66	100	100	-				
Pendimethalin F ₂		$C_8H_8N_3O_3$	194.0560	6	14	74	100	-	8	85	51				
Pendimethalin F ₃		$C_5H_{10}NO_4$	148.0604	-	-	-	-	-	-	15	100				
Phenmedipham	$C_{16}H_{16}N_2O_4$	$[M+H]^+$	301.1183	100	29	4	-	-	-	-	-				
Phenmedipham F ₁		$C_8H_{10}NO_3$	168.0655	61	100	80	18	100	18	-	-				
Phenmedipham F ₂		$C_7H_6NO_2$	136.0393	30	35	100	100	15	100	100	32				
Phenmedipham F ₃		C_6H_6NO	108.0444	-	-	-	-	-	6	56	64				
Phenmedipham F ₄		C_6H_5O	93.0335	-	-	-	-	-	-	44	100				
Phenmedipham	$C_{16}H_{16}N_2O_4$	$[M+Na]^+$	323.1002	12	26	60	84	-	-	-	-				
Phenothrin	$C_{23}H_{26}O_3$	$[M+H]^+$	351.1955	100	100	41	10	100	20	4	-				
Phenothrin F ₁		$C_{23}H_{25}O_2$	333.1849	-	-	-	-	57	34	10	-				
Phenothrin F ₂		$C_{22}H_{25}O$	305.1900	-	-	-	-	13	35	18	-				
Phenothrin F ₃		$C_{19}H_{19}O$	263.1430	-	-	-	-	-	7	14	3				
Phenothrin F ₄		$C_{18}H_{17}O$	249.1274	-	-	-	-	-	31	54	18				
Phenothrin F ₅		$C_{17}H_{17}O$	237.1274	-	-	-	-	40	100	95	19				
Phenothrin F ₆		$C_{17}H_{15}O$	235.1117	-	-	-	-	-	11	21	9				
Phenothrin F ₇		$C_{14}H_{13}O$	197.0961	-	-	-	-	-	7	18	5				

Phenothrin F ₈	C ₁₃ H ₁₀ O	183.0804	11	46	100	100	100	14	55	100	100	100
Phenothrin F ₉	C ₁₃ H ₉ O	181.0648	-	-	-	-	-	-	-	-	3	9
Phenothrin	[M+Na] ⁺	373.1774	-	-	-	-	-	18	43	57	30	30
	C ₂₃ H ₂₆ O ₃											
Pentoate	[M+H] ⁺	321.0379	100	22	1	-	100	2	-	-	-	-
Pentoate F ₁	C ₉ H ₁₂ O ₂ PS ₂	247.0011	-	-	-	-	34	100	22	-	-	-
Pentoate F ₂	C ₁₀ H ₁₁ O ₂	163.0754	34	100	16	5	9	34	-	-	-	-
Pentoate F ₃	C ₈ H ₇ O ₂	135.0441	-	-	-	-	-	20	100	59	-	-
Pentoate F ₄	C ₇ H ₇ O	107.0491	10	60	100	100	-	6	69	100	-	-
	C ₁₂ H ₁₅ ClNO ₄ PS ₂											
Phosalone	[M+H] ⁺	367.9941	100	41	2	-	100	20	-	-	-	-
Phosalone F ₁	C ₁₁ H ₁₄ ClNO ₄ PS	322.0064	1	2	2	-	3	29	-	-	-	-
Phosalone F ₂	C ₈ H ₅ ClNO ₂	182.0003	4	100	100	26	5	100	100	100	100	100
Phosalone F ₃	C ₈ H ₆ ClO	153.0102	-	-	-	-	-	7	5	-	-	-
Phosalone F ₄	C ₇ H ₅ NCI	138.0105	6	16	47	52	-	-	4	31	-	-
Phosalone F ₅	C ₆ H ₄ Cl	110.9996	-	-	-	-	-	-	3	32	-	-
Phosalone	[M+Na] ⁺	389.9761	60	74	99	100	25	42	21	18	-	-
	C ₁₂ H ₁₅ ClNO ₄ PS ₂											
Phosmet F ₁	C ₉ H ₆ NO ₂	160.0393	100	100	100	100	100	100	100	100	100	100
Phosmet F ₂	C ₈ H ₅ O ₂	133.0284	-	-	-	-	-	3	12	71	-	-
	C ₁₀ H ₁₉ ClNO ₅ P											
Phosphamidon	[M+H] ⁺	300.0762	100	100	100	12	100	100	8	-	-	-
Phosphamidon F ₁	C ₆ H ₉ ClO ₅ P	226.9871	-	-	-	-	-	-	23	-	-	-
Phosphamidon F ₂	C ₇ H ₁₃ NO ₂ P	174.0678	-	-	-	-	-	-	40	7	-	-
Phosphamidon F ₃	C ₂ H ₈ O ₄ P	127.0154	7	19	97	100	-	6	100	100	-	-
Phosphamidon F ₄	C ₅ H ₁₀ NO	100.0757	-	-	-	-	-	-	27	26	-	-
Phosphamidon	[M+NH ₄] ⁺	317.1028	-	-	-	-	-	22	-	-	-	-
	C ₁₀ H ₁₉ ClNO ₅ P											
Phosphonic acid	[M-H] ⁻	80.9747	100	100	-	-	100	100	-	-	-	-
	H ₃ O ₃ P											
Picloram	[M+H] ⁺	240.9333	100	59	5	-	100	27	-	-	-	-
Picloram F ₁	C ₆ H ₃ Cl ₃ N ₂ O ₂	222.9227	-	-	-	-	-	100	23	-	-	-
Picloram F ₂	C ₅ H ₂ Cl ₃ N ₂	194.9278	11	100	100	100	-	-	100	100	-	-
Picloram F ₃	C ₄ HCl ₃ N	167.9169	1	12	25	77	-	-	-	-	80	-
	C ₁₉ H ₁₂ F ₄ N ₂ O ₂											
Picolinafen	[M+H] ⁺	377.0908	100	100	100	100	100	100	-	-	-	-
Picolinafen F ₁	C ₁₉ H ₁₁ F ₄ N ₂ O	359.0802	-	-	-	-	-	-	9	25	-	-
Picolinafen F ₂	C ₁₂ H ₇ F ₃ NO	238.0474	-	6	52	95	-	-	100	100	-	-

Pretilachlor F ₂	C ₁₂ H ₁₈ N	176.1434	-	1	4	14	-	-	11	100
Pretilachlor F ₃	C ₁₁ H ₁₄ N	160.1121	-	-	-	-	-	-	1	10
Pretilachlor F ₄	C ₁₀ H ₁₄ N	148.1121	-	-	-	-	-	-	-	15
Pretilachlor F ₅	C ₈ H ₈ N	118.0651	-	-	-	-	-	-	1	16
Pretilachlor	[M+Na] ⁺	334.1544	-	-	-	-	3	16	15	26
Prochloraz	[M+H] ⁺	376.0381	100	14	3	8	100	9	-	-
Prochloraz F ₁	C ₁₂ H ₁₃ Cl ₃ NO ₂	308.0006	39	100	100	100	-	100	51	14
Prochloraz F ₂	C ₁₁ H ₁₃ Cl ₃ NO	280.0057	-	-	-	-	-	-	7	-
Prochloraz F ₃	C ₉ H ₇ Cl ₃ NO ₂	265.9536	-	-	-	-	-	14	18	3
Prochloraz F ₄	C ₁₁ H ₁₂ Cl ₂ NO	244.0288	-	-	-	-	-	-	10	-
Prochloraz F ₅	C ₈ H ₆ Cl ₂ NO	201.9821	-	-	-	-	-	-	9	4
Prochloraz F ₆	C ₄ H ₈ N	70.0651	-	-	-	-	-	-	37	76
Prochloraz F ₇	C ₃ H ₄ NO	70.0287	-	-	-	-	-	6	100	100
Procyimidone	[M+H] ⁺	284.0240	100	100	100	100	100	100	100	-
Procyimidone F ₁	C ₁₂ H ₁₇ Cl ₂ NO	256.0290	-	4	20	76	-	5	86	-
Profenofos	[M+H] ⁺	372.9424	100	100	38	9	100	100	9	-
Profenofos F ₁	C ₉ H ₁₂ BrClO ₃ PS	344.9111	-	-	-	-	-	59	15	6
Profenofos F ₂	C ₆ H ₆ BrClO ₃ PS	302.8642	3	22	100	100	-	37	100	100
Profenofos F ₃	C ₆ H ₄ BrClO ₂ PS	284.8533	-	-	-	-	-	-	5	26
Profenofos F ₄	C ₆ H ₄ BrClO ₃ P	268.8764	-	-	3	8	-	-	4	18
Profenofos F ₅	CH ₂ ClOS	96.9509	-	-	-	-	-	-	4	63
Profenofos	[M+Na] ⁺	394.9244	-	-	-	-	-	17	10	12
Prohexadione	[M+H] ⁻	211.0612	100	100	67	40	100	100	100	100
Prohexadione F ₁	C ₉ H ₁₁ O ₃	167.0764	12	43	100	100	1	17	39	70
Prohexadione F ₂	C ₈ H ₁₁ O	123.0815	5	23	47	41	-	21	31	77
Promecarb	[M+H] ⁺	208.1332	100	14	-	-	100	8	-	-
Promecarb F ₁	C ₁₁ H ₁₆ NO ₂	194.1176	2	-	-	-	-	-	-	-
Promecarb F ₂	C ₁₀ H ₁₅ O	151.1117	57	100	100	-	25	100	9	2
Promecarb F ₃	C ₇ H ₈ O	109.0648	-	-	-	-	-	68	100	100
Prometon	[M+H] ⁺	226.1662	100	100	100	66	100	100	45	2
Prometon F ₁	C ₇ H ₁₄ N ₂ O	184.1193	1	5	29	73	-	9	94	14

Prometon F ₂	C ₄ H ₈ N ₅ O	142.0723	-	2	16	100	-	-	100	100	100	100
Prometon F ₃	C ₃ H ₆ N ₃ O	100.0510	-	-	-	-	-	-	-	-	7	31
Prometon F ₄	C ₂ H ₄ N ₃ O	86.0356	-	-	-	-	-	-	-	-	11	66
Prometon F ₅	C ₂ H ₇ N ₃ O	75.0561	-	-	-	-	-	-	-	-	2	8
Prometon F ₆	C ₂ H ₅ N ₂	57.0458	-	-	-	-	-	-	-	-	2	22
Prometryn	[M+H] ⁺	242.1434	100	100	100	100	100	100	100	100	45	2
Prometryn F ₁	C ₇ H ₁₄ N ₅ O	200.0964	-	4	23	88	-	8	75	9		
Prometryn F ₂	C ₄ H ₈ N ₅ O	158.0495	-	1	11	96	-	-	100	100		
Prometryn F ₃	C ₃ H ₆ N ₃ S	116.0272	-	-	-	-	-	-	5	16		
Prometryn F ₄	C ₂ H ₅ N ₄	85.0509	-	-	-	-	-	-	-	17		
Propachlor	[M+H] ⁺	212.0837	100	56	6	1	100	56	6	2		
Propachlor F ₁	C ₈ H ₆ ClNO	170.0367	20	100	100	100	-	100	100	22		
Propachlor F ₂	C ₈ H ₇ ClN	152.0262	-	-	-	-	-	2	11	9		
Propachlor F ₃	C ₇ H ₈ N	106.0651	-	-	-	-	-	-	32	54		
Propachlor F ₄	C ₆ H ₈ N	94.0651	-	-	-	-	-	-	41	100		
Propamocarb	[M+H] ⁺	189.1598	100	100	31	10	100	100	1	-		
Propamocarb F ₁	C ₇ H ₁₄ NO ₂	144.1019	-	-	-	-	-	48	2	-		
Propamocarb F ₂	C ₉ H ₈ NO ₂	102.0550	4	41	100	100	-	90	100	52		
Propamocarb F ₃	C ₂ H ₄ NO ₂	74.0237	-	-	-	-	-	-	32	100		
Propamocarb F ₄	C ₃ H ₈ N	58.0651	-	-	-	-	-	-	8	25		
Propanil	[M+H] ⁺	218.0134	100	100	52	12	100	100	31	-		
Propanil F ₁	C ₈ H ₇ Cl ₂ O	188.9868	-	-	-	-	8	9	10	2		
Propanil F ₂	C ₆ H ₆ Cl ₂ N	161.9872	4	28	100	100	-	22	100	28		
Propanil F ₃	C ₉ H ₃ O	127.0178	-	-	-	-	-	-	47	100		
Propanil F ₄	C ₃ H ₅ O	57.0335	-	-	-	-	-	-	31	30		
Propaquizafop	[M+H] ⁺	444.1321	100	100	100	39	100	100	5	4		
Propaquizafop F ₁	C ₁₉ H ₁₆ ClN ₂ O ₄	371.0793	-	1	8	23	-	28	12	2		
Propaquizafop F ₂	C ₁₇ H ₁₂ ClN ₂ O ₃	327.0501	-	-	-	-	-	1	11	10		
Propaquizafop F ₃	C ₁₆ H ₁₂ ClN ₂ O ₂	299.0582	-	3	22	100	-	3	19	20		
Propaquizafop F ₄	C ₅ H ₁₀ NO	100.0757	-	2	13	43	-	81	100	100		
Propaquizafop	[M+Na] ⁺	466.1140	-	-	-	-	4	13	7	10		

Propisochlor F ₂	C ₁₁ H ₁₅ CINO	212.0837	12	24	36	20	-	12	6	-
Propisochlor F ₃	C ₁₀ H ₁₄ N	148.1121	62	100	100	100	5	100	100	53
Propisochlor F ₄	C ₉ H ₁₁ N	133.0884	-	-	-	-	-	-	32	100
Propisochlor	[M+Na] ⁺	306.1231	-	-	-	-	6	25	18	12
Propoxur	[M+H] ⁺	210.1125	23	8	-	-	71	1	1	-
Propoxur F ₁	C ₈ H ₁₀ NO ₃	168.0655	100	100	22	-	100	14	-	-
Propoxur F ₂	C ₉ H ₁₃ O ₂	153.0910	-	-	-	-	36	3	-	-
Propoxur F ₃	C ₆ H ₇ O ₂	111.0439	-	-	-	-	11	100	100	28
Propoxur F ₄	C ₆ H ₅ O	93.0332	-	-	-	-	-	3	66	100
Propoxur F ₅	C ₂ H ₄ NO	58.0287	-	-	-	-	-	-	10	19
Propoxur	[M+Na] ⁺	232.0944	5	41	100	100	3	3	3	2
Propylene thiourea (PTU)	[M+H] ⁺	117.0481	100	100	100	100	100	100	100	100
Propylene thiourea (PTU) F ₁	C ₄ H ₆ NS	100.0215	2	9	22	24	-	5	10	-
Propylene thiourea (PTU) F ₂	C ₃ H ₂ NS	71.9902	-	-	-	-	-	-	6	22
Propylene thiourea (PTU) F ₃	CH ₂ NS	59.9902	-	-	-	-	-	-	10	52
Propylene thiourea (PTU) F ₄	C ₃ H ₈ N	58.0651	-	-	-	-	-	41	80	63
Propyzamid	[M+H] ⁺	256.0290	100	50	9	5	100	40	2	-
Propyzamid F ₁	C ₇ H ₆ Cl ₂ NO	189.9821	23	100	100	100	16	100	100	18
Propyzamid F ₂	C ₇ H ₃ Cl ₂ O	172.9555	-	-	-	-	-	14	80	100
Propyzamid F ₃	C ₈ H ₅ Cl ₂	146.9763	-	-	-	-	-	-	8	-
Propyzamid F ₄	C ₆ H ₃ Cl ₂	144.9601	-	-	-	-	-	-	4	45
Propyzamid F ₅	C ₅ H ₇	67.0542	-	-	-	-	-	-	40	48
Proquinazid	[M+H] ⁺	373.0407	100	66	5	-	100	15	2	1
Proquinazid F ₁	C ₁₁ H ₁₂ IN ₂ O ₂	330.9938	16	100	100	32	5	100	85	11
Proquinazid F ₂	C ₈ H ₆ IN ₂ O ₂	288.9468	1	11	46	100	-	3	100	100
Proquinazid F ₃	C ₈ H ₃ INO ₂	271.9203	-	-	-	-	-	-	2	50
Prosulfocarb	[M+H] ⁺	252.1417	100	100	8	-	100	65	-	-
Prosulfocarb F ₁	C ₇ H ₁₄ NO	128.1070	-	-	-	-	-	64	2	-
Prosulfocarb F ₂	C ₇ H ₇	91.0542	6	61	100	100	-	100	100	100
Prosulfocarb F ₃	C ₄ H ₈ NO	86.0600	-	-	-	-	-	20	3	-
Prosulfuron	[M+H] ⁺	420.0948	100	100	100	17	100	100	3	2

Pyrazophos F ₆	C ₈ H ₈ N ₃ O ₃	194.0560	-	-	-	-	-	-	-	9	100
Pyridaben	[M+H] ⁺	365.1449	100	62	6	-	100	4	-	-	-
Pyridaben F ₁	C ₁₅ H ₁₈ ClN ₂ O ₅	309.0823	19	100	100	15	19	100	22	-	-
Pyridaben F ₂	C ₁₁ H ₁₅	147.1168	3	18	76	100	-	10	100	100	100
Pyridaben	[M+Na] ⁺	387.1268	-	-	-	-	-	5	5	-	-
Pyridaphenthion	[M+H] ⁺	341.0719	100	100	100	57	100	100	57	36	36
Pyridaphenthion F ₁	C ₁₂ H ₁₄ N ₂ O ₄ PS	313.0406	-	-	-	-	-	7	5	4	4
Pyridaphenthion F ₂	C ₁₀ H ₉ N ₂ O ₅	205.0430	-	-	-	-	-	-	51	37	37
Pyridaphenthion F ₃	C ₁₀ H ₉ N ₂ O ₂	189.0659	1	5	32	100	-	11	100	100	100
Pyridaphenthion F ₄	C ₆ H ₆ N	92.0495	-	-	-	-	-	-	-	19	19
Pyridaphenthion	[M+Na] ⁺	363.0539	-	-	-	-	-	8	13	10	10
Pyrifenox	[M+H] ⁺	295.0399	100	100	46	5	100	100	8	2	2
Pyrifenox F ₁	C ₁₃ H ₉ Cl ₂ N ₂	263.0137	-	-	1	1	-	-	-	-	-
Pyrifenox F ₂	C ₆ H ₆ N	93.0573	3	18	100	100	-	41	100	100	100
Pyrimethanil	[M+H] ⁺	200.1182	100	100	100	100	100	100	100	95	95
Pyrimethanil F ₁	C ₁₂ H ₁₁ N ₂	183.0917	-	-	5	20	-	-	23	58	58
Pyrimethanil F ₂	C ₆ H ₇ N ₂	107.0604	-	-	2	7	-	-	41	91	91
Pyrimethanil F ₃	C ₆ H ₇ N	82.0648	-	-	-	-	-	-	26	79	79
Pyriproxifen	[M+H] ⁺	322.1438	100	100	10	-	100	100	-	-	-
Pyriproxifen F ₁	C ₁₅ H ₁₅ O ₂	227.1067	2	25	36	11	-	24	6	11	11
Pyriproxifen F ₂	C ₁₂ H ₉ O ₂	185.0597	1	5	20	40	-	-	25	21	21
Pyriproxifen F ₃	C ₅ H ₆ NO	96.0440	4	53	100	100	-	100	100	100	100
Pyriproxifen F ₄	C ₅ H ₄ N	78.0338	1	5	14	59	-	-	-	5	5
Pyroquilon	[M+H] ⁺	174.0913	100	100	100	100	100	100	100	100	100
Pyroquilon F ₁	C ₉ H ₁₀ N	132.0808	1	2	9	38	-	-	33	100	100
Pyroquilon F ₂	C ₈ H ₇ N	117.0573	-	-	-	-	-	-	-	61	61
Quinalphos	[M+H] ⁺	299.0614	100	100	89	7	100	100	12	-	-
Quinalphos F ₁	C ₁₀ H ₁₂ N ₂ O ₃ PS	271.0301	-	-	-	-	-	22	-	-	-
Quinalphos F ₂	C ₈ H ₈ N ₂ O ₃ PS	242.9988	-	-	-	-	-	16	24	-	-
Quinalphos F ₃	C ₈ H ₇ N ₂ S	163.0320	-	-	-	-	-	16	95	79	79
Quinalphos F ₄	C ₈ H ₇ N ₂ O	147.0558	-	11	100	100	-	19	100	100	100

Secbumeton F ₁	C ₆ H ₁₂ N ₅ O	170.1036	2	8	43	100	-	13	100	100
Secbumeton F ₂	C ₄ H ₈ N ₅ O	142.0725	-	-	2	11	-	-	9	52
Secbumeton F ₃	C ₅ H ₁₀ N ₃ O	128.0818	-	-	-	-	-	-	3	25
Secbumeton F ₄	C ₄ H ₈ N ₃ O	114.0662	-	-	-	-	-	-	11	61
Secbumeton F ₅	C ₃ H ₆ N ₃ O	100.0505	-	1	4	20	-	-	8	96
Secbumeton F ₆	C ₄ H ₆ N ₃	96.0556	-	-	-	-	-	-	6	44
Secbumeton F ₇	C ₂ H ₄ N ₃ O	86.0349	-	-	-	-	-	-	4	51
Secbumeton F ₈	C ₂ H ₇ N ₂ O	75.0553	-	-	-	-	-	-	3	56
Secbumeton F ₉	C ₂ H ₅ N ₂	57.0447	-	-	-	-	-	-	-	48
Sethoxydim	C ₁₇ H ₂₉ NO ₃ S	328.1941	100	100	100	14	100	63	2	-
Sethoxydim F ₁	C ₁₅ H ₂₄ NO ₂ S	282.1522	5	17	78	27	2	100	5	-
Sethoxydim F ₂	C ₁₃ H ₁₈ NO ₂	220.1332	1	3	28	31	-	55	17	-
Sethoxydim F ₃	C ₁₀ H ₁₄ NO ₂	180.1019	-	-	-	-	-	18	43	88
Sethoxydim F ₄	C ₁₀ H ₁₂ NO ₂	178.0863	1	3	46	100	-	50	100	100
Siduron	[M+H] ⁺	233.1648	100	100	100	100	100	100	100	100
Siduron F ₁	C ₇ H ₉ N ₂ O	137.0709	2	10	38	59	-	10	40	37
Siduron F ₂	C ₆ H ₈ N	94.0651	2	5	22	78	-	7	43	95
Simazine	[M+H] ⁺	202.0854	100	100	100	83	100	100	90	6
Simazine F ₁	C ₄ H ₇ ClN ₃	132.0323	1	3	13	36	-	-	79	100
Simazine F ₂	C ₆ H ₁₀ N ₃	124.0869	-	-	-	-	-	7	100	7
Simazine F ₃	C ₂ H ₃ ClN ₃	105.0088	-	2	14	100	-	-	-	-
Spinosyn A	[M+H] ⁺	732.4681	100	100	100	100	100	100	74	4
Spinosyn A F ₁	C ₃₂ H ₅₀ NO ₆	544.3633	3	2	2	2	2	-	-	-
Spinosyn A F ₂	C ₈ H ₁₆ NO	142.1226	-	-	-	-	-	17	100	100
Spinosyn D	[M+H] ⁺	746.4838	100	100	100	100	100	100	100	100
Spinosyn D F ₁	C ₃₃ H ₅₂ NO ₆	558.3789	3	2	2	2	14	12	6	-
Spiromesifen	[M+H] ⁺	371.2217	18	6	1	4	25	3	1	-
Spiromesifen F ₁	C ₁₉ H ₁₉ O ₃	295.1329	-	-	-	-	-	-	7	46
Spiromesifen F ₂	C ₁₇ H ₂₁ O ₃	273.1485	100	100	100	100	100	100	100	100
Spiromesifen F ₃	C ₁₇ H ₁₉ O ₂	255.1380	2	6	16	39	-	13	32	86
Spiromesifen F ₄	C ₁₆ H ₁₉ O ₂	227.1430	-	-	-	-	-	-	8	23

Spiromesifen F ₅	C ₁₂ H ₁₁ O ₂	187.0754	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4	9	16	54
Spiromesifen F ₆	C ₁₁ H ₁₃ O	161.0961	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6	30
Spiromesifen F ₇	C ₅ H ₇	67.0542	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6	45
Spiromesifen F ₈	[M+Na] ⁺	393.2036	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4	9	16	33
Spirotetramat	C ₂₃ H ₃₀ O ₄	374.1962	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	70	30
Spirotetramat F ₁	[M+H] ⁺	330.2064	3	19	56	59	-	60	55	40													
Spirotetramat F ₂	C ₂₀ H ₂₈ NO ₃	302.1751	3	15	58	72	-	49	100	50													
Spirotetramat F ₃	C ₁₈ H ₂₄ NO ₃	216.1019	-	1	3	15	-	-	10	100													
Spirotetramat	C ₁₃ H ₁₄ NO ₂	396.1781	-	-	-	-	-	-	-	28													
Spiroxamine	[M+Na] ⁺	298.2741	100	100	100	100	42	100	100	12	2												
Spiroxamine F ₁	[M+H] ⁺	144.1383	2	18	55	100	-	24	100	100													
Spiroxamine F ₂	C ₈ H ₁₈ NO	100.1121	-	4	15	49	-	-	15	78													
Spiroxamine F ₃	C ₆ H ₁₄ N	72.0808	-	-	-	-	-	-	-	9													
Sulcotrione	C ₄ H ₁₀ N	329.0245	100	100	100	89	100	100	100	41	17												
Sulcotrione F ₁	[M+H] ⁺	293.0478	-	-	-	-	-	-	-	8	9												
Sulcotrione F ₂	C ₁₄ H ₁₃ O ₅ S	139.0390	2	4	25	100	-	12	100	100													
Sulcotrione F ₃	C ₇ H ₇ O ₃	111.0441	-	1	6	38	-	-	8	53													
Sulcotrione	C ₆ H ₇ O ₂	346.0510	-	-	-	-	-	-	38	1	-												
Sulcotrione	[M+MN ₄] ⁺	351.0064	-	-	-	-	-	-	-	7	10												
Sulcotrione	[M+Na] ⁺	301.0754	100	100	100	43	100	100	100	23	15												
Sulfaquinoxaline	[M+H] ⁺	156.0114	2	13	70	26	-	61	100	14													
Sulfaquinoxaline F ₁	C ₆ H ₆ NO ₂ S	146.0713	-	-	-	-	-	-	5	20	18												
Sulfaquinoxaline F ₂	C ₈ H ₈ N ₃	108.0444	-	4	46	94	-	2	73	85													
Sulfaquinoxaline F ₃	C ₆ H ₆ NO	92.0495	-	4	41	100	-	-	51	100													
Sulfaquinoxaline F ₄	C ₆ H ₆ N	323.0573	-	-	-	-	-	-	15	26	15												
Sulfaquinoxaline	[M+Na] ⁺	365.0914	100	100	37	3	100	21	1	-													
Sulfometuron methyl	[M+H] ⁺	263.9927	-	-	-	-	-	-	-	6													
Sulfometuron methyl F ₁	C ₁₄ H ₂ NO ₅	199.0060	-	3	9	6	-	-	7														
Sulfometuron methyl F ₂	C ₈ H ₇ O ₄ S	150.0662	4	23	100	100	1	100	100	100													
Sulfometuron methyl F ₃	C ₇ H ₈ N ₃ O	146.0713	-	-	-	-	-	-	-	27													
Sulfometuron methyl F ₄	C ₈ H ₈ N ₃	107.0604	-	2	6	14	-	-	-	10													
Sulfometuron methyl F ₅	C ₆ H ₇ N ₂		-	-	-	-	-	-	-	-													

Sulfometuron methyl	C ₁₅ H ₁₆ N ₄ O ₅ S	[M+Na] ⁺	387.0734	6	8	21	35	7	34	18	5
Sulfotep	C ₈ H ₂₀ O ₅ P ₂ S ₂	[M+H] ⁺	323.0300	100	100	22	9	100	15	-	-
Sulfotep F ₁	C ₆ H ₁₇ O ₅ P ₂ S ₂		294.9992	7	46	30	10	-	24	-	-
Sulfotep F ₂	C ₆ H ₁₇ O ₅ P ₂ S ₂		171.0239	3	36	100	100	-	100	45	-
Sulfotep F ₃	C ₂ H ₈ O ₃ PS		142.9926	-	-	-	-	-	22	100	20
Sulfotep F ₄	C ₇ H ₇ O ₂		123.0441	-	-	-	-	-	-	18	13
Sulfotep F ₅	H ₄ O ₃ PS		114.9613	-	-	-	-	-	-	64	81
Sulfotep F ₆	H ₂ O ₂ PS		96.9508	-	-	-	-	-	4	99	100
Sulprofos	C ₁₂ H ₁₉ O ₂ PS ₃	[M+H] ⁺	323.0358	100	100	-	-	100	30	5	-
Sulprofos F ₁	C ₇ H ₈ O ₂ PS ₂		218.9698	-	30	100	38	-	100	100	17
Sulprofos F ₂	C ₇ H ₇ OS		139.0212	-	-	70	100	-	-	43	100
TCPP	C ₉ H ₁₈ Cl ₃ O ₄ P	[M+H] ⁺	327.0081	100	38	-	-	100	4	-	-
TCPP F ₁	C ₇ H ₁₄ Cl ₃ O ₃		251.0003	28	70	40	-	26	18	-	-
TCPP F ₂	C ₄ H ₉ Cl ₂ O ₃		174.9923	15	100	100	-	5	65	4	-
TCPP F ₃	H ₄ O ₄ P		98.9842	-	-	-	-	-	100	100	100
Tebuconazole	C ₁₆ H ₂₂ ClN ₃ O	[M+H] ⁺	308.1524	100	100	100	49	100	100	13	-
Tebuconazole F ₁	C ₇ H ₆ Cl		125.0153	-	-	3	25	-	-	2	4
Tebuconazole F ₂	C ₂ H ₃ N ₃		70.0400	-	2	18	100	-	11	82	81
Tebuconazole F ₃	C ₄ H ₉		57.0699	-	-	-	-	-	17	100	100
Tebufenpyrad	C ₁₈ H ₂₄ ClN ₃ O	[M+H] ⁺	334.1681	100	100	100	100	100	100	100	56
Tebufenpyrad F ₁	C ₇ H ₈ ClN ₂ O		171.0320	-	-	-	-	-	-	5	18
Tebufenpyrad F ₂	C ₆ H ₁₀ ClN ₂		145.0527	-	-	1	6	-	-	13	100
Tebufenpyrad F ₃	C ₄ H ₆ ClN ₂		117.0214	-	-	-	-	-	-	2	50
Tebutam	C ₁₅ H ₂₃ NO	[M+H] ⁺	234.1852	100	100	59	3	100	100	3	-
Tebutam F ₁	C ₁₂ H ₁₈ NO		192.1383	1	8	16	5	-	6	3	-
Tebutam F ₂	C ₈ H ₇ O		119.0491	-	-	-	-	-	3	33	30
Tebutam F ₃	C ₇ H ₇		91.0542	5	28	100	100	-	30	100	100
Tebuthiuron	C ₉ H ₁₆ N ₄ OS	[M+H] ⁺	229.1118	100	100	29	5	100	100	4	-
Tebuthiuron F ₁	C ₇ H ₁₄ N ₃ S		172.0903	7	39	100	100	-	69	100	70
Tebuthiuron F ₂	C ₃ H ₆ N ₃ S		116.0277	-	2	8	31	-	-	12	100
Tebuthiuron F ₃	C ₂ H ₅ N ₂ S		89.0168	-	-	-	-	-	-	4	26

Terbumeton F ₃	C ₅ H ₁₀ N ₃ O	128.0818	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	22
Terbumeton F ₄	C ₄ H ₈ N ₃ O	114.0662	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	8	52
Terbumeton F ₅	C ₃ H ₆ N ₃ O	100.0505	-	-	2	11	-	-	-	-	-	-	-	-	-	-	-	3	50
Terbumeton F ₆	C ₄ H ₆ N ₃	96.0556	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	22
Terbumeton F ₇	C ₂ H ₄ N ₃ O	86.0349	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3	40
Terbumeton F ₈	C ₂ H ₇ N ₂ O	75.0553	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3	47
Terbumeton F ₉	C ₂ H ₅ N ₂	57.0447	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	32
Terbutylazine	C ₉ H ₁₆ CIN ₅	230.1167	100	100	19	4	100	100	100	100	100	100	100	100	100	100	100	8	17
Terbutylazine F ₁	[M+H] ⁺	174.0540	9	67	100	100	-	-	-	-	-	-	-	-	-	-	-	93	98
Terbutylazine F ₂	C ₅ H ₉ CIN ₅	138.0774	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3	16
Terbutylazine F ₃	C ₅ H ₈ N ₅	132.0323	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	8	51
Terbutylazine F ₄	C ₆ H ₇ CIN ₅	104.0010	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	57
Terbutylazine F ₅	C ₂ H ₃ CIN ₅	96.0556	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	9	100
Terbutylazine F ₆	C ₄ H ₆ N ₃	79.0058	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	7	61
Terbutryn	C ₁₀ H ₁₉ N ₅ S	242.1434	100	100	44	8	100	100	100	100	100	100	100	100	100	100	100	6	-
Terbutryn F ₁	[M+H] ⁺	186.0808	4	27	100	100	-	-	-	-	-	-	-	-	-	-	-	46	100
Terbutryn F ₂	C ₆ H ₁₂ N ₅ S	91.0324	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6	65
Tetrachovinphos	C ₁₀ H ₉ Cl ₄ O ₄ P	364.9065	100	52	6	2	100	20	1	-	-	-	-	-	-	-	-	1	-
Tetrachovinphos F ₁	[M+H] ⁺	238.8983	23	12	14	19	-	3	7	8	-	-	-	-	-	-	-	3	7
Tetrachovinphos F ₂	C ₈ H ₃ Cl ₄	127.0155	3	100	100	100	3	100	100	100	100	100	100	100	100	100	100	100	100
Tetrachovinphos F ₃	C ₂ H ₈ O ₄ P	109.0049	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	8
Tetrachovinphos	C ₂ H ₆ O ₃ P	386.8885	5	5	3	5	2	2	1	-	-	-	-	-	-	-	-	1	-
Thiabenzazole	C ₁₀ H ₉ Cl ₄ O ₄ P	202.0433	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	43
Thiabenzazole F ₁	[M+H] ⁺	175.0324	-	2	10	49	-	-	-	-	-	-	-	-	-	-	-	24	100
Thiabenzazole F ₂	C ₉ H ₇ N ₂ S	131.0602	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	46
Thiabenzazole F ₃	C ₈ H ₇ N ₂	92.0495	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	9
Thiacloprid	C ₁₀ H ₉ CIN ₄ S	253.0309	100	100	48	1	100	100	100	100	100	100	100	100	100	100	100	81	40
Thiacloprid F ₁	[M+H] ⁺	186.0139	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	5	4
Thiacloprid F ₂	C ₈ H ₉ CIN ₅	126.0105	5	35	100	100	-	17	100	100	100	100	100	100	100	100	100	100	100
Thiacloprid F ₃	C ₆ H ₅ CIN	98.9996	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4
Thiacloprid F ₄	C ₅ H ₄ Cl	90.0338	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	12

Thiacloprid	C ₁₀ H ₉ ClN ₄ S	[M+Na] ⁺	275.0129	-	-	-	-	2	10	15	8
Thiamethoxam	C ₈ H ₁₀ ClN ₅ O ₃ S	[M+H] ⁺	292.0266	100	51	24	6	100	28	10	3
Thiamethoxam F ₁		C ₈ H ₁₁ N ₄ OS	211.0648	77	100	100	100	24	100	100	100
Thiamethoxam F ₂		C ₇ H ₉ N ₄ S	181.0542	-	-	-	-	-	6	75	85
Thiamethoxam F ₃		C ₆ H ₆ N ₃ S	152.0277	-	-	-	-	-	-	3	31
Thiamethoxam F ₄		C ₄ H ₃ CINS	131.9669	-	-	-	-	-	8	27	56
Thidiazuron	C ₉ H ₈ N ₄ OS	[M+H] ⁺	221.0492	100	100	16	14	100	96	19	38
Thidiazuron F ₁		C ₃ HN ₃ OS	127.9913	-	-	-	-	-	10	11	14
Thidiazuron F ₂		C ₃ H ₄ N ₃ S	102.0120	9	97	100	100	-	100	100	100
Thidiazuron	C ₉ H ₈ N ₄ OS	[M+Na] ⁺	243.0311	-	-	-	-	4	9	5	12
Thifensulfuron-methyl	C ₁₂ H ₁₃ N ₅ O ₆ S ₂	[M+H] ⁺	388.0380	100	100	48	4	100	35	2	-
Thifensulfuron-methyl F ₁		C ₆ H ₅ O ₄ S ₂	204.9624	-	4	23	32	-	-	12	27
Thifensulfuron-methyl F ₂		C ₆ H ₇ N ₄ O ₂	167.0564	4	21	100	100	-	100	100	100
Thifensulfuron-methyl F ₃		C ₅ H ₉ N ₄ O	141.0771	1	12	65	64	-	12	17	29
Thifensulfuron-methyl	C ₁₂ H ₁₃ N ₅ O ₆ S ₂	[M+Na] ⁺	410.0199	4	7	38	79	2	13	4	-
Thiocyclam	C ₅ H ₁₁ NS ₃	[M+H] ⁺	182.0126	100	45	13	-	100	77	8	2
Thiocyclam F ₁		C ₅ H ₅ S ₃	136.9548	35	100	100	17	-	100	100	19
Thiocyclam F ₂		C ₃ H ₃ S ₂	102.9671	-	9	58	100	-	-	7	19
Thiocyclam F ₃		C ₅ H ₁₇ N	86.0964	-	7	12	3	-	30	18	-
Thiocyclam F ₄		C ₃ H ₅ S	73.0106	-	-	-	-	-	4	78	100
Thiodicarb	C ₁₀ H ₁₈ N ₄ O ₄ S ₃	[M+H] ⁺	355.0563	100	16	21	5	100	9	-	-
Thiodicarb F ₁		C ₅ H ₁₁ N ₂ O ₂ S	163.0536	-	-	-	-	32	7	-	-
Thiodicarb F ₂		C ₂ H ₆ NS ₂	107.9936	5	18	12	2	-	39	23	10
Thiodicarb F ₃		C ₃ H ₆ NS	88.0215	30	100	100	27	32	100	100	100
Thiodicarb F ₄		C ₄ H ₂ N	64.0182	-	-	-	-	-	-	4	17
Thiodicarb	C ₁₀ H ₁₈ N ₄ O ₄ S ₃	[M+Na] ⁺	377.0382	10	22	72	100	14	81	62	26
Thiofanox	C ₉ H ₁₈ N ₂ O ₂ S	[M+H] ⁺	219.1162	-	-	-	-	-	-	-	-
Thiofanox F ₁		C ₇ H ₁₄ NS	144.0841	-	-	-	-	18	1	-	-
Thiofanox F ₂		C ₂ H ₆ NO ₂	76.0393	-	-	-	-	33	25	17	-
Thiofanox F ₃		C ₄ H ₉	57.0699	-	-	-	-	100	100	100	-
Thiofanox	C ₉ H ₁₈ N ₂ O ₂ S	[M+Na] ⁺	241.0981	100	100	100	100	8	7	5	-

Thiophanate-methyl	C ₁₂ H ₁₄ N ₄ O ₄ S ₂	[M+H] ⁺	343.0529	100	100	7	-	100	-	-
Thiophanate-methyl F ₁	C ₁₁ H ₁₀ N ₄ O ₃ S ₂		311.0267	4	33	14	1	13	26	-
Thiophanate-methyl F ₂	C ₁₀ H ₁₀ N ₃ O ₃ S ₂		268.0209	-	-	-	-	-	12	-
Thiophanate-methyl F ₃	C ₉ H ₉ N ₃ O ₂		192.0768	-	5	6	3	-	6	3
Thiophanate-methyl F ₄	C ₇ H ₈ N ₂ S		151.0324	4	54	100	100	4	100	100
Tolclofos-methyl	C ₉ H ₁₁ Cl ₂ O ₃ PS	[M+H] ⁺	300.9616	100	100	100	24	100	100	3
Tolclofos-methyl F ₁	C ₈ H ₈ Cl ₂ O ₂ PS		268.9354	-	14	64	50	-	50	29
Tolclofos-methyl F ₂	C ₉ H ₁₁ ClO ₃ PS		264.9820	-	-	-	-	-	5	9
Tolclofos-methyl F ₃	C ₇ H ₅ Cl ₂ O		174.9712	-	4	37	100	-	-	26
Tolclofos-methyl F ₄	C ₂ H ₆ O ₂ PS		124.9821	-	-	-	-	-	88	100
Tralkoxidym	C ₂₀ H ₂₇ NO ₃	[M+H] ⁺	330.2064	100	100	74	13	100	31	4
Tralkoxidym F ₁	C ₁₈ H ₂₂ NO ₂		284.1645	6	30	100	100	2	100	26
Tralkoxidym F ₂	C ₈ H ₁₀ NO ₂		152.0706	-	-	-	-	-	1	9
Tralkoxidym F ₃	C ₇ H ₈ NO ₂		138.0550	-	2	21	94	-	14	100
Tralkoxidym F ₄	C ₆ H ₈ NO		110.0600	-	-	-	-	-	1	11
Tralkoxidym F ₅	C ₅ H ₈ NO		98.0600	-	-	-	-	-	1	17
Tralkoxidym F ₆	C ₅ H ₆ NO		96.0444	-	-	3	28	-	1	31
Tralkoxidym F ₇	C ₅ H ₈ N		82.0651	-	-	-	-	-	-	5
Tralkoxidym F ₈	C ₃ H ₆ NO		72.0444	-	-	-	-	-	-	7
Transfluthrin	C ₁₅ H ₁₂ Cl ₂ F ₄ O ₂	[M+H] ⁺	371.0223	100	30	2	-	100	10	-
Transfluthrin F ₁	C ₇ H ₃ F ₄		163.0165	32	100	100	100	-	100	100
Transfluthrin F ₂	C ₇ H ₂ F ₃		143.0103	-	-	5	10	-	7	-
Triadimefon	C ₁₄ H ₁₆ ClN ₃ O ₂	[M+H] ⁺	294.1004	100	100	28	10	100	100	27
Triadimefon F ₁	C ₁₂ H ₁₄ ClO ₂		225.0677	3	22	30	100	-	30	18
Triadimefon F ₂	C ₁₁ H ₁₄ ClO		197.0728	3	27	100	8	-	43	100
Triadimenol	C ₁₄ H ₁₈ ClN ₃ O ₂	[M+H] ⁺	296.1160	100	19	14	14	100	4	-
Triadimenol F ₁	C ₁₂ H ₁₆ ClO ₂		227.0833	8	22	-	4	3	2	-
Triadimenol F ₂	C ₆ H ₁₁ O		99.0804	1	9	5	1	-	6	5
Triadimenol F ₃	C ₂ H ₄ N ₃		70.0399	18	100	100	100	51	100	100
Triallat	C ₁₀ H ₁₆ Cl ₃ NOS	[M+H] ⁺	304.0091	100	100	100	7	100	64	2
Triallat F ₁	C ₇ H ₁₁ Cl ₃ NOS		261.9621	2	11	56	11	-	9	-

Triallat F ₂	C ₃ H ₂ Cl ₃	142.9217	-	6	89	100	-	3	28	100
Triallat F ₃	C ₇ H ₁₄ NO	128.1070	-	-	-	-	-	46	16	15
Triallat F ₄	C ₄ H ₈ NO	86.0600	-	-	28	6	-	100	100	75
Triasulfuron	[M+H] ⁺	402.0633	100	100	100	12	100	97	3	1
Triasulfuron F ₁	C ₁₁ H ₆ ClNO ₄ S	283.9769	-	-	-	-	-	-	8	33
Triasulfuron F ₁	C ₈ H ₈ ClO ₃ S	218.9877	-	-	-	-	-	-	6	-
Triasulfuron F ₃	C ₆ H ₇ N ₄ O ₂	167.0564	2	5	49	53	-	100	100	96
Triasulfuron F ₄	C ₈ H ₁₀ O ₅	163.0601	-	-	-	-	-	6	23	64
Triasulfuron F ₅	C ₅ H ₉ N ₄ O	141.0771	2	10	95	100	-	61	78	100
Triazophos	[M+H] ⁺	314.0723	100	100	20	2	100	80	-	-
Triazophos F ₁	C ₁₀ H ₁₂ N ₃ O ₃ PS	286.0410	-	-	-	-	-	16	1	-
Triazophos F ₂	C ₈ H ₈ N ₃ S	178.0430	-	-	-	-	-	3	7	-
Triazophos F ₃	C ₈ H ₈ N ₃ O	162.0662	4	36	100	100	-	100	100	100
Triazophos F ₄	C ₇ H ₂ N ₂	119.0604	-	-	-	-	-	-	3	33
Triazophos F ₅	H ₂ O ₂ PS	96.9508	-	-	-	-	-	-	6	26
Triazophos	[M+Na] ⁺	336.0542	-	-	-	-	1	7	4	-
Triazoxide	[M+H] ⁺	248.0334	100	100	100	100	100	100	100	100
Triazoxide F ₁	C ₉ H ₆ ClN ₄ O	221.0225	-	-	1	3	-	-	1	5
Triazoxide F ₃	C ₉ HO	125.0022	-	-	-	-	-	-	-	12
Triazoxide F ₄	C ₃ H ₆ ClN	123.9949	-	-	-	-	-	-	1	20
Triazoxide F ₇	C ₄ H ₃ N ₂	95.0240	-	-	-	-	-	-	5	49
Trichlorfon	[M+H] ⁺	256.9299	100	70	7	-	100	100	-	-
Trichlorfon F ₁	C ₄ H ₈ Cl ₃ O ₄ P	220.9531	10	34	9	3	-	64	4	-
Trichlorfon F ₂	C ₂ H ₆ O ₃ P	109.0051	11	100	100	100	-	95	100	100
Trichlorfon F ₃	CH ₄ O ₂ P	78.9943	-	-	-	-	-	-	-	6
Triclocarban	[M+H] ⁺	314.9853	100	100	100	99	100	100	57	25
Triclocarban F ₁	C ₆ H ₆ Cl ₂ N	161.9872	-	4	25	100	-	8	68	36
Triclocarban F ₂	C ₈ H ₇ ClN	128.0262	-	-	-	-	-	13	100	66
Triclocarban F ₃	C ₉ H ₇ O	127.0178	-	-	-	-	-	-	39	100
Triclocarban F ₄	C ₈ H ₅ ClN	126.0105	-	-	-	-	-	-	6	18

Tridemorph	$C_{19}H_{39}NO$	$[M+H]^+$	298.3105	84	100	100	72	100	100	100	100	100	100	100	100
Tridemorph F ₁		$C_{18}H_{38}NO$	284.2948	100	86	51	100	6	2	-	-	-	-	-	-
Tridemorph F ₂		$C_7H_{16}NO$	130.1226	-	-	-	-	-	-	-	-	-	-	2	42
Tridemorph F ₃		$C_6H_{14}NO$	116.1070	-	-	-	-	-	-	-	-	-	-	2	17
Trietazine	$C_9H_{16}ClN_5$	$[M+H]^+$	230.1167	100	100	100	100	100	100	100	100	100	100	100	100
Trietazine F ₁		$C_7H_{13}ClN_5$	202.0854	-	-	-	-	-	-	-	-	-	-	32	19
Trietazine F ₂		$C_4H_7ClN_3$	132.0323	-	-	1	5	-	-	-	-	-	-	26	37
Trietazine F ₃		$C_6H_{10}N_3$	124.0869	-	-	-	-	-	-	-	-	-	-	13	31
Trietazine F ₄		$C_2H_3ClN_3$	104.0010	-	-	-	-	-	-	-	-	-	-	7	48
Trietazine F ₅		$C_3H_{11}N_2$	99.0917	-	-	4	28	-	-	-	-	-	-	28	83
Trietazine F ₆		$C_3H_7N_2$	71.0604	-	-	-	-	-	-	-	-	-	-	7	77
Trifloxystrobin	$C_{20}H_{19}F_3N_2O_4$	$[M+H]^+$	409.1370	100	100	13	-	100	24	1	-	-	-	1	-
Trifloxystrobin F ₁		$C_9H_{11}F_3NO$	206.0812	-	-	-	-	-	48	18	5	-	-	18	5
Trifloxystrobin F ₂		$C_9H_7F_3N$	186.0525	4	43	100	100	100	-	100	100	100	100	100	100
Trifloxystrobin F ₃		$C_7H_4F_3$	145.0260	-	-	-	-	-	-	-	-	-	-	1	15
Trifloxystrobin F ₄		$C_9H_{10}N$	132.0808	-	-	-	-	-	-	6	11	11	11	11	11
Trifloxystrobin F ₅		C_8H_6N	116.0495	-	-	-	-	-	-	12	17	17	17	24	24
Trifloxysulfuron	$C_{14}H_{13}F_3N_5O_6S$	$[M+H]^+$	438.0690	100	100	90	7	100	56	1	1	-	-	1	1
Trifloxysulfuron F ₁		$C_7H_8F_3N_2O_3S$	257.0202	-	3	21	15	-	11	14	7	-	-	14	7
Trifloxysulfuron F ₂		$C_7H_8N_3O_3$	182.0560	2	12	100	100	-	100	100	100	-	-	100	100
Trifloxysulfuron F ₃		$C_7H_4F_3NO$	176.0313	-	-	-	-	-	-	-	-	-	-	2	13
Trifloxysulfuron F ₄		$C_6H_{10}N_3O_2$	156.0768	-	2	18	22	-	4	7	8	-	-	7	8
Trifloxysulfuron	$C_{14}H_{13}F_3N_5O_6S$	$[M+Na]^+$	460.0590	-	-	-	-	4	60	50	29	-	-	50	29
Triflumizole	$C_{15}H_{15}ClF_3N_3O$	$[M+H]^+$	346.0929	100	8	9	3	100	5	26	9	-	-	26	9
Triflumizole F ₁		$C_{12}H_{12}ClF_3NO$	278.0554	57	100	100	100	40	100	100	57	-	-	100	57
Triflumizole F ₂		$C_3H_5N_2$	69.0447	-	-	-	-	-	9	93	100	-	-	93	100
Triflumuron	$C_{15}H_{10}ClF_3N_2O_3$	$[M+H]^+$	357.0259	100	100	46	9	100	-	-	-	-	-	-	-
Triflumuron F ₁		$C_{10}H_4F_2N$	176.0317	2	23	100	41	-	-	-	-	-	-	-	-
Triflumuron F ₂		CHF_3O	84.9907	-	5	48	100	-	-	-	-	-	-	-	-
Trifluralin	$C_{13}H_{16}F_3N_3O_4$	$[M+H]^+$	336.1166	100	100	-	-	100	100	100	100	100	100	100	100

Zoxamide F ₃	C ₈ H ₅ Cl ₂ O	186.9712	5	33	100	100	100	100	45	100	100
Zoxamide F ₄	C ₆ H ₁₁ CIN	132.0575	-	-	-	-	-	-	-	20	7
Veterinary drugs											
Albendazole sulfone	C ₁₂ H ₁₅ N ₃ O ₄ S	298.0856	100	100	100	100	100	100	100	84	87
Albendazole sulfone F ₁	[M+H] ⁺	266.0594	1	4	22	89	-	8	100	100	100
Albendazole sulfone F ₂	C ₁₁ H ₁₂ N ₃ O ₃ S	224.0124	-	-	2	14	-	-	12	82	82
Albendazole sulfone F ₃	C ₈ H ₆ N ₃ O ₃ S	191.0703	-	-	-	-	-	-	-	6	6
Albendazole sulfone F ₄	C ₁₁ H ₁₁ O ₃	159.0441	-	-	-	-	-	-	-	75	75
Albendazole sulfone	C ₁₀ H ₇ O ₂	320.0675	-	-	-	-	1	2	5	6	6
Albendazole sulfone	[M+Na] ⁺	282.0907	100	100	66	41	100	51	42	22	22
Albendazole sulfoxide	C ₁₂ H ₁₅ N ₃ O ₃ S	240.0437	10	61	100	47	6	100	88	25	25
Albendazole sulfoxide F ₁	C ₉ H ₁₀ N ₃ O ₃ S	208.0175	1	7	40	100	-	4	100	100	100
Albendazole sulfoxide F ₂	C ₈ H ₆ N ₃ O ₂ S	191.0703	-	-	-	-	-	1	7	6	6
Albendazole sulfoxide F ₃	C ₁₁ H ₁₁ O ₃	191.0161	-	-	-	-	-	-	-	7	7
Albendazole sulfoxide F ₄	C ₁₀ H ₇ O ₂ S	159.0441	-	-	-	-	-	-	-	17	17
Albendazole sulfoxide F ₅	C ₁₀ H ₇ O ₂	366.1118	100	42	44	76	100	7	-	5	5
Amoxicillin	[M+H] ⁺	349.0853	33	100	100	100	-	1	-	-	-
Amoxicillin F ₁	C ₁₆ H ₁₇ N ₂ O ₅ S	207.0764	-	-	-	-	-	15	3	3	3
Amoxicillin F ₂	C ₁₀ H ₁₁ N ₂ O ₃	160.0427	-	-	-	-	16	100	100	100	100
Amoxicillin F ₃	C ₆ H ₁₀ NO ₂ S	388.0938	-	-	-	-	4	7	8	13	13
Amoxicillin	[M+Na] ⁺	350.1169	100	100	60	51	-	-	-	-	-
Ampicillin	C ₁₆ H ₁₉ N ₃ O ₄ S	175.0754	23	46	64	41	-	-	-	-	-
Ampicillin F ₁	C ₁₁ H ₁₁ O ₂	174.0550	-	-	-	-	-	20	100	62	62
Ampicillin F ₂	C ₁₀ H ₈ NO ₂	160.0427	-	-	-	-	-	100	64	54	54
Ampicillin F ₃	C ₆ H ₁₀ NO ₂ S	128.0528	-	-	-	-	-	-	30	100	100
Ampicillin F ₄	C ₆ H ₁₀ NS	106.0651	3	25	100	100	-	-	-	-	-
Ampicillin F ₅	C ₇ H ₈ N	136.0215	100	100	100	100	100	100	100	100	100
Benzothiazole	C ₇ H ₅ NS	310.1914	100	100	100	77	100	100	1	-	-
Benzylamine	C ₁₉ H ₂₃ N ₃ O	265.1335	-	2	10	7	-	9	4	-	-
Benzylamine F ₁	C ₁₇ H ₁₇ N ₂ O	86.0964	2	14	100	100	-	74	100	100	100
Benzylamine F ₂	C ₅ H ₁₂ N										

Ciprofloxacin F ₁	C ₁₆ H ₁₉ FN ₃ O ₂	314.1299	-	4	30	100	-	8	8	70
Ciprofloxacin F ₂	C ₁₆ H ₁₉ FN ₃ O	288.1507	-	2	17	57	-	9	9	49
Ciprofloxacin F ₃	C ₁₄ H ₁₄ FN ₂ O	245.1085	-	3	4	32	-	-	-	100
Ciprofloxacin F ₄	C ₁₂ H ₈ FN ₂ O ₂	231.0564	-	3	5	14	-	-	-	34
Ciprofloxacin F ₅	C ₁₁ H ₈ FN ₂ O	203.0615	-	-	1	3	-	-	-	14
Clarithromycin	[M+H] ⁺	748.4842	100	100	100	100	100	100	100	19
Clarithromycin F ₁	C ₃₀ H ₅₆ NO ₁₀	590.3899	-	-	2	6	1	23	72	4
Clarithromycin F ₂	C ₂₉ H ₅₂ NO ₉	558.3637	-	-	-	2	-	2	16	4
Clarithromycin F ₃	C ₈ H ₁₆ NO ₂	158.1176	-	-	-	5	-	4	100	100
Clarithromycin F ₄	C ₆ H ₁₄ NO	116.1070	-	-	-	1	-	-	9	13
Clenbuterol	[M+H] ⁺	277.0869	100	98	9	5	100	17	4	-
Clenbuterol F ₁	C ₁₂ H ₁₇ Cl ₂ N ₂	259.0763	7	38	8	3	8	64	3	-
Clenbuterol F ₂	C ₈ H ₉ Cl ₂ N ₂	203.0137	10	100	100	100	-	100	100	23
Clenbuterol F ₃	C ₁₁ H ₆ NO	168.0444	-	-	-	-	-	-	17	100
Clenbuterol F ₄	C ₈ H ₉	57.0699	-	-	-	-	-	-	13	40
Clofibric acid	[M-H] ⁻	213.0324	69	15	4	7	100	32	8	3
Clofibric acid F ₁	C ₆ H ₄ ClO	126.9951	100	100	100	100	7	100	100	100
Clofibric acid F ₂	C ₄ H ₅ O	85.0295	20	9	4	3	7	36	21	14
Cloxacillin	[M+H] ⁺	436.0728	-	6	55	100	-	20	12	-
Cloxacillin F ₁	C ₁₄ H ₁₄ ClN ₂ O	309.0637	-	-	-	-	-	17	5	-
Cloxacillin F ₂	C ₁₃ H ₁₀ O ₃ N ₂ Cl	277.0374	-	-	-	2	-	2	7	2
Cloxacillin F ₃	C ₁₁ H ₉ O ₂ NCl	222.0316	-	-	-	4	-	-	-	-
Cloxacillin F ₄	C ₉ H ₅ ONCl	178.0054	-	1	8	32	-	-	17	55
Cloxacillin F ₅	C ₆ H ₁₀ O ₂ SN	160.0427	-	4	33	52	-	100	100	100
Cloxacillin F ₆	C ₃ H ₈ NS	114.0372	-	-	-	-	-	-	4	26
Cloxacillin	[M+CH ₃ OH] ⁺	468.0991	100	100	100	19	100	69	2	-
Cotinine	[M+H] ⁺	177.1022	100	100	100	37	100	100	100	23
Cotinine F ₁	C ₉ H ₈ NO	146.0600	-	-	-	-	-	1	8	-
Cotinine F ₂	C ₈ H ₈ NO	134.0600	-	-	-	1	-	-	-	-
Cotinine F ₃	C ₇ H ₈ N	106.0561	-	-	1	2	-	-	-	-
Cotinine F ₄	C ₃ H ₈ NO	98.0600	-	-	-	-	-	2	32	23

Cotinine F ₅	C ₅ H ₆ N	80.0495	1	6	40	100	-	4	89	100
Danofloxacin	[M+H] ⁺	358.1561	100	100	100	100	100	100	100	100
Danofloxacin F ₁	C ₁₉ H ₂₀ FN ₃ O ₃	314.1663	-	1	4	14	-	-	24	20
Danofloxacin F ₂	C ₁₇ H ₁₅ FN ₂ O	283.1241	-	-	1	5	-	-	9	60
Danofloxacin F ₃	C ₆ H ₆ N	96.0808	-	1	1	3	-	-	12	48
Demeclocycline	[M+H] ⁺	465.1059	100	100	100	18	100	100	-	1
Demeclocycline F ₁	C ₂₁ H ₁₉ ClNO ₈	448.0794	1	10	80	100	-	78	78	2
Demeclocycline F ₂	C ₂₁ H ₁₇ ClNO ₇	430.0688	-	-	-	-	-	10	79	16
Demeclocycline F ₃	C ₆ H ₆ NO	108.0444	-	-	-	-	-	-	100	70
Demeclocycline F ₄	C ₆ H ₆ N	92.0495	-	-	-	-	-	-	90	100
Diclofenac	[M+H] ⁻	294.0094	59	4	2	9	100	6	-	-
Diclofenac F ₁	C ₁₃ H ₁₀ Cl ₂ N	250.0196	100	100	100	100	10	100	100	100
Diclofenac F ₂	C ₁₃ H ₁₀ ClN	214.0426	1	4	25	72	-	-	25	52
Dicloxacillin	[M+H] ⁺	470.0339	-	7	44	100	-	7	16	-
Dicloxacillin F ₁	C ₉ H ₄ Cl ₂ NO	211.9664	-	-	-	-	-	-	-	31
Dicloxacillin F ₂	C ₆ H ₁₀ NO ₂ S	160.0427	-	-	-	-	-	62	100	100
Dicloxacillin F ₃	C ₅ H ₁₀ NO ₂	116.0705	-	-	-	-	-	-	-	8
Dicloxacillin F ₄	C ₅ H ₈ NS	114.0372	-	-	-	-	-	-	-	12
Dicloxacillin	[M+CH ₃ OH] ⁺	502.0601	100	100	100	31	100	100	-	-
Difloxacin	[M+H] ⁺	400.1467	100	100	100	100	100	100	41	14
Difloxacin F ₁	C ₂₁ H ₁₈ F ₂ N ₃ O ₂	382.1362	-	1	10	65	-	4	40	85
Difloxacin F ₂	C ₂₀ H ₂₀ F ₂ N ₃ O	356.1569	-	1	10	64	-	7	100	100
Digoxin	[M+H] ⁺	781.4369	4	7	8	13	-	-	-	-
Digoxin F ₁	C ₃₅ H ₅₅ O ₁₁	651.3739	100	100	100	100	100	100	9	2
Digoxin F ₂	C ₂₉ H ₄₅ O ₈	521.3109	-	-	-	-	18	47	10	2
Digoxin F ₃	C ₂₃ H ₃₅ O ₅	391.2479	-	-	-	-	6	42	12	4
Digoxin	[M+Na] ⁺	798.4634	8	11	7	-	-	-	-	-
Dimetridazole	[M+H] ⁺	142.0611	100	100	41	6	100	100	88	23
Dimetridazole F ₁	C ₅ H ₇ N ₂	95.0604	2	16	100	100	-	2	100	10
Dimetridazole F ₂	C ₄ H ₅ N ₂	81.0447	-	9	36	78	-	-	45	68
Diphenhydramine	[M+H] ⁺	256.1696	62	7	1	-	100	1	-	-

Eprinomectin b _{1a} F ₄	C ₃₆ H ₅₂ NO ₉	642.3637	-	-	-	-	24	1	-	-		
Eprinomectin b _{1a} F ₅	C ₂₅ H ₄₂ NO ₇	468.2956	-	-	-	-	12	2	-	-		
Eprinomectin b _{1a} F ₆	C ₁₆ H ₂₈ NO ₆	330.1911	-	-	-	-	14	19	5	3		
Eprinomectin b _{1a} F ₇	C ₁₅ H ₂₄ NO ₅	298.1649	-	-	-	-	17	10	19	17		
Eprinomectin b _{1a} F ₈	C ₁₅ H ₁₅ O ₃	243.1016	-	-	-	-	3	5	13	19		
Eprinomectin b _{1a} F ₉	C ₉ H ₁₆ NO ₃	186.1125	-	-	-	-	67	100	100	100		
Eprinomectin b _{1a} F ₁₀	C ₇ H ₁₄ NO ₂	154.0863	-	-	-	-	21	23	52	91		
Eprinomectin b _{1a} F ₁₁	C ₇ H ₁₄ NO ₂	144.1019	-	-	-	-	4	11	27	60		
Eprinomectin b _{1a} F ₁₂	C ₆ H ₁₀ NO	112.0757	-	-	-	-	-	8	15	32		
Eprinomectin b _{1a}	[M+Na] ⁺	936.5080	98	100	100	100	100	100	57	29	40	64
Eprinomectin b _{1b}	[M+H] ⁺	900.5104	38	53	27	13	-	-	-	-	-	-
Eprinomectin b _{1b} F ₁	C ₄₉ H ₇₂ NO ₁₃	882.4998	44	40	27	17	-	-	-	-	-	-
Eprinomectin b _{1b} F ₂	C ₄₉ H ₇₀ NO ₁₂	864.4893	65	66	49	30	-	-	-	-	-	-
Eprinomectin b _{1b} F ₃	C ₃₄ H ₄₉ O ₇	569.3473	-	-	-	-	10	50	26	-	-	-
Eprinomectin b _{1b} F ₄	C ₃₄ H ₄₇ O ₆	551.3367	-	-	-	-	100	69	60	29	-	-
Eprinomectin b _{1b} F ₅	C ₁₉ H ₃₁ O ₃	307.2268	-	-	-	-	63	100	100	100	-	-
Eprinomectin b _{1b}	[M+Na] ⁺	922.4923	100	100	100	100	100	-	-	-	-	-
Erythromycin	[M+H] ⁺	734.4685	100	100	100	100	100	100	16	-	-	-
Erythromycin F ₁	C ₂₉ H ₅₃ NO ₁₀	576.3742	-	1	3	9	1	30	76	11	-	-
Erythromycin F ₂	C ₂₉ H ₅₂ NO ₉	558.3637	-	-	-	-	-	9	24	2	-	-
Erythromycin F ₃	C ₂₉ H ₄₈ NO ₇	522.3495	-	-	-	-	-	5	17	3	-	-
Erythromycin F ₄	C ₈ H ₁₆ NO ₂	158.1176	-	-	1	4	-	5	100	100	-	-
Erythromycin F ₅	C ₆ H ₁₄ NO	116.1070	-	-	-	-	1	-	10	16	-	-
Erythromycin F ₆	C ₅ H ₇ O	83.0491	-	-	-	-	1	4	-	11	-	-
Estrone	[M+H] ⁺	271.1693	100	100	100	73	100	81	35	-	-	-
Estrone F ₁	C ₁₈ H ₂₁ O	253.1587	5	20	65	100	-	71	100	27	-	-
Estrone F ₂	C ₁₄ H ₁₃ O	197.0961	-	-	-	-	-	-	52	41	-	-
Estrone F ₃	C ₁₁ H ₉ O	157.0648	-	-	-	-	-	-	81	100	-	-
Estrone F ₄	C ₉ H ₈ O	133.0648	1	5	30	96	-	9	62	100	-	-
Febantel	[M+H] ⁺	447.1333	-	-	-	-	-	-	-	-	-	-
Febantel 1 F ₁	C ₁₈ H ₂₁ N ₄ O ₄ S	389.1278	100	100	100	100	100	100	100	8	-	-

Febantel 1 F ₂	C ₁₇ H ₁₇ N ₄ O ₃ S	357.1016	-	4	18	72	-	65	100	7
Febantel 1 F ₃	C ₁₆ H ₁₄ N ₃ O ₂ S	312.0802	-	-	-	-	4	7	80	23
Febantel 1 F ₄	C ₁₅ H ₁₅ O ₅ S	307.0635	-	-	-	-	-	-	5	15
Febantel 1 F ₅	C ₁₄ H ₁₂ N ₃ S	254.0746	-	-	1	16	-	-	40	100
Febantel 1 F ₆	C ₁₄ H ₁₁ NS	239.0637	-	-	-	-	-	-	15	83
Fleroxacin	[M+H] ⁺	370.1373	100	100	100	85	100	100	39	12
Fleroxacin F ₁	C ₁₇ H ₁₇ F ₃ N ₃ O ₂	352.1267	-	1	6	24	-	3	14	13
Fleroxacin F ₂	C ₁₆ H ₁₉ F ₃ N ₃ O	326.1475	-	3	21	100	-	11	100	55
Fleroxacin F ₃	C ₁₃ H ₁₂ F ₃ N ₂ O	269.0896	-	-	2	25	-	-	21	100
Fleroxacin F ₄	C ₁₁ H ₉ F ₂ N ₂ O	223.0677	-	-	-	-	-	-	-	10
Fleroxacin F ₅	C ₃ H ₈ N	58.0651	-	-	-	-	-	-	3	27
Flufenamic acid	[M+H] ⁺	282.0736	100	35	2	-	100	14	-	-
Flufenamic acid F ₁	C ₁₄ H ₉ F ₃ NO	264.0631	21	100	100	100	7	100	100	100
Flufenamic acid F ₂	C ₁₃ H ₁₀ N	180.0808	-	-	-	-	-	-	-	27
Flumequine	[M+H] ⁺	262.0874	100	100	20	9	100	63	9	11
Flumequine F ₁	C ₁₄ H ₁₁ FNO ₂	244.0768	10	89	100	100	-	100	100	100
Flumequine F ₂	C ₁₁ H ₅ FNO ₂	202.0299	-	2	6	26	-	-	3	80
Flumequine F ₃	C ₁₀ H ₅ FNO	174.0350	-	-	1	4	-	-	-	-
Fluoxetine	[M+H] ⁺	310.1413	100	100	100	100	100	100	100	100
Fluoxetine F ₁	C ₁₀ H ₁₄ N	148.1121	1	4	3	6	19	18	16	11
Furosemide	[M-H] ⁻	329.0040	100	100	66	30	100	100	100	100
Furosemide F ₁	C ₁₁ H ₁₀ ClN ₂ O ₃ S	285.0106	11	63	100	100	-	19	25	77
Furosemide F ₂	C ₆ H ₇ ClN ₂ O ₂ S	204.9844	1	4	12	24	-	-	27	36
Gemfibrozil	[M+H] ⁺	251.1642	-	-	-	-	67	1	-	-
Gemfibrozil F ₁	C ₁₅ H ₂₁ O ₂	233.1536	62	13	7	18	100	12	-	-
Gemfibrozil F ₂	C ₁₄ H ₂₁ O	205.1587	-	-	-	-	22	8	-	-
Gemfibrozil F ₃	C ₇ H ₁₃ O ₂	129.0910	100	100	92	22	48	78	59	25
Gemfibrozil F ₄	C ₆ H ₁₁	83.0855	-	-	-	-	35	100	100	100
Gemfibrozil	[M+Na] ⁺	273.1461	27	42	100	100	20	18	21	26
Hydrochlorothiazide	[M-H] ⁻	295.9572	100	100	100	100	100	100	100	100
Hydrochlorothiazide F ₁	C ₆ H ₆ ClN ₂ O ₄ S ₂	268.9536	1	4	11	18	-	-	40	19

Hydrochlorothiazide F ₂	C ₆ H ₆ ClN ₂ O ₂ S	204.9844	-	2	10	28	-	25	40
Hydroflumethiazide	[M+H] ⁺	331.9981	100	33	35	30	100	30	38
Hydroflumethiazide F ₁	C ₈ H ₆ F ₃ N ₂ O ₄ S ₂	314.9716	60	100	100	45	-	100	100
Hydroflumethiazide F ₂	C ₈ H ₇ FN ₃ O ₄ S ₂	291.9857	4	12	23	37	-	24	67
Hydroflumethiazide F ₃	C ₈ H ₆ F ₃ N ₂ O ₃ S	267.0046	-	-	41	47	-	-	50
Hydroflumethiazide F ₄	C ₈ H ₆ F ₃ N ₂ O ₂ S	251.0097	-	-	48	62	-	-	38
Hydroflumethiazide F ₅	C ₈ H ₆ F ₃ N ₂	187.0478	-	-	31	100	-	-	23
Hydroflumethiazide	[M+Na] ⁺	353.9801	-	-	-	-	20	45	92
Ibuprofen	[M+H] ⁺	207.1380	87	10	2	-	69	6	-
Ibuprofen F ₁	C ₁₂ H ₁₇	161.1325	100	100	100	100	50	100	100
Ibuprofen	[M+NH ₄] ⁺	224.1645	-	-	-	-	100	-	-
Indomethacine	[M+H] ⁺	358.0841	100	100	15	1	100	82	4
Indomethacine F ₁	C ₁₁ H ₁₂ NO	174.0913	1	3	4	5	1	49	19
Indomethacine F ₂	C ₇ H ₄ ClO	138.9945	7	53	100	100	1	100	100
Indomethacine F ₃	C ₆ H ₄ Cl	110.9996	-	-	-	-	-	-	13
Irgasan	[M+H] ⁺	288.9584	100	28	-	-	100	41	-
Irgasan F ₁	C ₆ H ₃ Cl ₂ O	160.9555	56	100	62	10	-	-	-
Irgasan F ₂	C ₅ H ₃ Cl ₂	132.9606	18	42	100	100	-	-	-
Josamycin	[M+H] ⁺	828.4740	100	100	100	100	100	100	100
Josamycin F ₁	C ₃₀ H ₅₀ NO ₁₁	600.3378	-	-	-	-	-	-	25
Josamycin F ₂	C ₁₂ H ₂₁ O ₄	229.1431	-	-	-	-	-	-	27
Josamycin F ₃	C ₈ H ₁₆ NO ₃	174.1125	-	-	-	-	-	-	78
Josamycin F ₄	C ₇ H ₉ O	109.0648	-	-	-	-	-	-	34
Ketoprofen	[M+H] ⁺	255.1016	100	100	100	9	100	100	7
Ketoprofen F ₁	C ₁₅ H ₁₃ O	209.0961	3	12	71	37	1	64	100
Ketoprofen F ₂	C ₁₄ H ₁₀ O	194.0726	-	-	2	5	-	-	5
Ketoprofen F ₃	C ₁₀ H ₉ O ₃	177.0546	-	-	-	-	-	-	10
Ketoprofen F ₄	C ₇ H ₅ O	105.0335	1	7	70	100	-	6	49
Ketoprofen	[M+Na] ⁺	277.0835	6	10	20	6	-	4	4
Leucomalachite green	[M+H] ⁺	331.2169	100	100	100	100	51	100	100
Leucomalachite green F ₁	C ₂₃ H ₂₆ N ₂	316.1934	-	-	4	22	-	-	45

Leucomalachite green F ₂	C ₁₆ H ₁₉ N ₂	239.1543	-	-	2	20	-	-	23	100
Leucomalachite green F ₃	C ₁₄ H ₁₄ N	196.1121	9	40	45	34	-	9	57	26
Leucomalachite green F ₄	C ₁₃ H ₁₀ N	180.0808	-	-	4	16	-	-	3	18
Leucomalachite green	[M+2H] ²⁺	166.1121	-	-	-	-	100	70	-	-
Levamisole	C ₂₃ H ₂₆ N ₂	205.0794	100	100	100	100	100	100	100	28
Levamisole F ₁	[M+H] ⁺	178.0685	1	3	16	60	-	1	69	100
Levamisole F ₂	C ₁₀ H ₁₂ NS	150.0372	-	-	-	-	-	-	2	10
Levamisole F ₃	C ₈ H ₈ NS	146.0964	-	1	8	32	-	-	7	9
Levamisole F ₄	C ₁₀ H ₁₂ N	123.0263	-	-	-	-	-	-	6	77
Lincomycin	C ₇ H ₇ S	407.221	100	100	100	76	100	100	27	2
Lincomycin F ₁	[M+H] ⁺	389.2105	-	-	-	1	-	1	2	-
Lincomycin F ₂	C ₁₈ H ₃₃ N ₂ O ₅ S	359.2177	-	-	2	6	-	3	14	-
Lincomycin F ₃	C ₁₇ H ₃₁ N ₂ O ₆	126.1277	-	1	14	100	-	4	100	100
Lomefloxacin	C ₈ H ₁₆ N	352.1467	100	100	100	100	100	100	83	11
Lomefloxacin F ₁	[M+H] ⁺	334.1362	-	1	8	41	-	3	30	13
Lomefloxacin F ₂	C ₁₇ H ₁₈ F ₂ N ₃ O ₂	308.1569	-	2	15	67	-	10	100	17
Lomefloxacin F ₃	C ₁₆ H ₂₀ F ₂ N ₃ O	288.1507	-	-	-	-	-	-	17	9
Lomefloxacin F ₄	C ₁₆ H ₁₉ FN ₃ O	265.1147	-	1	5	57	-	1	91	100
Malachite green	C ₁₄ H ₁₅ F ₂ N ₂ O	329.2012	100	100	100	100	100	100	100	100
Malachite green F ₁	[M+H] ⁺	313.1699	-	-	-	-	-	-	-	17
Malachite green F ₂	C ₂₂ H ₂₁ N ₂	208.1121	-	-	-	-	-	-	-	9
Marbofloxacin	C ₁₅ H ₁₄ N	363.1463	100	100	100	100	100	100	100	100
Marbofloxacin F ₁	[M+H] ⁺	320.1041	1	6	34	74	-	15	47	58
Mebendazole	C ₁₅ H ₁₅ FN ₃ O ₄	296.1030	100	100	100	53	100	100	38	24
Mebendazole F ₁	[M+H] ⁺	264.0768	1	5	33	100	-	13	100	100
Mebendazole F ₂	C ₁₅ H ₉ N ₃ O ₂	105.0335	-	-	-	-	-	-	-	23
Meclofenamic acid	C ₇ H ₅ O	296.0240	100	34	-	-	100	7	-	-
Meclofenamic acid F ₁	[M+H] ⁺	278.0134	28	100	49	28	13	100	59	12
Meclofenamic acid F ₂	C ₁₄ H ₁₀ Cl ₂ NO	243.0445	46	76	100	100	-	48	100	100
Mefenamic acid	C ₁₄ H ₁₀ ClNO	242.1176	100	41	2	-	100	11	1	2
Mefenamic acid F ₁	[M+H] ⁺	224.1070	23	100	100	100	5	100	100	67
	C ₁₅ H ₁₄ NO ₂									

Mefenamic acid F ₂	C ₁₄ H ₁₁ NO	209.0835	-	1	4	21	-	-	10	100
Mefenamic acid F ₃	C ₁₃ H ₁₀ N	180.0808	-	-	1	5	-	-	-	9
Menadione	[M-H] ⁻	253.0171	100	51	46	66	100	27	14	9
Menadione F ₁	H ₃ O ₃	80.9652	23	100	100	100	5	100	100	100
Metformin	[M+H] ⁺	130.1087	100	100	35	15	73	100	5	8
Metformin F ₁	C ₄ H ₉ N ₄	113.0822	2	21	31	16	-	15	5	1
Metformin F ₂	C ₃ H ₁₀ N ₃	88.0869	3	32	44	14	-	28	13	1
Metformin F ₃	C ₂ H ₅ N ₄	85.0509	3	25	45	21	-	31	18	6
Metformin F ₄	C ₃ H ₇ N ₂	71.0604	2	27	100	10	-	39	100	100
Metformin F ₅	C ₄ H ₂ N	64.0182	-	-	-	-	100	49	4	-
Metronidazole	[M+H] ⁺	172.0717	100	51	20	18	100	66	15	9
Metronidazole F ₁	C ₄ H ₆ N ₃ O ₂	128.0456	23	100	100	58	-	100	100	20
Metronidazole F ₂	C ₆ H ₇ O ₂	111.0441	-	-	-	-	-	-	6	6
Metronidazole F ₃	C ₄ H ₆ N ₂	82.0525	2	11	52	100	-	3	61	100
Miconazole	[M+H] ⁺	414.9933	100	100	100	100	100	100	83	5
Miconazole F ₁	C ₁₀ H ₉ Cl ₂ N ₂	227.0137	-	-	-	-	-	1	11	1
Miconazole F ₂	C ₇ H ₅ Cl ₂	158.9760	-	-	10	83	-	1	100	100
Miconazole F ₃	C ₃ H ₅ N ₂	69.0447	-	-	-	-	-	-	21	11
Minocycline	[M+H] ⁺	458.1922	100	100	100	100	53	30	56	100
Minocycline F ₁	C ₁₉ H ₁₈ N	250.0651	-	-	-	-	100	100	100	10
Minocycline F ₂	C ₂₃ H ₂₆ N ₂ O ₇	221.0865	89	36	2	-	16	43	61	45
Minocycline F ₃	C ₂₂ H ₂₃ N ₂ O ₇	213.5746	5	15	2	-	-	3	30	17
Monensin	[M+H] ⁺	671.4635	-	-	-	-	-	-	-	-
Monensin F ₁	C ₃₆ H ₆₁ O ₁₀	653.4154	1	2	3	13	8	38	-	-
Monensin F ₂	C ₃₆ H ₅₉ O ₉	635.4154	9	10	15	41	12	100	72	-
Monensin F ₃	C ₃₆ H ₅₇ O ₈	617.4048	3	3	5	13	9	30	87	56
Monensin F ₄	C ₃₆ H ₅₅ O ₇	599.3942	-	-	-	-	-	-	7	7
Monensin F ₅	C ₂₈ H ₄₅ O ₅	461.3262	-	-	-	-	4	16	100	100
Monensin F ₆	C ₂₈ H ₄₃ O ₄	443.3156	-	-	-	-	-	-	7	30
Monensin F ₇	C ₁₇ H ₇ O ₃	279.1953	-	-	-	-	-	-	5	-
Monensin F ₈	C ₁₅ H ₂₇ O ₄	267.1591	-	-	-	-	-	-	-	12

Monensin	$C_{36}H_{62}O_{11}$	$[M+NH_4]^+$	688.4633	100	100	100	100	100	100	50	-	-
Naproxen	$C_{14}H_{14}O_3$	$[M+H]^+$	231.1016	100	57	5	-	100	45	2	-	-
Naproxen F ₁	$C_{13}H_{13}O$	$C_{13}H_{13}O$	185.0961	36	100	100	100	7	100	100	100	100
Naproxen F ₂	$C_{12}H_{10}O$	$C_{12}H_{10}O$	170.0726	-	3	8	28	-	-	-	11	64
Naproxen F ₃	$C_{12}H_9$	$C_{12}H_9$	153.0699	-	1	4	24	-	-	-	-	27
Naproxen F ₄	$C_{11}H_9$	$C_{11}H_9$	141.0699	-	1	3	19	-	-	-	-	-
Naproxen	$C_{14}H_{14}O_3$	$[M+Na]^+$	253.0835	-	7	2	1	5	5	3	-	3
Natamycin	$C_{33}H_{47}NO_{13}$	$[M+H]^+$	666.3120	100	100	98	7	100	-	-	-	12
Natamycin F ₁	$C_{33}H_{46}NO_{12}$	$C_{33}H_{46}NO_{12}$	648.3015	7	12	34	10	33	31	15	23	23
Natamycin F ₂	$C_{27}H_{35}O_9$	$C_{27}H_{35}O_9$	503.2276	8	19	100	100	33	93	39	50	50
Natamycin F ₃	$C_{27}H_{33}O_8$	$C_{27}H_{33}O_8$	485.2170	1	4	30	43	7	100	100	52	52
Natamycin F ₄	$C_{27}H_{31}O_7$	$C_{27}H_{31}O_7$	467.2060	-	-	-	-	3	42	76	-	-
Natamycin	$C_{33}H_{47}NO_{13}$	$[M+Na]^+$	688.2940	-	-	-	-	5	17	46	-	100
Nicotine	$C_{10}H_{14}N_2$	$[M+H]^+$	163.1230	100	100	22	5	100	100	23	8	8
Nicotine F ₁	$C_9H_{10}N$	$C_9H_{10}N$	132.0808	7	57	100	100	-	30	62	18	18
Nicotine F ₂	C_9H_8N	C_9H_8N	130.0651	-	-	-	-	-	10	100	100	100
Nicotine F ₃	C_7H_8N	C_7H_8N	106.0651	-	-	-	-	-	13	35	28	28
Nifuroxazide	$C_{12}H_9N_3O_5$	$[M+H]^+$	276.0615	100	100	61	13	100	100	50	-	-
Nifuroxazide	$C_{12}H_9N_3O_5$	$[M+Na]^+$	298.0434	10	13	100	100	10	22	100	100	100
Norfloxacina	$C_{16}H_{18}FN_3O_3$	$[M+H]^+$	320.1405	100	100	100	43	100	100	47	9	9
Norfloxacina F ₁	$C_{16}H_{17}FN_3O_2$	$C_{16}H_{17}FN_3O_2$	302.1299	1	6	35	100	-	9	73	70	70
Norfloxacina F ₂	$C_{15}H_{19}FN_3O$	$C_{15}H_{19}FN_3O$	276.1507	-	3	26	58	-	12	100	44	44
Norfloxacina F ₃	$C_{15}H_{18}N_3O$	$C_{15}H_{18}N_3O$	256.1444	-	-	-	-	-	-	15	26	26
Norfloxacina F ₄	$C_{13}H_{14}FN_2O$	$C_{13}H_{14}FN_2O$	233.1085	-	1	6	43	-	-	36	100	100
Norfloxacina F ₅	$C_{12}H_8FN_2O_2$	$C_{12}H_8FN_2O_2$	231.0564	-	2	3	5	-	-	1	9	9
Norfloxacina F ₆	$C_{12}H_{12}FN_2O$	$C_{12}H_{12}FN_2O$	219.0928	-	-	-	-	-	-	7	22	22
Norfloxacina F ₇	$C_{11}H_{10}FN_2O$	$C_{11}H_{10}FN_2O$	205.0772	-	-	-	-	-	-	-	23	23
Orbifloxacina	$C_{19}H_{20}F_3N_3O_3$	$[M+H]^+$	396.1530	100	100	100	100	100	100	100	100	100
Orbifloxacina F ₁	$C_{18}H_{21}F_3N_3O$	$C_{18}H_{21}F_3N_3O$	352.1631	-	2	12	60	-	12	100	26	26
Orbifloxacina F ₂	$C_{15}H_{14}F_3N_2O$	$C_{15}H_{14}F_3N_2O$	295.1093	-	-	3	30	-	-	50	100	100
Orbifloxacina F ₃	$C_{14}H_6N_2O_3$	$C_{14}H_6N_2O_3$	267.0400	-	-	-	-	-	-	-	17	17

Oxacillin	$C_{19}H_{19}N_3O_5S$	$[M+H]^+$	402.1118	59	36	88	100	40	13	10	12
Oxacillin F ₁	$C_{13}H_{11}N_2O_3$		243.0764	6	12	25	15	6	41	25	12
Oxacillin F ₂	$C_6H_{10}NO_2S$		160.0427	11	21	82	52	13	100	100	100
Oxacillin F ₃	C_9H_6NO		144.0444	-	5	30	65	1	-	34	100
Oxacillin	$C_{20}H_{22}N_3O_5S$	$[M+CH_3OH]^+$	434.1380	100	100	100	16	100	32	2	-
Oxolinic acid	$C_{13}H_{11}NO_5$	$[M+H]^+$	262.0710	100	81	6	1	100	48	4	-
Oxolinic acid F ₁	$C_{13}H_{10}NO_4$		244.0604	12	100	100	100	1	100	100	100
Oxolinic acid F ₂	$C_{11}H_6NO_4$		216.0291	-	1	3	18	-	-	2	30
Oxolinic acid F ₃	$C_{11}H_5NO_4$		215.0213	-	-	1	6	-	-	-	-
Oxolinic acid F ₄	$C_{10}H_6NO_2$		172.0393	-	-	-	1	-	-	-	-
Oxolinic acid F ₅	$C_9H_6NO_2$		160.0393	-	-	1	-	-	-	-	-
Oxybendazole	$C_{12}H_{15}N_3O_3$	$[M+H]^+$	250.1186	100	100	100	62	100	100	100	39
Oxybendazole F ₁	$C_{11}H_{12}N_3O_2$		218.0924	4	26	86	100	-	19	100	100
Oxybendazole F ₂	$C_8H_6N_3O_3$		176.0455	1	5	29	98	-	-	22	77
Oxytetracycline	$C_{22}H_{24}N_2O_9$	$[M+H]^+$	461.1555	100	100	100	22	100	79	-	-
Oxytetracycline F ₁	$C_{22}H_{22}NO_9$		444.1289	1	7	54	61	-	53	4	11
Oxytetracycline F ₂	$C_{22}H_{20}NO_8$		426.1183	-	4	40	100	-	100	100	100
Oxytetracycline F ₃	$C_{22}H_{18}NO_7$		408.1078	-	-	-	-	-	-	5	24
Oxytetracycline F ₄	$C_{20}H_{13}O_8$		381.0605	-	-	-	-	-	-	8	47
Oxytetracycline F ₅	$C_{20}H_{13}O_7$		365.0656	-	-	-	-	-	9	2	67
Oxytetracycline F ₆	$C_{19}H_{13}O_6$		337.0707	-	-	-	-	-	-	3	98
Oxytetracycline F ₇	$C_{10}H_{13}NO_5$		226.0710	-	-	-	-	-	-	6	29
Penicillin G	$C_{16}H_{18}N_2O_4S$	$[M+H]^+$	335.1060	100	100	100	100	-	24	6	-
Penicillin G F ₁	$C_{10}H_{10}NO_2$		176.0706	-	3	2	4	-	-	6	7
Penicillin G F ₂	$C_6H_{10}NO_2S$		160.0427	72	49	41	51	8	100	100	100
Penicillin G F ₃	C_3H_8NS		114.0372	-	7	6	28	-	-	8	67
Penicillin G	$C_{16}H_{18}N_2O_4S$	$[M+CH_3OH]^+$	367.1322	-	-	-	-	100	52	1	2
Penicillin V	$C_{16}H_{18}N_2O_5S$	$[M+H]^+$	351.1009	2	14	100	83	-	20	-	-
Penicillin V F ₁	$C_6H_{10}NO_2S$		160.0427	2	11	72	100	-	100	100	100
Penicillin V	$C_{16}H_{18}N_2O_5S$	$[M+CH_3OH]^+$	383.1271	100	100	77	22	100	40	-	-
Pentylentetrazole	$C_6H_{10}N_4$	$[M+H]^+$	139.0978	100	100	95	66	100	100	79	53

Pentylentetrazole F ₁	C ₆ H ₁₀ N	96.0808	9	42	100	100	100	100	100	100	100	100	100	100
Phenylbutazone	[M+] ⁺	309.1598	100	100	100	100	100	100	100	100	100	100	100	100
Phenylbutazone F ₁	C ₁₃ H ₁₁ N ₂ O	211.0866	-	-	-	-	-	-	-	-	-	-	-	66
Phenylbutazone F ₂	C ₁₂ H ₁₄ NO	188.1070	-	1	9	27	-	12	59	29	9	46	31	31
Phenylbutazone F ₃	C ₁₁ H ₁₄ N	160.1121	-	-	5	40	-	2	41	39	2	41	39	29
Phenylbutazone F ₄	C ₈ H ₆ NO	132.0444	-	-	2	14	-	-	13	26	-	13	26	26
Phenylbutazone F ₅	C ₇ H ₆ NO	120.0444	-	2	15	58	-	9	100	91	9	100	91	91
Phenylbutazone F ₆	C ₆ H ₆ N	92.0495	-	-	4	37	-	-	24	100	-	24	100	100
Phenylbutazone F ₇	C ₆ H ₅	77.0386	-	-	-	4	-	-	6	45	-	6	45	45
Pravastatin	[M+] ⁻	423.2388	100	100	100	100	100	100	100	100	100	100	100	100
Pravastatin F ₁	C ₁₈ H ₂₅ O ₅	321.1707	1	3	10	21	-	8	7	27	-	7	27	27
Pravastatin F ₂	C ₅ H ₉ O ₂	101.0608	-	-	3	17	-	-	8	24	-	8	24	24
Prednisolone	[M+] ⁺	361.2010	100	100	32	31	100	90	43	7	100	90	43	7
Prednisolone F ₁	C ₂₁ H ₂₆ O ₄	343.1904	11	72	100	100	-	100	100	52	-	100	100	52
Prednisolone F ₂	C ₂₁ H ₂₄ O ₃	325.1798	3	18	38	43	7	37	35	19	7	37	35	19
Prednisolone F ₃	C ₂₁ H ₂₃ O ₂	307.1685	-	-	-	-	4	31	35	17	4	31	35	17
Prednisolone F ₄	C ₂₁ H ₂₁ O	289.1578	-	-	-	-	1	17	31	16	1	17	31	16
Prednisolone F ₅	C ₁₀ H ₁₁ O	147.0797	-	-	-	-	1	22	89	100	1	22	89	100
Promethazine	[M+] ⁺	198.0372	100	100	100	100	100	100	100	100	100	100	100	100
Promethazine F ₁	C ₁₁ H ₈ N	154.0651	-	-	-	2	-	-	-	-	2	-	-	-
Promethazine F ₂	C ₄ H ₉ N	71.0730	-	-	-	-	-	-	-	38	-	-	-	38
Propranolol	[M+] ⁺	260.1645	100	100	100	100	100	100	42	21	100	100	42	21
Propranolol F ₁	C ₁₃ H ₁₁ O	183.0804	-	2	13	70	-	4	57	19	2	13	70	19
Propranolol F ₂	C ₁₂ H ₁₁	157.0648	-	-	9	100	-	2	32	34	9	100	32	34
Propranolol F ₃	C ₆ H ₁₄ NO	116.1070	-	1	10	38	-	7	100	50	1	10	38	50
Propranolol F ₄	C ₃ H ₈ NO	74.0600	-	-	3	23	-	-	55	100	-	3	23	100
Ranitidine	[M+] ⁺	315.1485	100	100	30	13	100	100	1	-	100	100	1	-
Ranitidine F ₁	C ₁₁ H ₁₆ N ₃ O ₃ S	270.0907	5	54	100	25	-	30	-	-	5	54	100	25
Ranitidine F ₂	C ₅ H ₁₀ N ₃ O ₂ S	176.0488	2	16	86	100	-	1	100	23	2	16	86	100
Ranitidine F ₃	C ₆ H ₅ OS	125.0056	-	-	-	-	-	1	26	81	-	-	-	81
Ranitidine F ₄	C ₄ H ₈ NS	102.0372	-	-	-	-	-	-	9	100	-	-	-	100

Ranitidine	$C_{13}H_{22}N_4O_3S$	$[M+2H]^{2+}$	158.0779	-	-	-	-	-	3	-	-	-
Robenidine	$C_{18}H_{23}NO_3$	$[M+H]^+$	302.1751	100	100	41	11	100	32	14	7	-
Robenidine F ₁	$C_{18}H_{22}NO_2$	$C_{18}H_{22}NO_2$	284.1605	8	50	100	28	-	100	14	-	-
Robenidine F ₂	$C_8H_{10}O_2$	$C_8H_{10}O_2$	136.0757	1	4	35	56	-	-	-	26	-
Robenidine F ₃	C_7H_7O	C_7H_7O	107.0491	1	4	41	100	-	-	100	100	-
Ronidazole	$C_6H_8N_4O_4$	$[M+H]^+$	201.0618	51	8	35	100	100	6	20	55	-
Ronidazole F ₁	$C_5H_6N_3O_2$	$C_5H_6N_3O_2$	140.0455	100	100	100	97	24	100	100	100	-
Ronidazole	$C_6H_8N_4O_4$	$[M+Na]^+$	223.0438	-	-	-	-	9	8	33	77	-
Roxithromycin	$C_{41}H_{76}N_2O_{15}$	$[M+H]^+$	837.5318	100	100	100	100	100	100	19	-	-
Roxithromycin F ₁	$C_{33}H_{63}N_2O_{12}$	$C_{33}H_{63}N_2O_{12}$	679.4376	-	-	1	6	-	19	100	44	-
Roxithromycin F ₂	$C_8H_{16}NO_2$	$C_8H_{16}NO_2$	158.1176	-	-	-	-	-	5	21	100	-
Roxithromycin	$C_{41}H_{76}N_2O_{15}$	$[M+2H]^{2+}$	419.2696	21	7	-	-	12	-	-	-	-
Salbutamol	$C_{13}H_{21}NO_3$	$[M+H]^+$	240.1594	100	100	8	5	100	20	2	8	-
Salbutamol F ₁	$C_{13}H_{20}NO_2$	$C_{13}H_{20}NO_2$	222.1489	9	54	8	2	10	93	2	-	-
Salbutamol F ₂	$C_9H_{12}NO_2$	$C_9H_{12}NO_2$	166.0863	7	92	49	14	1	72	4	-	-
Salbutamol F ₃	$C_9H_{10}NO$	$C_9H_{10}NO$	148.0757	6	66	100	100	-	100	100	100	-
Sarafloxacin	$C_{20}H_{17}F_2N_3O_3$	$[M+H]^+$	386.1311	100	100	100	100	100	100	69	4	-
Sarafloxacin F ₁	$C_{20}H_{16}F_2N_3O_2$	$C_{20}H_{16}F_2N_3O_2$	368.1205	-	2	12	69	-	4	54	26	-
Sarafloxacin F ₂	$C_{19}H_{18}F_2N_3O$	$C_{19}H_{18}F_2N_3O$	342.1412	-	1	10	57	-	5	100	24	-
Sarafloxacin F ₃	$C_{20}H_{12}FN_2$	$C_{20}H_{12}FN_2$	299.0979	-	-	2	25	-	-	34	100	-
Spiramycin	$C_{43}H_{74}N_2O_{14}$	$[M+H]^+$	843.5213	19	26	92	63	8	72	30	20	-
Spiramycin F ₁	$C_{36}H_{63}N_2O_{11}$	$C_{36}H_{63}N_2O_{11}$	699.4426	1	8	39	4	-	22	-	-	-
Spiramycin F ₂	$C_{28}H_{46}NO_9$	$C_{28}H_{46}NO_9$	540.3167	-	4	43	12	-	83	5	5	-
Spiramycin F ₃	$C_{19}H_{38}N_2O_8$	$C_{19}H_{38}N_2O_8$	422.2623	-	-	-	-	100	9	-	-	-
Spiramycin F ₄	$C_8H_{16}NO_3$	$C_8H_{16}NO_3$	174.1125	-	-	-	-	-	40	100	100	-
Spiramycin F ₅	$C_5H_6O_2$	$C_5H_6O_2$	101.0597	-	-	-	-	-	10	54	51	-
Spiramycin	$C_{43}H_{74}N_2O_{14}$	$[M+2H]^{2+}$	342.7000	-	-	-	-	-	-	7	-	-
Streptomycin	$C_{21}H_{39}N_7O_{12}$	$[M+H]^+$	582.2729	-	-	11	28	100	100	100	100	-
Streptomycin F ₁	$C_8H_{19}N_6O_4$	$C_8H_{19}N_6O_4$	263.1462	100	100	100	100	-	-	37	-	-
Streptomycin F ₂	$C_8H_{16}N_5O_4$	$C_8H_{16}N_5O_4$	246.1197	-	20	36	45	-	-	-	-	-
Sulfabenzamide	$C_{13}H_{12}N_2O_3S$	$[M+H]^+$	277.0641	100	32	3	-	100	122	1	-	-

Sulfabenzamide F ₁	C ₆ H ₆ NO ₂ S	156.0114	23	100	12	-	8	100	78	31
Sulfabenzamide F ₂	C ₆ H ₆ NO	108.0444	5	31	59	68	-	8	65	65
Sulfabenzamide	[M+Na] ⁺	299.0460	9	33	100	100	10	52	100	35
Sulfacetamide	[M+H] ⁺	215.0485	83	6	-	-	100	12	-	-
Sulfacetamide F ₁	C ₆ H ₆ NO ₂ S	156.0114	100	100	12	5	17	100	61	6
Sulfacetamide F ₂	C ₆ H ₆ NO	108.0444	-	-	-	-	-	11	8	62
Sulfacetamide F ₃	C ₆ H ₆ N	92.0495	17	63	100	100	-	7	100	100
Sulfacetamide	[M+Na] ⁺	237.0304	17	42	37	52	-	39	39	11
Sulfachloropyridazine	[M+H] ⁺	285.0208	100	100	33	10	100	44	14	5
Sulfachloropyridazine F ₁	C ₆ H ₆ NO ₂ S	156.0114	9	93	78	22	-	100	100	18
Sulfachloropyridazine F ₂	C ₆ H ₆ NO	108.0444	3	30	88	92	-	6	93	72
Sulfachloropyridazine F ₃	C ₆ H ₆ N	92.0495	2	25	100	100	-	-	84	100
Sulfachloropyridazine	[M+Na] ⁺	307.0027	-	-	-	-	6	14	22	9
Sulfadiazine	[M+H] ⁺	251.0597	100	100	42	28	100	100	12	7
Sulfadiazine F ₁	C ₁₀ H ₉ N ₄	185.0822	-	-	11	12	3	1	7	4
Sulfadiazine F ₂	C ₄ H ₄ N ₃ O ₂ S	158.0019	2	5	12	6	-	13	16	3
Sulfadiazine F ₃	C ₆ H ₆ NO ₂ S	156.0114	4	37	61	13	-	89	74	14
Sulfadiazine F ₄	C ₆ H ₆ NO	108.0444	2	17	100	100	-	10	100	70
Sulfadiazine F ₅	C ₆ H ₆ N	92.0495	-	-	-	-	-	7	92	100
Sulfadiazine F ₆	[M+Na] ⁺	273.0417	-	-	-	-	6	43	47	11
Sulfadimethoxyn	[M+H] ⁺	311.0809	100	100	100	50	100	100	39	10
Sulfadimethoxyn F ₁	C ₁₂ H ₁₃ N ₄ O ₂	245.1033	-	1	3	10	-	2	27	-
Sulfadimethoxyn F ₂	C ₆ H ₁₀ N ₃ O ₂	156.0768	-	-	-	-	-	5	100	100
Sulfadimethoxyn F ₃	C ₆ H ₆ NO ₂ S	156.0114	-	1	24	100	-	5	60	18
Sulfadimethoxyn F ₄	C ₆ H ₆ NO	108.0444	-	-	-	-	-	1	34	88
Sulfadimethoxyn F ₅	C ₆ H ₆ N	92.0495	-	-	-	-	-	-	25	90
Sulfadimethoxyn	[M+Na] ⁺	333.0628	3	11	30	65	3	9	28	29
Sulfadoxine	[M+H] ⁺	311.0809	100	100	100	46	100	100	21	12
Sulfadoxine F ₁	C ₁₂ H ₁₃ N ₄ O ₂	245.1033	-	-	-	-	-	3	12	-
Sulfadoxine F ₂	C ₁₁ H ₁₂ N ₃ O ₂	218.0924	-	-	5	63	-	-	-	-
Sulfadoxine F ₃	C ₆ H ₁₀ N ₃ O ₂	156.0768	-	-	-	-	-	-	-	27

Sulfadoxine F ₄	C ₆ H ₆ NO ₂ S	156.0114	-	-	16	42	-	24	100	20
Sulfadoxine F ₅	C ₅ H ₆ N ₃ O ₂	140.0448	-	-	-	-	-	-	29	31
Sulfadoxine F ₆	C ₆ H ₆ NO	108.0444	-	-	-	-	-	1	56	94
Sulfadoxine F ₇	C ₆ H ₆ N	92.0495	-	-	-	-	-	-	40	100
Sulfadoxine	[M+Na] ⁺	333.0628	2	8	32	100	2	23	60	39
Sulfaguandine	C ₁₂ H ₁₄ N ₄ O ₂ S	215.0547	100	100	100	30	100	100	100	9
Sulfaguandine F ₁	[M+H] ⁺	156.0114	11	36	59	43	-	21	38	76
Sulfaguandine F ₂	C ₆ H ₆ NO ₂ S	108.0444	-	-	-	-	-	-	35	60
Sulfaguandine F ₃	C ₆ H ₆ NO	92.0495	3	14	75	100	-	-	40	100
Sulfaguandine F ₄	C ₆ H ₆ N	60.0556	-	-	-	-	-	24	61	98
Sulfaguandine	CH ₆ N ₃	237.0417	-	-	-	-	-	6	15	22
Sulfaguandine	[M+Na] ⁺	265.0754	100	100	100	24	100	100	23	9
Sufamerazine	[M+H] ⁺	172.0175	1	4	28	13	-	33	84	11
Sufamerazine F ₁	C ₅ H ₆ N ₃ O ₂ S	156.0114	1	9	55	14	-	33	90	9
Sufamerazine F ₂	C ₆ H ₆ NO ₂ S	110.0713	-	9	99	100	-	8	84	49
Sufamerazine F ₃	C ₅ H ₈ N ₃	108.0444	-	-	-	-	-	-	100	74
Sufamerazine F ₄	C ₆ H ₆ NO	92.0495	-	-	-	-	-	-	94	100
Sufamerazine F ₅	C ₆ H ₆ N	287.0573	-	-	-	-	2	12	27	8
Sufamerazine	[M+Na] ⁺	281.0703	100	100	100	68	100	100	25	7
Sulfameter	[M+H] ⁺	215.0926	-	-	-	-	-	4	38	17
Sulfameter F ₁	C ₁₁ H ₁₁ N ₄ O	188.0124	-	-	-	-	-	6	27	5
Sulfameter F ₂	C ₅ H ₇ N ₃ O ₃ S	172.0717	-	-	-	-	-	-	-	6
Sulfameter F ₃	C ₆ H ₁₀ N ₃ O ₃	156.0114	-	6	42	19	-	11	100	26
Sulfameter F ₄	C ₆ H ₆ NO ₂ S	126.0662	-	5	57	100	-	-	44	55
Sulfameter F ₅	C ₅ H ₈ N ₃ O	124.0505	-	-	-	-	-	-	3	5
Sulfameter F ₆	C ₅ H ₆ N ₃ O	108.0444	-	3	36	75	-	-	55	100
Sulfameter F ₇	C ₆ H ₆ NO	92.0495	-	2	31	70	-	-	-	-
Sulfameter F ₈	C ₆ H ₆ N	80.0495	-	-	3	15	-	-	-	-
Sulfameter F ₉	C ₅ H ₆ N	303.0522	-	-	-	-	-	5	23	16
Sulfameter	[M+Na] ⁺	279.0910	100	100	100	27	100	100	17	13
Sulfamethazine	[M+H] ⁺	213.1135	-	-	4	10	-	-	10	11
Sulfamethazine F ₁	C ₁₂ H ₁₃ N ₄									

Sulfamethazine F ₂	C ₆ H ₈ N ₃ O ₂ S	186.0332	-	3	19	20	-	35	100	29
Sulfamethazine F ₃	C ₆ H ₆ NO ₂ S	156.0114	-	2	13	12	-	8	34	100
Sulfamethazine F ₄	C ₆ H ₁₀ N ₃	124.0869	-	5	45	100	-	5	52	93
Sulfamethazine F ₅	C ₆ H ₆ NO	108.0444	-	1	11	29	-	-	30	82
Sulfamethazine F ₆	C ₆ H ₆ N	92.0495	-	-	-	-	-	-	26	100
Sulfamethazine	[M+Na] ⁺	301.0730	-	-	-	-	2	8	12	14
Sulfamethizole	[M+H] ⁺	271.0318	100	100	100	44	100	100	92	24
Sulfamethizole F ₁	C ₆ H ₆ NO ₂ S	156.0114	11	48	48	71	1	93	100	77
Sulfamethizole F ₂	C ₃ H ₆ N ₃ S	116.0277	-	3	10	20	-	-	-	8
Sulfamethizole F ₃	C ₆ H ₆ NO	108.0444	3	15	52	95	-	-	81	71
Sulfamethizole F ₄	C ₆ H ₆ N	92.0495	3	14	59	100	-	-	80	100
Sulfamethoxazole	[M+H] ⁺	254.0594	100	100	38	5	100	100	13	-
Sulfamethoxazole F ₁	C ₆ H ₆ NO ₂ S	156.0114	3	31	62	10	-	68	68	6
Sulfamethoxazole F ₂	C ₆ H ₆ NO	108.0444	1	13	92	92	-	9	100	71
Sulfamethoxazole F ₃	C ₄ H ₇ N ₂ O	99.0553	-	8	33	14	-	7	28	13
Sulfamethoxazole F ₄	C ₆ H ₆ N	92.0495	1	12	100	100	-	6	100	100
Sulfamethoxazole	[M+Na] ⁺	276.0413	-	-	-	-	13	64	82	23
Sulfamethoxypridazine	C ₁₀ H ₁₁ N ₃ O ₃ S	281.0703	100	100	100	68	100	100	91	69
Sulfamethoxypridazine F ₁	C ₁₁ H ₁₁ N ₄ O	215.0926	-	-	-	-	-	1	6	3
Sulfamethoxypridazine F ₂	C ₃ H ₇ N ₃ O ₃ S	188.0124	-	-	-	-	-	1	6	3
Sulfamethoxypridazine F ₃	C ₆ H ₁₀ N ₃ O ₃	172.0717	-	-	-	-	-	-	-	1
Sulfamethoxypridazine F ₄	C ₆ H ₆ NO ₂ S	156.0114	-	6	35	41	-	18	100	39
Sulfamethoxypridazine F ₅	C ₅ H ₈ N ₃ O	126.0667	-	5	39	100	-	6	50	59
Sulfamethoxypridazine F ₆	C ₅ H ₆ N ₃ O	124.0505	-	-	-	-	-	-	1	1
Sulfamethoxypridazine F ₇	C ₆ H ₆ NO	108.0444	-	3	25	83	-	-	44	100
Sulfamethoxypridazine F ₈	C ₆ H ₆ N	92.0495	-	2	21	78	-	-	-	-
Sulfamethoxypridazine F ₉	C ₅ H ₆ N	80.0495	-	-	3	15	-	-	-	-
Sulfamethoxypridazine	[M+Na] ⁺	303.0522	-	-	-	-	-	3	5	5
Sulfamonomethoxyne	[M+H] ⁺	281.0703	100	100	100	28	100	100	35	12
Sulfamonomethoxyne F ₁	C ₁₁ H ₁₁ N ₄ O	215.0927	-	-	-	-	-	7	41	5
Sulfamonomethoxyne F ₂	C ₃ H ₆ N ₃ O ₃ S	188.0124	-	-	-	-	-	3	17	2

Sulfamonomethoxyne F ₃	C ₆ H ₆ NO ₂ S	156.0114	2	9	33	27	-	93	100	14
Sulfamonomethoxyne F ₄	C ₅ H ₈ N ₃ O	126.0667	1	7	55	100	-	6	81	41
Sulfamonomethoxyne F ₅	C ₆ H ₆ NO	108.0444	-	3	25	88	-	2	85	84
Sulfamonomethoxyne F ₆	C ₆ H ₆ N	92.0495	-	3	26	96	-	-	70	100
Sulfamonomethoxyne F ₇	C ₅ H ₆ N	80.0495	-	-	3	18	-	-	-	-
Sulfamonomethoxyne	[M+Na] ⁺	303.1512	-	-	-	-	3	7	20	6
Sulfanilamide	[M+H] ⁺	173.0379	100	100	100	29	100	100	100	31
Sulfanilamide F ₁	C ₆ H ₆ NO ₂ S	156.0114	-	-	-	-	69	78	26	4
Sulfanilamide F ₂	C ₆ H ₆ NO	108.0444	35	58	54	25	-	24	57	33
Sulfanilamide F ₃	C ₆ H ₇ N	93.0573	3	13	61	100	-	-	58	100
Sulfanilamide F ₄	C ₆ H ₆ N	92.0495	35	63	59	22	-	29	85	55
Sulfanilamide F ₅	C ₅ H ₆ N	80.0495	5	13	39	42	-	-	6	9
Sulfanilamide F ₆	C ₆ H ₄	76.0308	-	-	2	6	-	-	-	3
Sulfanilamide F ₇	C ₅ H ₆	66.0464	-	-	-	3	-	-	-	7
Sulfanilamide	[M+Na] ⁺	195.0199	-	-	-	-	9	11	8	6
Sulfapyridine	[M+H] ⁺	250.0645	100	100	100	40	100	40	9	39
Sulfapyridine F ₁	C ₁₁ H ₁₀ N ₃	184.0869	-	6	50	65	14	42	16	42
Sulfapyridine F ₂	C ₆ H ₆ NO ₂ S	156.0114	-	13	61	18	81	100	30	100
Sulfapyridine F ₃	C ₆ H ₆ NO	108.0444	-	5	65	91	6	99	76	100
Sulfapyridine F ₄	C ₆ H ₆ N	92.0495	-	-	70	100	-	95	100	97
Sulfathiazole	[M+H] ⁺	256.0209	100	100	100	17	100	59	34	9
Sulfathiazole F ₁	C ₆ H ₆ NO ₂ S	156.0114	9	33	58	75	-	100	99	29
Sulfathiazole F ₂	C ₆ H ₆ NO	108.0444	2	11	51	100	-	7	100	75
Sulfathiazole F ₃	C ₃ H ₅ N ₂ S	101.0168	1	5	17	42	-	-	6	5
Sulfathiazole F ₄	C ₆ H ₆ N	92.0495	-	-	-	-	-	4	97	100
Sulfathiazole	[M+Na] ⁺	278.0028	-	-	-	-	1	7	9	4
Sulfisoxazol	[M+H] ⁺	268.0750	100	100	29	32	100	57	7	-
Sulfisoxazol F ₁	C ₆ H ₆ NO ₂ S	156.0114	-	-	-	-	-	100	61	8
Sulfisoxazol F ₂	C ₆ H ₆ NOS	140.0165	-	-	-	-	-	-	5	5
Sulfisoxazol F ₃	C ₅ H ₉ N ₂ O	113.0709	3	39	100	100	-	60	100	26
Sulfisoxazol F ₄	C ₆ H ₆ NO	108.0444	-	-	-	-	-	11	88	72

Sulfisoxazol F ₅	C ₆ H ₆ N	92.0495	-	-	-	-	-	-	-	-	-	6	87	100
Sulfisoxazol F ₆	C ₄ H ₈ NO	86.0600	-	-	-	-	-	-	-	-	-	-	6	-
Sulfisoxazol F ₇	C ₃ H ₆ N ₂	71.0604	-	-	-	-	-	-	-	-	-	-	6	7
Sulfisoxazol	[M+Na] ⁺	290.0570	-	-	-	-	-	-	-	-	5	32	41	18
Sulindac	[M+H] ⁺	357.0955	100	100	100	100	100	100	100	100	100	100	100	63
Sulindac F ₁	C ₂₀ H ₁₇ FO ₃ S	340.0928	-	-	-	-	-	7	9	88	50	15	19	19
Sulindac F ₂	C ₁₈ H ₁₄ FOS	297.0744	-	-	-	-	-	-	-	-	-	-	14	52
Sulindac F ₃	C ₁₉ H ₁₆ FS	295.0951	-	-	-	-	-	-	-	-	-	-	9	24
Sulindac F ₄	C ₁₈ H ₁₃ FS	280.0717	-	-	-	-	-	-	-	-	-	-	6	21
Sulindac F ₅	C ₁₈ H ₁₃ F	248.0996	-	-	-	-	-	-	-	-	-	18	19	55
Sulindac F ₆	C ₁₄ H ₁₀ F	233.0761	-	-	-	-	-	-	-	-	-	-	3	5
Sulindac	[M+Na] ⁺	379.0775	-	-	-	-	-	-	-	-	-	-	3	9
Tetracycline	[M+H] ⁺	445.1605	100	100	100	100	13	100	100	100	100	100	3	-
Tetracycline F ₁	C ₂₂ H ₂₄ N ₂ O ₈	428.1340	-	6	50	30	-	-	-	-	-	-	-	-
Tetracycline F ₂	C ₂₂ H ₂₃ N ₂ O ₇	427.1500	-	-	-	-	-	-	-	69	10	-	-	-
Tetracycline F ₃	C ₂₂ H ₂₀ NO ₇	410.1234	-	5	58	100	-	-	-	22	100	22	100	58
Tetracycline F ₄	C ₇ H ₈ NO ₃	154.0499	-	-	2	6	-	-	-	-	-	-	17	100
Theobromine	[M+H] ⁺	181.0720	100	100	100	100	100	100	100	100	100	100	100	100
Theobromine F ₁	C ₆ H ₈ N ₃ O	138.0662	2	12	42	63	-	6	6	57	47	-	-	-
Theobromine F ₂	C ₅ H ₈ N ₃	110.0713	-	-	-	-	-	-	-	21	34	-	-	-
Theobromine	[M+Na] ⁺	203.0539	-	-	-	-	-	-	5	3	5	12	-	-
Theophylline	[M+H] ⁺	181.072	100	100	95	40	100	100	100	100	100	100	46	-
Theophylline F ₁	C ₅ H ₆ N ₃ O	124.0506	3	18	100	100	-	7	92	100	100	100	100	100
Theophylline	[M+Na] ⁺	203.0539	-	-	-	-	-	5	8	23	41	-	-	-
Thiamphenicol	[M-H] ⁻	353.9975	100	100	100	30	100	100	100	100	47	39	-	-
Thiamphenicol F ₁	C ₁₁ H ₁₂ NO ₅ S	270.0442	2	5	19	10	-	8	-	-	-	-	-	-
Thiamphenicol F ₂	C ₈ H ₉ O ₃ S	185.0278	2	7	54	100	-	-	-	100	100	100	100	100
Thiamphenicol	[M-Cl] ⁻	389.9742	30	5	1	-	-	-	-	-	-	-	-	-
Tilmicosin	[M+H] ⁺	869.5733	31	31	54	100	22	39	100	100	100	100	100	100
Tilmicosin F ₁	C ₃₈ H ₆₇ N ₂ O ₉	695.4849	-	-	-	-	-	-	-	11	37	-	-	-
Tilmicosin F ₂	C ₈ H ₁₆ NO ₃	174.1125	-	-	-	-	-	-	-	-	-	-	29	33

Tilmicosin	$C_{46}H_{80}N_2O_{13}$	$[M+2H]^{2+}$	435.2903	100	100	100	100	38	100	100	100	-	-
Tolfenamic acid	$C_{14}H_{12}ClNO_2$	$[M+H]^+$	262.0629	100	33	2	100	-	100	11	-	-	-
Tolfenamic acid F ₁	$C_{14}H_{11}ClNO$		244.0524	27	100	100	100	100	6	100	100	33	-
Tolfenamic acid F ₂	$C_{11}H_{14}ClN_2$		209.0480	-	-	-	-	-	-	-	17	54	-
Tolfenamic acid F ₃	$C_{13}H_{10}N$		180.0808	-	-	-	-	-	-	-	-	9	-
Tolmetin	$C_{15}H_{15}NO_3$	$[M+H]^+$	258.1125	100	100	46	100	8	100	30	13	-	-
Tolmetin F ₁		C_8H_7O	119.0491	5	27	100	100	100	-	100	100	100	100
Trimethoprim	$C_{14}H_{18}N_4O_3$	$[M+H]^+$	291.1451	100	100	100	100	100	100	100	100	100	100
Trimethoprim F ₁	$C_{13}H_{15}N_4O_3$		275.1139	-	-	-	-	-	-	-	14	55	-
Trimethoprim F ₂	$C_{12}H_{13}N_4O_3$		261.0982	-	-	-	-	-	-	-	21	94	-
Trimethoprim F ₃	$C_{15}H_{16}NO_3$		258.1125	-	-	-	-	-	-	-	6	8	-
Trimethoprim F ₄	$C_{13}H_{13}N_4O_2$		257.1033	-	-	-	-	-	-	-	-	45	-
Trimethoprim F ₅	$C_{12}H_{14}N_4O$		230.1162	-	-	-	-	-	-	-	41	100	-
Tylosin	$C_{46}H_{77}NO_{17}$	$[M+H]^+$	916.5264	100	100	100	100	100	100	100	100	100	100
Tylosin F ₁	$C_8H_{16}NO_3$		174.1125	-	-	-	-	-	-	-	-	15	-
Tylosin F ₂	$C_7H_{13}O_3$		145.0859	-	-	-	-	-	-	-	5	4	-
Tylosin F ₃	$C_5H_{11}NO$		101.0835	-	-	-	-	-	-	-	-	-	-
Tylosin F ₄	$C_5H_9O_2$		101.0597	-	-	-	-	-	-	-	-	13	29
β-Estradiol	$C_{18}H_{24}O_2$	$[M+H]^+$	273.1849	31	23	7	-	-	6	6	-	-	-
β-Estradiol F ₁	$C_{18}H_{23}O$		255.1743	100	100	45	10	43	81	-	-	-	-
β-Estradiol F ₂	$C_{11}H_{11}O$		159.0804	-	33	77	100	-	6	100	100	100	100
β-Estradiol F ₃	C_7H_7O		107.0491	61	88	100	71	-	-	-	13	12	-
Food packaging contaminants													
1,3-Phenylenediamine	$C_6H_8N_2$	$[M+H]^+$	109.0760	100	100	72	53	-	-	-	-	-	-
1,3-Phenylenediamine F ₁	C_6H_6N		92.0495	8	41	100	100	-	-	-	-	-	-
2-Ethylhexyl diphenyl phosphate	$C_{20}H_{27}O_4P$	$[M+H]^+$	363.1720	71	5	2	-	-	9	6	-	-	-
2-Ethylhexyl diphenyl phosphate F ₁	$C_{14}H_{10}O_4P$		273.0311	-	-	-	-	-	-	5	18	93	-
2-Ethylhexyl diphenyl phosphate F ₂	$C_{12}H_{12}O_4P$		251.0468	100	100	100	100	100	100	100	100	100	100
2-Ethylhexyl diphenyl phosphate F ₃	$C_{12}H_8O_2P$		215.0256	-	-	-	-	-	-	-	6	12	-
2-Ethylhexyl diphenyl phosphate F ₄	$C_6H_8O_4P$		175.0155	-	-	-	-	-	-	-	4	13	-

2-Ethylhexyl diphenyl phosphate F ₅	C ₅ H ₁₃ O ₃ P	153.0675	-	-	-	-	-	-	-	-	-	15	24
2-Ethylhexyl diphenyl phosphate F ₆	C ₆ H ₆ O	95.0491	-	-	-	-	-	-	-	-	-	6	18
2-Ethylhexyl diphenyl phosphate	[M+Na] ⁺	385.1539	23	16	18	39	26	58	92	93			
2-Methoxy-5-methylalanine	[M+H] ⁺	138.0913	100	73	10	2	100	90	12	21			
2-Methoxy-5-methylalanine F ₁	C ₇ H ₉ NO	123.0679	18	100	100	85	8	62	100	83			
2-Methoxy-5-methylalanine F ₂	C ₈ H ₁₁ N	122.0964	-	-	-	-	89	100	30	23			
2-Methoxy-5-methylalanine F ₃	C ₇ H ₈ NO	122.0600	2	9	23	100	-	1	10	85			
2-Methoxy-5-methylalanine F ₄	C ₇ H ₈ N	106.0651	1	7	10	25	1	3	18	100			
2-Methoxy-5-methylalanine F ₅	C ₆ H ₈ N	94.0651	-	2	5	23	-	-	-	19			
2-Methoxy-5-methylalanine F ₆	C ₆ H ₆	78.0474	-	2	5	24	-	-	8	83			
2,4-Diaminoanisole	[M+H] ⁺	139.0866	100	100	44	32	100	100	100	100			
2,4-Diaminoanisole F ₁	C ₆ H ₈ N ₂ O	124.0631	10	53	100	100	-	18	50	58			
2,4-Diaminoanisole F ₂	C ₇ H ₈ NO	122.0600	2	15	17	14	-	-	-	-			
2,4-Diaminotoluene	[M+H] ⁺	123.0917	100	100	66	39	100	100	98	48			
2,4-Diaminotoluene F ₁	C ₆ H ₉ N ₂	108.0685	-	-	-	-	-	-	-	100			
2,4-Diaminotoluene F ₂	C ₇ H ₈ N	106.0651	7	36	100	100	-	-	90	54			
2,4-Dimethylaniline	[M+H] ⁺	122.0964	100	100	70	23	100	100	100	53			
2,4-Dimethylaniline F ₁	C ₈ H ₉	105.0699	4	5	100	100	-	5	45	100			
2,4-Dimethylaniline F ₂		103.0542	-	-	-	-	-	-	11	59			
2,4,5-Trimethylaniline	[M+H] ⁺	136.1120	100	100	99	24	86	-	-	-			
2,4,5-Trimethylaniline F ₁	C ₉ H ₁₁	119.0855	4	17	100	74	-	-	-	-			
2,4,5-Trimethylaniline F ₂	C ₇ H ₇	91.0542	2	4	37	100	100	100	100	100			
2,6-Diaminotoluene	[M+H] ⁺	123.0917	100	100	42	17	100	100	74	30			
2,6-Diaminotoluene F ₁	C ₆ H ₉ N ₂	108.0685	-	-	-	-	-	-	46	77			
2,6-Diaminotoluene F ₂	C ₇ H ₈ N	106.0651	9	53	100	100	-	-	100	100			
2,6-Dimethylaniline	[M+H] ⁺	122.0964	100	100	43	17	-	-	-	-			
2,6-Dimethylaniline F ₁	C ₈ H ₉	105.0699	8	41	100	100	-	-	-	-			
4-Aminobiphenyl	[M+H] ⁺	170.0964	100	100	100	33	100	100	100	90			
4-Aminobiphenyl F ₁	C ₁₂ H ₉	153.0699	1	6	43	68	-	-	29	100			
4-Aminobiphenyl F ₂	C ₁₂ H ₈	152.0621	1	3	24	100	-	-	8	89			
4-Chloroaniline	[M+H] ⁺	128.0262	100	100	28	5	100	100	22	5			

4-Chloroaniline F ₁	C ₆ H ₄ Cl	110.9996	-	-	-	-	-	-	-	-	-	1	17	30
4-Chloroaniline F ₂	C ₆ H ₇ N	93.0573	9	52	100	100	100	100	100	100	100	1	32	100
4-Hexyiresorcinol	[M+H] ⁺	195.1380	100	100	40	-	100	100	-	100	100	100	17	-
4-Hexyiresorcinol F ₁	C ₁₂ H ₁₈ O ₂	111.0441	5	33	100	100	100	100	100	-	100	41	100	100
Aniline	[M+H] ⁺	94.0651	100	100	100	100	84	100	100	100	100	100	28	25
Aniline F ₁	C ₆ H ₇ N	93.0578	1	3	20	100	34	-	-	-	-	-	-	-
Aniline F ₂	C ₆ H ₅	77.0386	-	2	22	84	2	84	2	51	100	100	100	100
Benzyl butyl phthalate	[M+H] ⁺	313.1433	100	6	-	-	100	-	-	-	-	-	-	-
Benzyl butyl phthalate F ₁	C ₁₉ H ₂₀ O ₄	149.0233	-	-	-	-	20	67	35	19	-	-	-	-
Benzyl butyl phthalate F ₂	C ₇ H ₇	91.0542	44	100	100	67	-	100	100	100	100	100	100	100
Benzyl butyl phthalate	[M+Na] ⁺	335.1254	28	49	78	100	30	39	15	9	-	-	-	-
Bisphenol A	[M-H] ⁻	227.1078	100	100	100	100	100	100	100	100	100	100	100	100
⁵ BA2-3-DHGE	[M+H] ⁺	359.1853	6	5	-	-	-	-	-	-	-	-	-	-
BA2-3-DHGE	C ₁₀ H ₁₇ O ₅	217.1071	-	-	-	-	-	3	100	100	-	-	-	-
BA2-3-DHGE F ₁	C ₁₂ H ₁₇ O ₃	209.1172	15	54	66	33	-	34	21	9	-	-	-	-
BA2-3-DHGE F ₂	C ₁₂ H ₁₅ O ₂	191.1067	8	45	98	67	-	16	20	11	-	-	-	-
BA2-3-DHGE F ₃	C ₉ H ₁₁ O	135.0804	3	25	50	100	-	6	-	-	-	-	-	-
BA2-3-DHGE	[M+NH ₄] ⁺	376.2118	100	100	11	-	100	-	-	-	-	-	-	-
BA2-3-DHGE	[M+Na] ⁺	381.1672	44	97	100	44	100	100	100	100	100	100	39	16
⁶ BA3-Cl-2H-2-3DHPE	[M+COOH] ⁻	439.1529	100	100	100	-	100	-	100	100	-	-	-	-
BA3-Cl-2H-2-3DHPE F ₁	[M+Cl] ⁻	429.1241	10	11	-	-	11	-	14	-	-	-	-	-
BA 3-Cl-2-HPGE F ₁	C ₁₂ H ₁₆ ClO ₂	227.0833	19	38	79	47	-	-	-	-	-	-	-	-
BA 3-Cl-2-HPGE F ₂	C ₁₂ H ₁₅ O ₂	191.1067	5	20	86	57	-	-	-	-	-	-	-	-
BA 3-Cl-2-HPGE F ₃	C ₉ H ₁₁ O	135.0804	3	26	100	100	-	-	-	-	-	-	-	-
⁷ BA 3-Cl-2-HPGE	[M+NH ₄] ⁺	394.1780	100	100	21	1	-	-	-	-	-	-	-	-
⁸ BAB 2,3-DHE	[M+H] ⁺	377.1959	45	21	4	1	100	100	100	46	10	100	100	100

⁵ BA2-3-DHGE : Bisphenol A (2,3-dihydroxypropyl) Glycidyl Ether

⁶ BA3-Cl-2H-2-3DHPE : Bisphenol A (3-chloro-2-hydroxypropyl) (2,3-dihydroxypropyl) ether

⁷ BA 3-Cl-2-HPGE : Bisphenol A (3-chloro-2-hydroxypropyl) glycidil ether

⁸ BAB 2,3-DHE: Bisphenol A bis(2,3-dihydroxypropyl) Ether

BAB 2,3-DHE F ₁	C ₁₈ H ₂₃ O ₄	303.1591	-	-	-	-	-	-	-	50	36	-	-
BAB 2,3-DHE F ₂	C ₁₂ H ₁₇ O ₃	209.1172	27	100	100	51	-	-	-	-	-	-	4
BAB 2,3-DHE F ₃	C ₉ H ₁₃ O	137.0961	-	-	-	-	-	-	-	6	56	100	100
BAB 2,3-DHE F ₄	C ₉ H ₁₁ O	135.0804	5	19	40	100	-	-	-	-	-	-	16
BAB 2,3-DHE	[M+NH ₄] ⁺	394.2224	100	60	5	-	-	-	-	-	-	-	-
BAB 2,3-DHE	[M+Na] ⁺	399.1778	27	100	100	51	-	-	-	-	-	-	-
⁹ BADGE	C ₂₁ H ₂₄ O ₄	341.1747	2	9	10	-	-	-	-	-	-	-	-
BADGE F ₁	[M+H] ⁺	191.1067	100	100	11	-	-	5	100	100	100	100	100
BADGE F ₂	C ₉ H ₁₁ O	135.0804	14	57	100	100	-	-	4	14	68	-	68
BADGE	[M+NH ₄] ⁺	358.2013	1	9	23	81	-	-	74	4	5	-	5
Butyl-p-hydroxybenzoate	[M-H] ⁻	193.0870	100	100	85	15	-	-	100	100	32	-	8
Butyl-p-hydroxybenzoate F ₁	C ₇ H ₅ O ₃	137.0244	1	4	13	4	-	-	7	19	2	-	2
Butyl-p-hydroxybenzoate F ₂	C ₇ H ₄ O ₃	136.0166	1	5	14	4	-	-	5	20	2	-	2
Butyl-p-hydroxybenzoate F ₃	C ₆ H ₃ O	92.0262	2	12	100	100	-	-	3	100	100	-	100
Di-(2-ethylhexyl)adipate	[M+H] ⁺	371.3156	100	100	33	-	-	-	100	-	-	-	-
Di-(2-ethylhexyl)adipate F ₁	C ₆ H ₉ O ₃	129.0546	8	35	100	100	-	-	-	-	-	-	-
Dibutyl sebacate	[M+H] ⁺	315.2530	100	70	9	-	-	-	100	27	-	-	-
Dibutyl sebacate F ₁	C ₁₄ H ₂₅ O ₃	241.1798	22	100	100	14	-	-	75	82	8	-	-
Dibutyl sebacate F ₂	C ₁₀ H ₁₇ O ₃	185.1172	5	20	59	27	-	-	62	100	11	-	11
Dibutyl sebacate F ₃	C ₉ H ₁₅ O	139.1117	3	10	61	100	-	-	-	-	85	-	100
Dibutyl sebacate	[M+Na] ⁺	337.2349	-	-	-	-	-	-	61	100	12	-	68
Dibutyl sebacate	[M+NH ₄] ⁺	332.2797	-	-	-	-	-	-	16	-	-	-	-
Dicyclohexyl phthalate	[M+H] ⁺	331.1904	100	14	-	-	-	-	100	4	-	-	-
Dicyclohexyl phthalate F ₁	C ₁₆ H ₁₅ O ₄	271.0965	-	-	-	-	-	-	-	-	11	-	8
Dicyclohexyl phthalate F ₂	C ₁₄ H ₁₇ O ₄	249.1121	12	15	1	-	-	-	9	19	-	-	-
Dicyclohexyl phthalate F ₃	C ₈ H ₇ O ₄	167.0339	9	34	5	-	-	-	6	50	20	-	1
Dicyclohexyl phthalate F ₄	C ₈ H ₅ O ₃	149.0233	32	100	100	100	-	-	9	46	94	-	100
Dicyclohexyl phthalate	[M+Na] ⁺	353.1723	-	-	-	-	-	-	52	100	100	-	82
Diethyl phthalate	[M+H] ⁺	223.0965	13	-	-	-	-	-	-	-	-	-	-

⁹ BADGE: Bisphenol A diglycidyl ether

Diethyl phthalate F ₁	C ₁₀ H ₉ O ₃	177.0546	100	7	-	-	100	50	-	-
Diethyl phthalate F ₂	C ₈ H ₅ O ₃	149.0233	96	100	100	100	33	100	100	100
Diethyl phthalate	[M+Na] ⁺	245.0784	11	8	5	5	-	-	-	-
Diisodecyl phthalate	C ₂₈ H ₄₆ O ₄	447.3469	81	45	11	-	-	-	-	-
Diisodecyl phthalate	[M+H] ⁺	469.3288	100	100	100	100	-	-	-	-
Diisodecyl phthalate	[M+Na] ⁺	419.3156	100	100	100	-	-	-	-	-
Diisononyl phthalate F ₁	C ₂₀ H ₂₁ O ₃	309.1485	-	-	-	-	100	10	-	-
Diisononyl phthalate F ₂	C ₁₇ H ₂₅ O ₄	293.1747	-	5	26	-	72	100	100	100
Diisononyl phthalate F ₃	C ₁₇ H ₂₃ O ₃	275.1642	1	8	31	-	-	-	-	-
Dimethyl phthalate	[M+H] ⁺	195.0652	-	-	-	-	47	-	-	-
Dimethyl phthalate F ₁	C ₉ H ₇ O ₃	163.0390	100	100	100	84	100	100	92	-
Dimethyl phthalate F ₂	C ₈ H ₇ O ₂	135.0441	2	8	45	100	-	-	-	-
Dimethyl phthalate F ₃	C ₈ H ₅ O ₂	133.0284	-	2	9	21	-	-	-	-
Dimethyl phthalate F ₄	C ₆ H ₅	77.0386	-	-	3	50	-	-	100	100
Dimethyl phthalate	[M+Na] ⁺	217.0471	4	2	1	-	19	-	-	-
Di-N-butyl phthalate	[M+H] ⁺	279.1591	81	-	-	-	100	-	-	-
Di-N-butyl phthalate F ₁	C ₁₂ H ₁₅ O ₄	223.0965	-	-	-	-	-	-	-	-
Di-N-butyl phthalate F ₂	C ₁₂ H ₁₃ O ₃	205.0859	37	4	-	-	33	10	-	-
Di-N-butyl phthalate F ₃	C ₈ H ₅ O ₃	149.0233	100	100	100	100	37	100	100	100
Di-N-butyl phthalate	[M+Na] ⁺	301.1410	-	-	-	-	30	40	21	15
Di-n-octyl-phthalate	[M+H] ⁺	391.2843	100	100	5	-	100	2	-	-
Di-n-octyl-phthalate F ₁	C ₁₆ H ₂₃ O ₄	279.1591	-	-	-	-	4	4	-	-
Di-n-octyl-phthalate F ₂	C ₈ H ₇ O ₄	167.0339	-	-	-	-	6	10	3	-
Di-n-octyl-phthalate F ₃	C ₈ H ₅ O ₃	149.0233	11	86	100	100	6	22	28	34
Di-n-octyl-phthalate F ₄	C ₅ H ₁₁	71.0855	-	-	-	-	-	9	6	7
Di-n-octyl-phthalate F ₅	C ₄ H ₉	57.0699	-	-	-	-	-	4	5	6
Di-n-octyl-phthalate	[M+Na] ⁺	413.2662	-	-	-	-	94	100	100	100
Dipropyl phthalate	[M+H] ⁺	251.1278	100	100	100	42	100	-	-	-
Dipropyl phthalate F ₁	C ₁₃ H ₁₇ O ₂	205.1223	4	15	67	53	-	-	-	-
Dipropyl phthalate F ₂	C ₁₁ H ₁₁ O ₃	191.0703	-	-	-	-	41	21	-	-
Dipropyl phthalate F ₃	C ₁₂ H ₁₇ O	177.1274	1	6	37	100	-	-	-	-

Dipropyl phtalate F ₄			149.0233	-	-	-	-	3	100	100	100	100	100
Dipropyl phtalate	C ₁₄ H ₁₈ O ₄	C ₈ H ₅ O ₃ [M+Na] ⁺	273.1097	-	-	-	-	-	14	4	4	4	4
Ethyl 4-hydroxybenzoate	C ₉ H ₁₀ O ₃	[M-H] ⁻	165.0557	100	100	32	4	100	100	38	17	17	17
Ethyl 4-hydroxybenzoate F ₁		C ₇ H ₅ O ₃	137.0244	4	19	13	2	-	31	33	11	11	11
Ethyl 4-hydroxybenzoate F ₂		C ₇ H ₄ O ₃	136.0160	3	19	5	-	-	11	16	4	4	4
Ethyl 4-hydroxybenzoate F ₃		C ₆ H ₅ O	93.0346	3	27	100	100	-	9	100	100	100	100
Melamine	C ₃ H ₆ N ₆	[M+H] ⁺	127.0727	100	100	100	99	100	100	63	47	47	47
Melamine F ₁		C ₂ H ₅ N	85.0509	3	15	56	100	-	7	100	100	100	100
Methyl paraben	C ₈ H ₈ O ₃	[M-H] ⁻	151.0401	6	90	11	7	100	100	16	9	9	9
Methyl paraben F ₁		C ₇ H ₃ O ₃	136.0160	100	18	4	-	-	26	10	4	4	4
Methyl paraben F ₂		C ₆ H ₂ O	92.0262	11	100	100	100	-	22	100	100	100	100
Nordihydroguaiaretic acid	C ₁₈ H ₂₂ O ₄	[M-H] ⁻	301.1445	100	100	100	100	100	-	-	-	-	-
Nordihydroguaiaretic acid F ₁		C ₁₃ H ₁₇ O ₃	221.1183	6	8	13	10	-	-	-	-	-	-
o-Anisidine	C ₇ H ₉ ON	[M+H] ⁺	124.0757	100	60	7	1	100	100	27	17	17	17
o-Anisidine F ₁		C ₆ H ₇ ON	109.0522	21	100	100	100	19	91	100	100	100	100
o-Anisidine F ₂		C ₅ H ₆ N	80.0495	1	4	12	58	-	1	20	89	89	89
o-Toluidine	C ₇ H ₉ N	[M+H] ⁺	108.0808	100	100	31	7	100	100	48	20	20	20
o-Toluidine F ₁		C ₆ H ₇ N	93.0573	3	15	33	55	3	30	51	41	41	41
o-Toluidine F ₂		C ₇ H ₇	91.0542	8	44	100	100	9	53	100	100	100	100
Propyl 4-hydroxybenzoate	C ₁₀ H ₁₂ O ₃	[M-H] ⁻	179.0714	100	100	41	11	100	100	76	33	33	33
Propyl 4-hydroxybenzoate F ₁		C ₇ H ₅ O ₃	137.0244	1	7	7	3	-	11	45	7	7	7
Propyl 4-hydroxybenzoate F ₂		C ₇ H ₄ O ₃	136.0160	2	9	9	1	-	10	48	8	8	8
Propyl 4-hydroxybenzoate F ₃		C ₆ H ₅ O	93.0346	2	14	100	100	-	3	100	100	100	100
Tributyl-o-acetyl citrate	C ₂₀ H ₃₄ O ₈	[M+H] ⁺	403.2326	100	100	9	-	100	-	-	-	-	-
Tributyl-o-acetyl citrate F ₁		C ₂₀ H ₂₉ O ₆	365.1959	-	-	-	-	-	-	24	8	8	8
Tributyl-o-acetyl citrate F ₂		C ₁₈ H ₃₃ O ₇	361.2221	5	60	30	-	3	50	-	-	-	-
Tributyl-o-acetyl citrate F ₃		C ₁₆ H ₂₅ O ₇	329.1595	7	52	13	-	16	73	7	-	-	-
Tributyl-o-acetyl citrate F ₄		C ₁₃ H ₂₃ O ₅	259.1531	3	33	100	100	-	100	12	-	-	-
Tributyl-o-acetyl citrate F ₅		C ₉ H ₁₃ O ₄	185.0808	-	-	-	-	-	61	100	24	24	24
Tributyl-o-acetyl citrate F ₆		C ₆ H ₅ O ₅	157.0131	-	-	-	-	-	67	45	8	8	8
Tributyl-o-acetyl citrate F ₇		C ₆ H ₃ O ₄	139.0026	-	-	-	-	-	11	30	42	42	42

Aflatoxin G ₁	C ₁₇ H ₁₂ O ₇	[M+Na] ⁺	351.0475	2	6	19	54	17	88	100	100	100
Aflatoxin G ₂	C ₁₇ H ₁₄ O ₇	[M+H] ⁺	331.0812	100	100	100	100	100	100	100	41	22
Aflatoxin G ₂ F ₁	C ₁₇ H ₁₃ O ₆	C ₁₇ H ₁₃ O ₆	313.0707	-	-	-	-	-	-	-	2	8
Aflatoxin G ₂ F ₂	C ₁₄ H ₁₃ O ₄	C ₁₄ H ₁₃ O ₄	245.0808	-	-	-	1	-	-	-	-	2
Aflatoxin G ₂	C ₁₇ H ₁₄ O ₇	[M+Na] ⁺	353.0632	5	10	21	52	31	88	100	100	100
Aflatoxin G ₂	C ₁₇ H ₁₄ O ₇	[M+K] ⁺	369.0371	-	-	-	-	3	8	3	4	4
Aflatoxin M ₁	C ₁₇ H ₁₂ O ₇	[M+H] ⁺	329.0656	100	100	100	49	100	100	100	100	100
Aflatoxin M ₁ F ₁	C ₁₇ H ₁₂ O ₇	[M+Na] ⁺	351.0475	4	46	99	100	-	2	6	3	3
α-Zearalenol	C ₁₈ H ₂₄ O ₅	[M+H] ⁺	321.1697	100	18	1	-	100	8	-	-	-
α-Zearalenol F ₁	C ₁₈ H ₂₃ O ₄	C ₁₈ H ₂₃ O ₄	303.1591	66	100	40	19	58	52	12	-	-
α-Zearalenol F ₂	C ₁₈ H ₂₁ O ₃	C ₁₈ H ₂₁ O ₃	285.1485	18	66	100	98	5	100	100	9	9
α-Zearalenol F ₃	C ₁₈ H ₁₉ O ₂	C ₁₈ H ₁₉ O ₂	267.1380	-	-	-	-	-	19	79	14	14
α-Zearalenol F ₄	C ₁₇ H ₂₁ O ₂	C ₁₇ H ₂₁ O ₂	257.1536	-	-	-	-	-	11	30	4	4
α-Zearalenol F ₅	C ₁₀ H ₇ O ₃	C ₁₀ H ₇ O ₃	175.0390	-	-	-	-	-	2	65	100	100
α-Zearalenol	C ₁₈ H ₂₄ O ₅	[M+Na] ⁺	343.1516	16	21	31	100	2	4	10	4	4
Cyclopiazonic acid	C ₂₀ H ₂₀ N ₂ O ₃	[M+H] ⁺	337.1547	100	100	100	45	-	-	-	-	-
Cyclopiazonic acid F ₁	C ₉ H ₁₂ NO ₃	C ₉ H ₁₂ NO ₃	182.0812	-	7	36	100	-	-	-	-	-
Deoxynivalenol	C ₁₅ H ₂₀ O ₆	[M+H] ⁺	297.1340	100	100	53	-	100	43	25	24	24
Deoxynivalenol F ₁	C ₁₄ H ₁₇ O ₄	C ₁₄ H ₁₇ O ₄	249.1121	6	34	100	-	-	27	14	-	-
Deoxynivalenol	C ₁₅ H ₂₀ O ₆	[M+Na] ⁺	319.1152	-	-	-	-	30	100	100	100	100
Diacetoxyscirpenol	C ₁₉ H ₂₆ O ₇	[M+H] ⁺	367.1751	12	17	5	-	5	4	-	-	-
Diacetoxyscirpenol F ₁	C ₁₇ H ₂₃ O ₅	C ₁₇ H ₂₃ O ₅	307.1540	17	91	100	10	10	46	-	-	-
Diacetoxyscirpenol F ₂	C ₁₅ H ₁₉ O ₃	C ₁₅ H ₁₉ O ₃	247.1329	5	33	77	16	-	32	17	-	-
Diacetoxyscirpenol	C ₁₉ H ₂₆ O ₇	[M+NH ₄] ⁺	384.2017	100	100	8	1	100	25	-	-	-
Diacetoxyscirpenol	C ₁₉ H ₂₆ O ₇	[M+Na] ⁺	389.1571	4	19	96	100	39	100	100	100	-
Ergocornine	C ₃₁ H ₃₉ N ₅ O ₅	[M+H] ⁺	562.3024	100	100	100	100	100	100	100	100	25
Ergocornine F ₁	C ₃₁ H ₃₈ N ₅ O ₄	C ₃₁ H ₃₈ N ₅ O ₄	544.2918	-	2	6	16	1	30	73	13	13
Ergocornine F ₂	C ₂₆ H ₂₂ N	C ₂₆ H ₂₂ N	348.1747	-	-	-	-	-	-	17	25	25
Ergocornine F ₃	C ₂₀ H ₂₁ O	C ₂₀ H ₂₁ O	277.1587	-	-	-	-	-	-	10	41	41
Ergocornine F ₄	C ₁₆ H ₁₈ N ₃ O	C ₁₆ H ₁₈ N ₃ O	268.1444	-	-	-	-	1	2	41	98	98
Ergocornine F ₅	C ₈ H ₁₉ N ₂ O ₅	C ₈ H ₁₉ N ₂ O ₅	223.1288	-	-	-	-	-	-	7	55	55

Fumonisin B ₁	C ₃₄ H ₅₉ NO ₁₅	[M+H] ⁺	722.3957	100	100	100	100	100	100	100	100	100	100
Fumonisin B ₁ F ₁	C ₃₄ H ₅₈ NO ₁₄		704.3852	-	-	-	-	-	-	-	-	-	29
Fumonisin B ₁ F ₂	C ₃₄ H ₅₆ NO ₁₃		686.3746	-	-	-	-	-	-	-	-	-	6
Fumonisin B ₁ F ₃	C ₂₈ H ₅₂ NO ₉		546.3637	-	-	-	-	-	-	-	-	-	6
Fumonisin B ₁ F ₄	C ₂₈ H ₅₀ NO ₈		528.3531	-	-	-	-	-	-	-	-	-	4
Fumonisin B ₁ F ₅	C ₂₂ H ₄₄ NO ₃		370.3316	-	-	-	-	-	-	-	-	-	5
Fumonisin B ₁ F ₆	C ₂₂ H ₄₂ NO ₂		352.3137	-	-	-	-	-	-	-	-	-	6
Fumonisin B ₂	C ₃₄ H ₅₉ NO ₁₄	[M+H] ⁺	706.4008	100	100	100	100	100	100	100	100	100	-
Fumonisin B ₂ F ₁	C ₃₄ H ₅₈ NO ₁₃		688.3903	-	-	-	-	-	-	-	-	-	-
Gliotoxin	C ₁₃ H ₁₄ N ₂ O ₄ S ₂	[M+H] ⁺	327.0478	100	5	-	-	100	-	-	-	-	-
Gliotoxin F ₁	C ₁₃ H ₁₅ N ₂ O ₄		263.1026	98	100	88	33	75	74	56	48	48	48
Gliotoxin F ₂	C ₁₃ H ₁₃ N ₂ O ₃		245.0921	27	30	100	100	-	100	100	100	100	100
HT-2 toxin	C ₂₂ H ₃₂ O ₈	[M+H] ⁺	425.2170	19	57	13	-	15	12	3	4	4	4
HT-2 toxin F ₁	C ₁₇ H ₂₃ O ₆		323.1489	-	-	-	-	6	14	5	2	2	2
HT-2 toxin F ₂	C ₁₅ H ₁₉ O ₄		263.1278	14	69	100	68	11	100	100	38	38	38
HT-2 toxin F ₃	C ₁₅ H ₁₅ O ₂		227.1067	-	7	9	9	2	22	27	16	16	16
HT-2 toxin F ₄	C ₁₄ H ₁₅ O ₂		215.1067	-	-	-	-	5	81	91	53	53	53
HT-2 toxin F ₅	C ₁₄ H ₁₃ O		197.0961	-	-	-	-	1	40	72	57	57	57
HT-2 toxin F ₆	C ₁₃ H ₁₅ O		187.1117	-	-	-	-	-	21	55	49	49	49
HT-2 toxin F ₇	C ₁₃ H ₁₂		169.1012	-	-	-	-	-	22	61	81	81	81
HT-2 toxin F ₈	C ₁₂ H ₁₃		157.1012	-	-	-	-	-	16	56	78	78	78
HT-2 toxin F ₉	C ₁₁ H ₁₃		145.1012	-	-	-	-	-	9	43	76	76	76
HT-2 toxin F ₁₀	C ₇ H ₉ O ₂		125.0597	-	-	-	-	-	6	17	18	18	18
HT-2 toxin F ₁₁	C ₈ H ₉		105.0699	-	-	-	-	-	16	52	100	100	100
HT-2 toxin	C ₂₂ H ₃₂ O ₈	[M+NH ₄] ⁺	442.2437	100	100	5	-	100	8	3	4	4	4
HT-2 toxin	C ₂₂ H ₃₂ O ₈	[M+Na] ⁺	447.1989	6	24	44	100	2	17	31	43	43	43
Ochratoxin A	C ₂₀ H ₁₈ ClNO ₆	[M+H] ⁺	404.0895	100	100	33	2	100	77	4	4	4	4
Ochratoxin A F ₁	C ₂₀ H ₁₇ ClNO ₅		386.0879	-	-	-	-	-	-	-	10	10	10
Ochratoxin A F ₂	C ₁₉ H ₁₇ ClNO ₄		358.0841	1	5	12	2	-	49	30	2	2	2
Ochratoxin A F ₃	C ₁₉ H ₁₄ ClO ₄		341.0575	-	-	-	-	-	2	16	7	7	7
Ochratoxin A F ₄	C ₁₁ H ₈ ClO ₄		239.0106	3	21	100	100	-	9	100	100	100	100

N-nitrosomorpholine F ₁	C ₄ H ₇ NO	86.0606	5	5	9	1	16	100	-
N-nitroso-n-diphenylamine	[M+H] ⁺	199.0866	100	11	1	-	-	-	-
N-nitroso-n-diphenylamine F ₁	C ₉ H ₁₁ N	169.0886	71	100	100	100	100	100	100
N-nitrosopiperidine	[M+H] ⁺	115.0866	100	100	100	-	100	100	47
N-nitrosopiperidine F ₁	C ₅ H ₁₀ N ₂ O	69.0699	1	5	12	-	1	26	100
N-nitrosopyrrolidine	[M+H] ⁺	101.0709	100	100	100	-	100	100	57
N-nitrosopyrrolidine F ₁	C ₄ H ₇	55.0542	-	1	1	-	1	25	100
Perfluorinated compounds									
Pentafluoropropionic acid	[M-H] ⁻	162.9824	15	10	27	64	100	18	26
Pentafluoropropionic acid F ₁	C ₃ F ₅	118.9926	100	100	100	100	38	100	100
Perfluorobutyric acid	[M-H] ⁻	212.9792	11	15	17	61	100	15	53
Perfluorobutyric acid F ₁	C ₃ F ₇	168.9894	100	100	100	100	51	100	100
Perfluoropentanoic acid	[M-H] ⁻	262.9760	14	34	21	37	100	27	38
Perfluoropentanoic acid F ₁	C ₄ F ₉	218.9862	100	100	100	100	71	100	100
Perfluoroheptanoic acid	[M-H] ⁻	362.9696	22	6	44	16	100	19	21
Perfluoroheptanoic acid F ₁	C ₆ F ₁₃	318.9798	100	100	100	100	67	100	81
Perfluoroheptanoic acid F ₂	C ₃ F ₇	168.9894	5	31	63	24	-	19	100
Perfluoroheptanoic acid F ₃	C ₂ F ₅	118.9926	1	10	27	9	-	3	32
Perfluorooctanoic acid	[M-H] ⁻	412.9664	72	5	17	28	100	18	14
Perfluorooctanoic acid F ₁	C ₇ F ₁₅	368.9766	100	100	92	100	58	100	57
Perfluorooctanoic acid F ₂	C ₃ F ₇	168.9894	8	27	100	48	-	19	100
Perfluorooctanoic acid F ₃	C ₂ F ₅	118.9926	1	2	13	8	-	-	24
Perfluorononanoic acid	[M-H] ⁻	462.9632	80	8	5	45	100	15	24
Perfluorononanoic acid F ₁	C ₈ F ₁₇	418.9734	100	100	100	100	46	100	100
Perfluorononanoic acid F ₂	C ₅ F ₁₁	268.9830	-	-	-	-	-	3	15
Perfluorononanoic acid F ₃	C ₄ F ₉	218.9862	3	11	45	34	-	13	81
Perfluorononanoic acid F ₄	C ₃ F ₇	168.9894	2	8	51	56	-	6	85
Perfluorononanoic acid F ₅	C ₂ F ₅	118.9926	-	-	6	14	-	-	14
Perfluorodecanoic acid	[M-H] ⁻	512.9600	100	11	3	35	100	14	24
	C ₁₀ HO ₂ F ₁₉								13

Perfluorodecanoic acid F ₁	C ₉ F ₁₉	468.9702	73	100	100	100	100	100	100	100	100	100	100	100
Perfluorodecanoic acid F ₂	C ₅ F ₁₁	268.9830	-	-	-	-	-	-	-	-	-	-	7	57
Perfluorodecanoic acid F ₃	C ₄ F ₉	218.9862	2	5	26	47	-	8	66	66	36	65	44	65
Perfluorodecanoic acid F ₄	C ₃ F ₇	168.9894	1	3	20	60	-	-	44	44	65	19	-	19
Perfluorodecanoic acid F ₅	C ₂ F ₅	118.9926	-	-	4	29	-	-	-	-	-	-	-	-
Perfluoroundecanoic acid	[M-H] ⁻	562.9568	100	20	3	11	100	11	17	17	-	-	-	-
Perfluoroundecanoic acid F ₁	C ₁₀ F ₂₁	518.9670	45	100	100	100	100	100	100	100	91	91	100	91
Perfluoroundecanoic acid F ₂	C ₇ F ₁₅	368.9766	-	-	-	-	-	-	4	4	-	-	-	-
Perfluoroundecanoic acid F ₃	C ₅ F ₁₁	268.9830	-	-	-	-	-	-	55	55	39	39	-	39
Perfluoroundecanoic acid F ₄	C ₄ F ₉	218.9862	1	2	10	40	-	-	43	43	37	37	-	37
Perfluoroundecanoic acid F ₅	C ₃ F ₇	168.9894	1	2	9	68	-	-	32	32	100	100	-	100
Perfluoroundecanoic acid F ₆	C ₂ F ₅	118.9926	-	-	2	27	-	-	-	-	27	27	-	27
Perfluorododecanoic acid	[M-H] ⁻	612.9537	100	37	3	3	100	13	12	12	-	-	-	-
Perfluorododecanoic acid F ₁	C ₁₁ HF ₂₃	568.9638	32	100	100	100	100	26	100	100	59	59	100	59
Perfluorododecanoic acid F ₂	C ₇ F ₁₅	368.9766	-	-	-	-	-	-	1	1	17	17	-	17
Perfluorododecanoic acid F ₃	C ₆ F ₁₃	318.9798	-	-	-	-	-	-	2	2	38	38	-	38
Perfluorododecanoic acid F ₃	C ₅ F ₁₁	268.9830	-	-	-	-	-	-	2	2	34	34	-	34
Perfluorododecanoic acid F ₄	C ₄ F ₉	218.9862	-	1	5	25	-	-	25	25	31	31	-	31
Perfluorododecanoic acid F ₅	C ₃ F ₇	168.9894	1	2	6	45	-	-	26	26	100	100	-	100
Perfluorododecanoic acid F ₆	C ₂ F ₅	118.9926	-	-	1	12	-	-	-	-	12	12	-	12
Heptadecafluorooctanesulfonic acid	C ₈ HO ₃ F ₁₇ S	498.9302	100	100	100	100	100	100	100	100	100	100	100	100
Sweeteners														
Aspartame	[M-H] ⁻	293.1143	100	100	100	100	100	100	100	100	100	100	100	100
Aspartame F ₁	C ₁₄ H ₁₈ N ₂ O ₅	261.0881	3	6	8	10	-	62	80	80	100	100	-	100
Aspartame F ₂	C ₁₂ H ₁₃ N ₂ O ₂	217.0983	1	6	17	21	-	-	-	-	44	44	-	44
Acesulfame-K	[M-H] ⁻	161.9867	100	50	45	100	100	63	41	41	89	89	-	89
Acesulfame-K F ₁	C ₄ H ₄ NO	82.0298	31	100	100	33	-	100	100	100	100	100	-	100
Saccharin	[M-H] ⁻	181.9917	100	100	100	100	100	100	100	100	100	100	100	100
Saccharin F ₁	CHNO ₃ S	105.9604	-	1	2	2	-	-	6	6	5	5	-	5
Sucralose	[M-H] ⁻	395.0073	63	100	100	-	-	100	100	100	100	100	-	100

Sucralose F ₁	C ₁₂ H ₁₉ Cl ₃ O ₈	[M+Cl] ⁻	430.9840	100	48	50	-	-	19	-	-
Sucralose F ₂	C ₁₂ H ₁₉ Cl ₃ O ₈	[M+COOH] ⁻	441.0128	29	28	-	-	100	4	-	-
Cyclamate	C ₆ H ₁₂ NO ₃ S	[M-H] ⁻	178.0538	100	100	100	57	100	100	100	54
Cyclamate F ₁		HSO ₃	79.9574	2	7	36	100	-	-	44	100

Table S3. Isobaric compounds of the database developed which could not be distinguished by retention time, resolving power, isotopic pattern or fragment ions.

Group	Compound	Theoretical mass	RT (min) ($\Delta RT \leq 0.2$ min)
1	2,4-Diaminotoluene	123.0917	0.29
	2,6-Diaminotoluene	123.0917	0.29
2	Secbumeton	226.1662	4.05
	Terbumeton	226.1662	4.10
3	Sulfameter	281.0703	3.51
	Sulfamethoxy pyridazine	281.0703	3.53

Table S4. Compounds without fragmentation or whose relative abundance to the most intensity ion was lower than 10% (employing 220 V as fragmentation voltage). Compounds in bold contains chlorine or bromine atoms in their structure.

Pesticides		
4-Chloro-2-methylphenol	Ethiprole	Metaflumizone
Acibenzolar s-methyl	Ethoxyquin	Methoprotryne
Amitrol	Etoazole	Norfluzurone
Ampa	Fenarimol	Nuarimol
Anilazine	Fenhexamid	Oryzalin
Brodifacoum	Fenpropidine	Oxfendazole
Bromadiolone	Fenpropimorph	Phosphonic acid
Bromophos methyl	Fenthion	Pyrimethanil
Bromoxynil	Fentin*	Pyroquilon
Chlordimeform	Fipronil	Quinoxifen
Chloridazon	Fluazinam	Rotenone
Chlormequat chloride	Fludioxonil	Spinosyn A
Chlorpyrifos methyl	Fonofos	Spinosyn d
Cyprodinil	Hydramethylnon	Tebufenpyrad
Dazomet	Imazalil	Temephos
Dicloran	Imazalil metabolite	Terbufos
Difenacoum	Imazamox	Thiofanox
Difenzoquat	Maleic hydrazide	Triazoxide
Diflufenican	Mepanipyrim	Trietazine
Emamectin	Mepiquat chloride	Trifluralin
Epoiconazole		
Veterinary drugs		
Benzothiazole	Fluoxetine	Roxithromycin
Clarithromycin	Malachite green	Sulindac
Danofloxacin	Minocycline	Tylosin
Erythromycin	Promethazine	
Plasticizers		
Bisphenol A	*BA(3Cl-2-HP)(2,3-DHP)E	
Mycotoxins		
Ergocornine	Fumonisin B ₁	Fumonisin B ₂
Perfluorinated compounds		
Heptadecafluorooctanesulfonic acid		
N-nitrosodimethylamine	N-nitrosomethylethylamine	N-nitrosomorpholine

*BA(3Cl-2-HP)(2,3-DHP)E Bisphenol A (3-chloro-2-hydroxypropyl) (2,3-dihydroxypropyl) ether

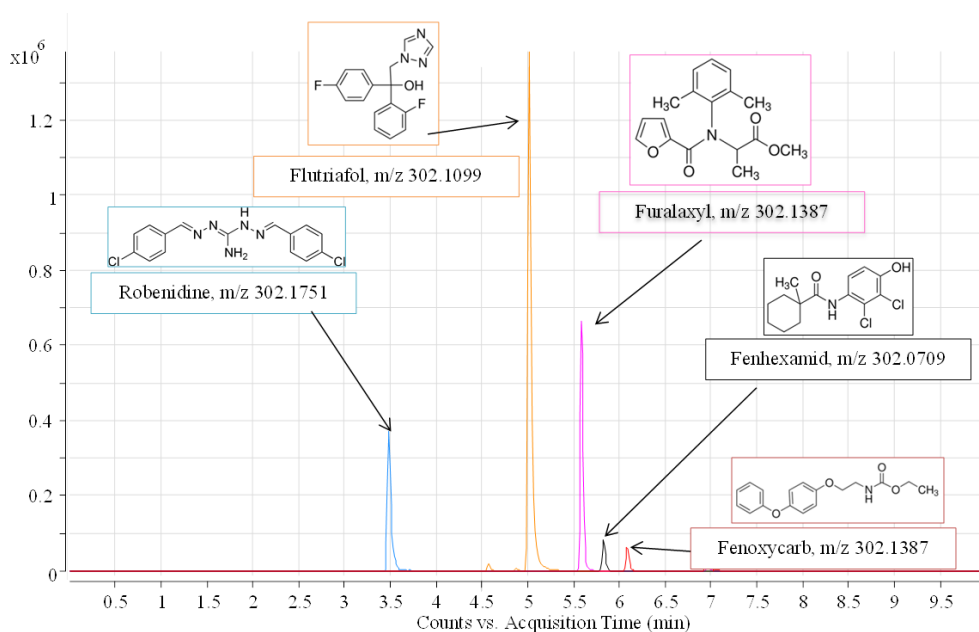


Figure S1. Overlapped EICs (extracted ion chromatograms) from isobaric species that could be distinguished by retention time (robenidine, flutriafol, furalaxyl, fenhexamid and fenoxycarb)

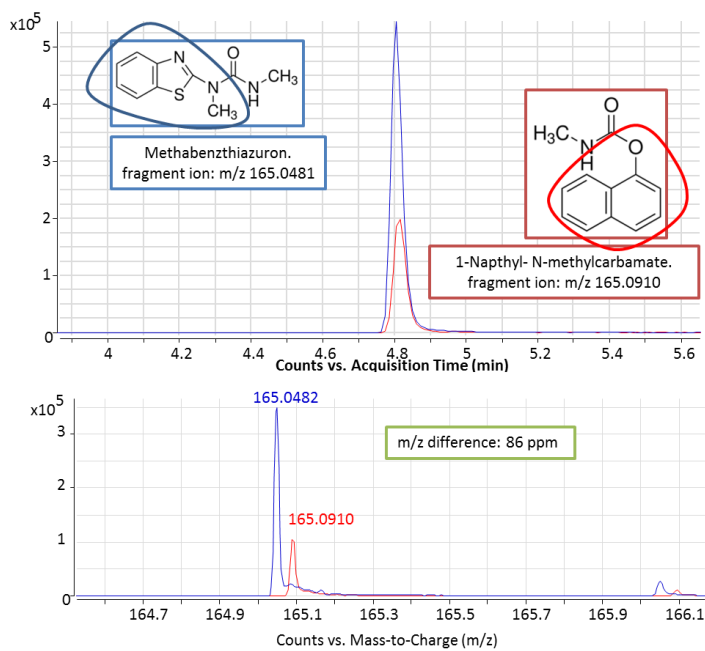


Figure S2. Overlapped EICs and mass spectrums of isobaric compound distinguished by resolving power (methabenzthiazuron and 1-naphthyl-n-methylcarbamate fragments).

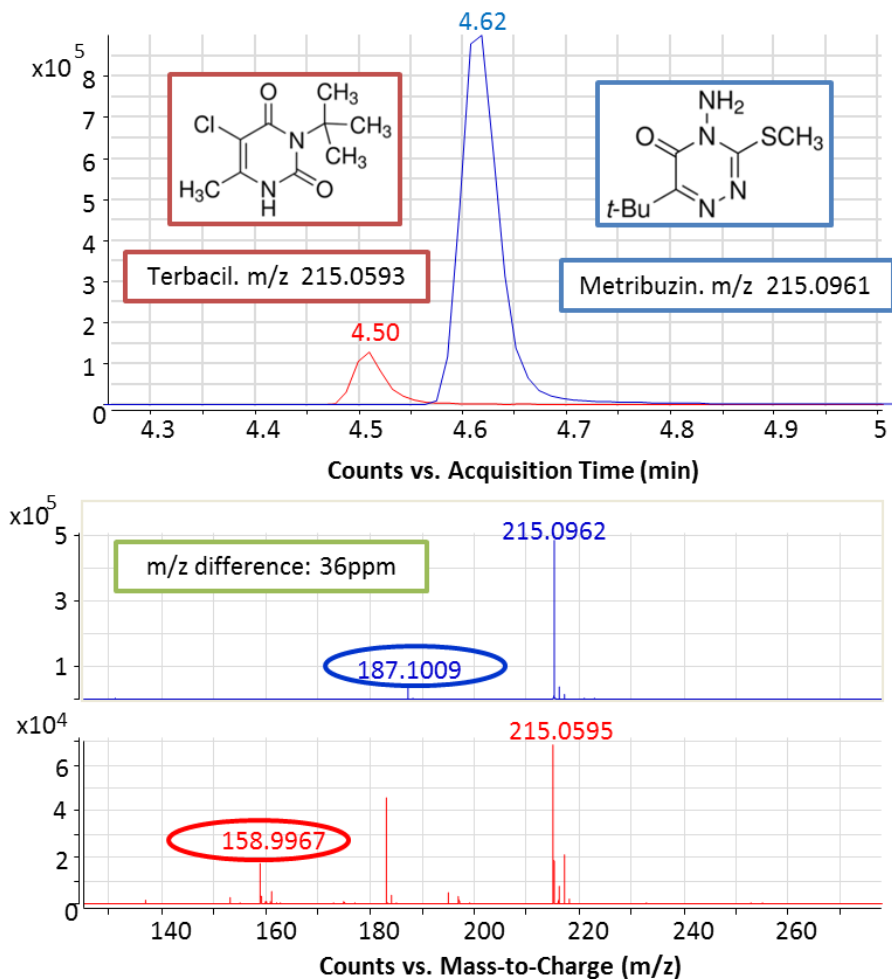


Figure S3. Overlapped EICs and mass spectrums of isobaric species that could be distinguished by resolving power and additional ions (fragment ions: terbacil, m/z 158; metribuzin, m/z 187)

III.2. DESARROLLO DE UN MÉTODO PARA LA DETECCIÓN DE MÁS DE 600 CONTAMINANTES (PESTICIDAS, PRODUCTOS VETERINARIOS, MICOTOXINAS Y OTRAS ESPECIES) EN ALIMENTOS MEDIANTE CROMATOGRAFÍA DE LÍQUIDOS DE ULTRAELEVADA RESOLUCIÓN Y ESPECTROMETRÍA DE MASAS DE TIEMPO DE VUELO (UHPLC-TOFMS).

III.2. Desarrollo de un método para la detección de más de 600 contaminantes (pesticidas, productos veterinarios, micotoxinas y otras especies) en alimentos mediante cromatografía de líquidos de ultraelevada resolución y espectrometría de masas de tiempo de vuelo (UHPLC-TOFMS).

III.2.1. Resumen

El control de la calidad de los alimentos que consumimos ha crecido exponencialmente en los últimos años. En particular, la presencia de contaminantes orgánicos nocivos para la salud a niveles de trazas supone una gran preocupación tanto para el consumidor como para los agentes involucrados en el negocio. Por este motivo, tanto las normas que regulan la presencia de los contaminantes como las herramientas que se emplean para su control en los laboratorios oficiales han mejorado sustancialmente en los últimos años. La tendencia es emplear métodos los más genéricos e universales, que permitan la detección rápida de centenares de compuestos de interés en un único análisis. Por poner un ejemplo relevante, los productos infantiles elaborados pueden contener frutas, verduras, carne y pescado, por lo que es necesario controlar la presencia de pesticidas, micotoxinas o productos veterinarios entre otras familias de contaminantes. Para llevar a cabo este tipo de métodos de *screening* rápidos se emplea cromatografía de líquidos/espectrometría de masas de alta resolución, teniendo en cuenta la naturaleza relativamente polar de la mayoría de los contaminantes orgánicos en alimentos que nos preocupan.

En este trabajo de investigación se ha desarrollado un método de *screening* empleando cromatografía de líquidos de ultraelevada resolución (UHPLC) y espectrometría de masas de alta resolución con analizador de tiempo-de-vuelo (UHPLC-(Q)TOFMS) para la detección de más de 625 contaminantes orgánicos de distintas familias en alimentos. En total se incluyeron 426

pesticidas, 117 productos veterinarios, 42 residuos de envases alimentarios, 21 micotoxinas, 10 compuestos perfluorados, 9 nitrosaminas y 5 edulcorantes. La separación de los analitos se llevó a cabo empleando un sistema UHPLC con una columna C₁₈ (2.1 x 50 mm, 1.8 µm de tamaño de partícula). Se ensayaron diferentes gradientes de elución empleando agua con 0.1 % de ácido fórmico y acetonitrilo con 0.1 % de ácido fórmico como fases móviles. El método final seleccionado (gradiente de 10 minutos) permitía una separación adecuada de los analitos en un tiempo corto. La identificación de los compuestos se llevó a cabo mediante medidas de masas exactas de los iones característicos de cada analito (principalmente molécula (de)protonada), e información de tiempo de retención junto con la fragmentación característica para cada especie, todo ello llevado a cabo de forma automatizada a través de un programa informático específico. El método propuesto permite la detección de la mayoría de los compuestos estudiados a niveles de concentración muy bajos del orden de 1 a 10 µg Kg⁻¹. Para una caracterización completa del rendimiento del método, se llevó a cabo el estudio de los límites de cuantificación de los compuestos estudiados. Para el caso particular de los pesticidas, se estudiaron tres matrices representativas (tomate naranja y productos infantiles combinando verduras y carne), encontrándose que los valores de detección empeoran conforme la matriz es más compleja de forma que para un porcentaje de entre el 10 y el 15 % de los compuestos, no se llega a cumplir los valores de límite máximo de residuos (LMRs) establecidos para la combinaciones pesticida/matriz estudiadas. Éste hecho se agudizaba para el caso de la matriz de naranja, mucho más compleja y que presentaba efectos matriz mucho mas significativos. La sensibilidad es quizás la principal debilidad del método propuesto, ya que es difícil que absolutamente todos los compuestos sean sensibles para unas condiciones instrumentales concretas (ionización mediante *electrospray*). El empleo de instrumentación con

transmisión de iones y fuentes de ionización asistidas térmicamente optimizadas podría mejorar esta situación aunque es difícil en cualquier caso para los analitos que por su naturaleza presentan unas características incompatibles con la ionización mediante *electrospray*.

III.2.2. Artículo

Abstract

In this article, an accurate-mass multi-residue screening method has been developed for the determination of over 625 multiclass food contaminants in different matrices using Ultrahigh Performance Liquid Chromatography/(Quadrupole)-Time-of-Flight Mass Spectrometry (UHPLC-(Q)TOFMS). The compounds included in the study were 426 pesticides, 117 veterinary drugs, 42 food packaging contaminants, 21 mycotoxins, 10 perfluorinated compounds, 9 nitrosamines and 5 sweeteners. The separation of the targeted compounds was carried out by liquid chromatography using a C₁₈ column (50 mm x 2.1 mm and 1.8 μm particle size). Three different elution gradients were assayed (5, 10 and 15 minutes) to develop a rapid screening method, which allowed the separation and identification of the highest number of compounds in a short single run. The identification of the targeted species was accomplished using accurate masses of the targeted ions (protonated molecule) along with retention time data and characteristic in-source fragment ions, using specific software for automated data mining and exploitation. The performance of the screening method was validated in terms of linearity, matrix effect and limits of quantification (LOQs) for three representative food matrices (tomato, orange and baby food) using a generic sample treatment based on liquid partitioning with acetonitrile (QuEChERS). The overall method performance was satisfactory with limits of quantification lower than 10 μg kg⁻¹ for the 44% of studied compounds. In some cases (ca. 10 % of the pesticides), (non-authorized pesticides with 10 μg kg⁻¹ default level set) MRLS were not fulfilled. Matrix effects occurring were also examined. Orange was the matrix which produced limits of quantification > 100 μg kg⁻¹ more frequently. Signal suppression was the

most common effect produced. In general, orange was the matrix with produced the highest matrix effect and baby food, the lowest.

Introduction

Food quality and safety have become increasing concerns for consumers, governments and producers in such globalized market, where commodities are produced and distributed throughout the World [1-2]. Chemical contaminants in food have been defined as “any chemical not intentionally added to food but present from many potential sources [3]”, including residues from the application of pesticides and veterinary medicines, those entering the food chain from the environment, those formed during the processing of food, natural toxins, accidental contamination or adulteration.

To protect the health of consumers, stringent regulations enforced with diligent monitoring of foods have been recently established. The need of methods covering multiclass contaminants such as pesticides, veterinary drugs and mycotoxins is illustrated by selected recent examples in the literature [4-9]. For instance, derivate food products such as baby food combine different matrices: cereal-based food, meat-based food, powdered milk based infant formulae and fruit and vegetable-based food [10]. Thus, they should be tested keeping in mind the potential simultaneous presence of both pesticides and veterinary drugs. In addition, the presence of emerging contaminants such as parabens, human pharmaceuticals and antibiotics, and veterinary drugs has been recently reported in processed food [11] due to contamination either during farming/ crop production -as the use of reclaimed water is becoming more common-, [12] or in the food-producing scenarios. Furthermore, contaminants can also enter the food chain through adulteration of food (international contamination, eg. melamine in milk formulae) [13]. To cope with these huge numbers of

contaminants/commodity combinations, residue laboratories are forced to employ multi-residue methods.

The monitoring of residues from either pesticides or other contaminants in produce of both plant and animal origin is of great interest for the protection of human health. It is currently addressed by means of a plethora of regulations worldwide [14-25]. Laboratories monitoring these chemicals must have cost-effective, rapid and comprehensive methods for detecting their presence so that further actions can be taken in a timely manner. Current food safety methods are aimed at the simultaneous determination of several families of contaminants and/or residues. These methods increase sample throughput and the capabilities of routine laboratories [1-3].

The prevailing method for determining pesticides, veterinary drugs and other relevant contaminants is a targeted approach (multi-residue methods (MRMs)) using liquid chromatography/tandem mass spectrometry (LC-MS/MS) or/and gas chromatography/tandem mass spectrometry (GC-MS/MS). The scope of the targeted analysis is usually limited to a list of compounds (typically one-two hundreds), usually selected on the basis of their frequency of occurrence, contribution to the residue definition and legislation requirements. However, the main flaw of the approach is the previous knowledge required to set-up the acquisition method (retention time and optimized MS/MS transitions for each analyte sought). Consequently, LC-MS/MS multi-residue methods are blind to compounds not defined in the MRM method (non-targeted analysis), so that none or scarce information on possible non-target or unknown pesticides or their degradation products are available when using these techniques. MRMs also require dedicated validation and Quality Control (QC) (due to the large number of species). In quantitative MRM, valuable time and effort is wasted in generating ongoing QC data for many compounds that are not frequently

detected. Besides, handling and preservation of standard mixtures containing hundreds of compounds, which are barely stable over long periods, constitutes a compelling effort required. Therefore, screening methods skipping such reference materials and all ongoing QC measurements associated are desirable.

Liquid chromatography combined with full-scan high-resolution mass spectrometry (LC-full-scan HRMS) has shown to be an effective approach to screen food samples for the presence of high number of analytes. In contrast to the various modes of MS/MS acquisition, LC-full scan HRMS enables a fully untargeted measurement with the ability to retrospectively detect additional compounds in the raw data, which were not anticipated to be of interest at the time of sample analysis [25-28]. It is a challenging effort to keep the integrity of mixed standard solutions containing hundred of compounds. The shelf life will be obviously determined by the most labile species. This forces the storage of standard solutions at very low temperature, which may prompt the partial precipitation of poorly soluble compounds. Therefore, screening methods skipping reference materials are desirable. Besides, although the interrogation of the data is performed against the list of compounds included in the database or library, retrospective evaluation is always possible as data for all compounds that have given sufficient detector response was acquired [25-28].

The development of accurate-mass LC-HRMS screening methods has been addressed by different authors, using either time-of-flight [26-31] or orbitrap mass spectrometers [32-33]. These methodologies include typically between 200 and 450 pesticides, although there are also a few examples covering other contaminants such as veterinary drugs. The qualitative information regarding collision induced dissociation (CID) fragmentation for confirmatory purposes is not addressed in most of these previous works. In this article, an

accurate-mass multiresidue screening method using liquid chromatography high-resolution mass spectrometry has been developed and its performance evaluated for the determination of over 600 multiclass food contaminants (pesticides, veterinary drugs, mycotoxins, nitrosamines and food packaging contaminants) in food, using tomato, orange and baby food as model matrices.

Experimental Section

Chemicals and Reagents. Pesticides, veterinary drugs, food-packaging contaminants, perfluorinated compounds, mycotoxins, nitrosamines and sweeteners analytical-grade standards were purchased from Fluka (Pestanal quality) (Madrid, Spain), Sigma-Aldrich (Madrid, Spain) or Dr. Ehrenstorfer (Augsburg, Germany). Individual stock solutions (*ca.* 500 mg L⁻¹ each) were prepared in different solvents depending on compound solubility and stability (acetonitrile, metanol MeOH, and/or water in basic or acidic media) and were stored at -20°C. Working solutions containing *ca.* 30 compounds each were prepared by appropriate dilution of the stock solutions with MeOH at 10 mg L⁻¹. HPLC-grade acetonitrile and methanol were obtained from Merck (Darmstadt, Germany). Formic acid was obtained from Fluka (Buchs, Switzerland). Primary-secondary amine (PSA) Bond Elut was obtained from Varian, Inc. (Palo Alto, CA, USA). Acetic acid was from Panreac (Barcelona, Spain). Anhydrous magnesium sulfate anhydrous (MgSO₄) and sodium acetate (NaCOOCH₃) were from Sigma-Aldrich (Madrid, Spain). A Milli-Q-Plus ultrapure water system from Millipore (Milford, MA, USA) was used throughout the study to obtain the HPLC-grade water used during the analyses.

Selection of the studied compounds. The 630 compounds included in the screening method were carefully selected considering different lists

established by official bodies from the European Union and The United States, previous relevant literature, and thus, their potential presence in different types of foodstuffs and water. Up to 426 pesticides, 117 veterinary drugs and pharmaceuticals, 43 food-packaging contaminants, 10 perfluorinated compounds 21 mycotoxins, 9 nitrosamines and 5 sweeteners were included. From the 426 pesticides included, most of them are covered in Annex 1 of Directive 396/2005 for several commodities [34]. A significant number (over 130 species), of priority pesticides (according to Annex I of Commission Implementing Regulation 788/2012 due to their usage and frequency of detection), were also included in the targeted list [36]. Most of the selected food-packaging contaminants and perfluorinated compounds are regulated by different documents [35-42]. With regards to the veterinary drugs and pharmaceuticals, most of the selected substances are US FDA approved veterinary drugs for animal use [38] or authorized products in the European Union. It should be noted that some of the species are included in **Table 1** as pesticides although they can be also classified as veterinary drugs such as albendazole, fenbendazole, fenthion, ivermectin, lufenuron, spinosad, sulfaquinoxaline, thiabendazole and trichlorfon, all of them included in US FDA approved list for animal use. Along with the veterinary drugs, other human pharmaceuticals were included due to their ubiquitous presence in the environment. Besides, all the main mycotoxins including those regulated in Commission Regulation EC 1881/2006 [39] are amongst those 21 substances selected. The 11 nitrosamines selected are included in US EPA final Drinking Water Contaminant Candidate lists (CCL-3)[40,41]. Finally, all the sweeteners included are DG SANCO authorized food additives [42].

Sample treatment. Different baby food samples from different local markets containing meat and vegetables were pooled and used as model matrix,

along with tomato and orange. Extraction was accomplished using QuEChERS approach described elsewhere and detailed in the Supplementary material [43]. A representative 10-g portion of homogenized sample was weighed in a 50-mL PTFE centrifuge tube and mixed with 10 mL of 0.1% acetic acid in acetonitrile, being the tube vigorously shaken for 1 minute. Then, 1 g of NaCOOCH₃ and 4 g of MgSO₄ anhydrous were added, and the tube was shaken again to prevent coagulation of MgSO₄. The extract was centrifuged (3700rpm) for 3 minutes. A 5-mL aliquot of supernatant (acetonitrile phase) was taken with a pipette and transferred to a 15 mL centrifuge tube containing 250 mg of PSA and 750 mg of MgSO₄ anhydrous that was energetically shaken for 20 seconds. The extract was centrifuged again (3700 rpm) for 3 minutes. 3 mL of supernatant were taken and evaporated to near dryness and reconstituted to 3mL of 20% MeOH. Prior UHPLC–MS analysis, the extract was filter through a 0.45µm PTFE filter and transfer into a vial. Tomato, orange and baby food extracts were obtained. These extracts were used for method performance evaluation by appropriate spiking with the compounds mixtures.

Ultra-high Performance Liquid Chromatography-Electrospray-(Quadrupole)-Time-of-Flight Mass Spectrometry. The separation and identification of the analytical standards was carried out using a reversed phase C₁₈ column (50 mm x 2.1 mm and 1.8 µm particle size, Zorbax Rapid Resolution High Definition (RRHD) Eclipse-Plus C₁₈) by means of an Agilent UHPLC system (Agilent 1290 Infinity, Agilent Technologies, Santa Clara, CA, USA), consisting of vacuum degasser, auto-sampler and a binary pump. Mobile phases A and B were water and acetonitrile respectively, both with 0.1% formic acid. The flow-rate used was 0.5 mL min⁻¹. The chromatographic method held the initial mobile phase composition (5% B) constant for 2 min, followed by a linear gradient to 100 % B at 8 min and held constant for a 2 min at 100 % B.

20 μL of extract were injected in each study. A 5-min post-time was used for each analysis.

The UHPLC system was connected to a time-of-flight mass spectrometer Agilent TOF 6220 (Agilent Technologies, Santa Clara, CA, USA) equipped with an electrospray interface operated in either positive or negative ionization mode, using the following operation parameters: capillary voltage, 4000 V; nebulizer pressure, 40 psig; drying gas, 9 L min^{-1} ; gas temperature, 325 $^{\circ}\text{C}$; fragmentor voltage (in-source CID fragmentation), 190 V. 160, 190, 220 and 250V were used for fragments evaluation. LC-MS accurate mass spectra were recorded across the range m/z 50-1000. 1.5 spectra per second was employed as acquisition time with full-scan acquisition.

For comparison purposes, additional experiments were accomplished using ultra-high performance liquid chromatography quadrupole-time-of-flight mass spectrometry (UHPLC-QTOF-MS/MS), acquiring simultaneously at two different experiments: full-scan acquisition, and *all-ion mode* MS/MS, in order to perform CID experiments in a dedicated collision cell with no precursor ion isolation along with high-resolution full-scan acquisition. For this purpose, an Agilent 1260 Infinity HPLC system was connected to a hybrid quadrupole time-of-flight (Q-TOF) mass spectrometer Agilent 6530 (Agilent Technologies, Santa Clara, CA), equipped with the same dual spray interface, applying the same chromatographic method and MS parameters described for the TOF instrument except fragmentor voltage, set at 90 V. "*All-ion mode*" full-scan acquisition was used at two different collision energy conditions (0 (no fragmentation) and 20 V), using 400 milliseconds for each experiment (1.25 spectra/acquisition points per second). Accurate mass measurements of each peak from the total ion chromatograms were obtained by means of an automated calibrant delivery system using a dual-nebulizer electrospray source that introduces the flow from the outlet of the

chromatograph together with a low flow of a calibrating solution (calibrant solution A, Agilent Technologies), which contains the internal reference masses (purine ($C_5H_4N_4$ at m/z 121.050873 and HP-0921 [hexakis-(1H,1H,3H-tetrafluoropentoxy)-phosphazene] ($C_{18}H_{18}O_6N_3P_3F_{24}$) at m/z 922.009798). All data was recorded with Agilent Mass Hunter Data Acquisition software (version B.04.00) and processed with Agilent Mass Hunter Qualitative Analysis software (version B.04.00), which included both “*Molecular Feature Extractor*” and “*Find by Formula*” applications used.

Development of an accurate-mass database of 630 multiclass food contaminants pollutants. Mixtures containing *ca.* 30-50 compounds, at individual concentrations of $200 \mu\text{g L}^{-1}$ each were injected in the LC-TOFMS system to collect retention time (t_R) data and the accurate masses of target ions together with the elemental composition. For confirmatory purposes of the compounds detected in real samples, the mass spectrum was carefully investigated to identify characteristic fragment ions produced by in-source collision induced dissociation (in-source CID). In some cases, individual standards of priority and emerging compounds were required for further confirmation of diagnostic fragment ions. For the screening method step, an Excel spreadsheet was constructed containing for each analyte the compound name, molecular formula, theoretical exact mass, fragment ions and retention time. This file was converted into csv format for use by the Agilent Mass Hunter Data Acquisition software (version B.04.00). When a sample run is completed and the corresponding raw data acquired, its components are automatically matched against the csv file (Find by formula application) by the Mass Hunter software taking into account a defined tolerance for mass and retention time deviations ($t_R \pm 0.2$ min and ion exact mass ± 20 ppm), and a report is generated with the compounds tentatively found in the analyzed sample data file.

Results and discussion

Screening method development and general acquisition method considerations

Selection of UHPLC gradient. Before developing the screening method, different elution gradients were assayed in representative matrices (such as tomato and orange) in order to obtain appropriate separation of analytes and matrix components within the shortest period of time and also displaying relatively low or moderate signal suppression effects. Three methods (A, B and C) were assayed and the only difference was elution gradient (total time of 5, 10 min and 15 minutes respectively). Mobile phases were 0.1% HCOOH in water (A) and 0.1% HCOOH in acetonitrile (B). The details of the different gradient elution programs are shown in **Table S1**. The flow rate was 0.5 mL min⁻¹. An example on the analysis of a mixture of selected pesticides and some representative extracted ion chromatograms (EICs) (100 µg L⁻¹) in orange are shown in **Figure 1**. Different criteria were employed to select the most appropriate elution gradient to develop the screening method. The comparison of the total ion chromatograms (TICs) revealed that the matrix components and analytes were not separated properly in such reduced run time. The number of coelutions and thus, the possibility of interferences and quantitation issues due to matrix effects would be clearly increased under these conditions (method A). It must be taken into account the large number of components from a matrix (typically with 5000-10000 [25]) at relevant concentrations which must be separated from potentially over 600 species. For this reason, the shortest method (method A) was discarded. Given the differences of run time, it would be expected that coelutions with method B were more frequent than with method C. This fact was examined using matrix effects.

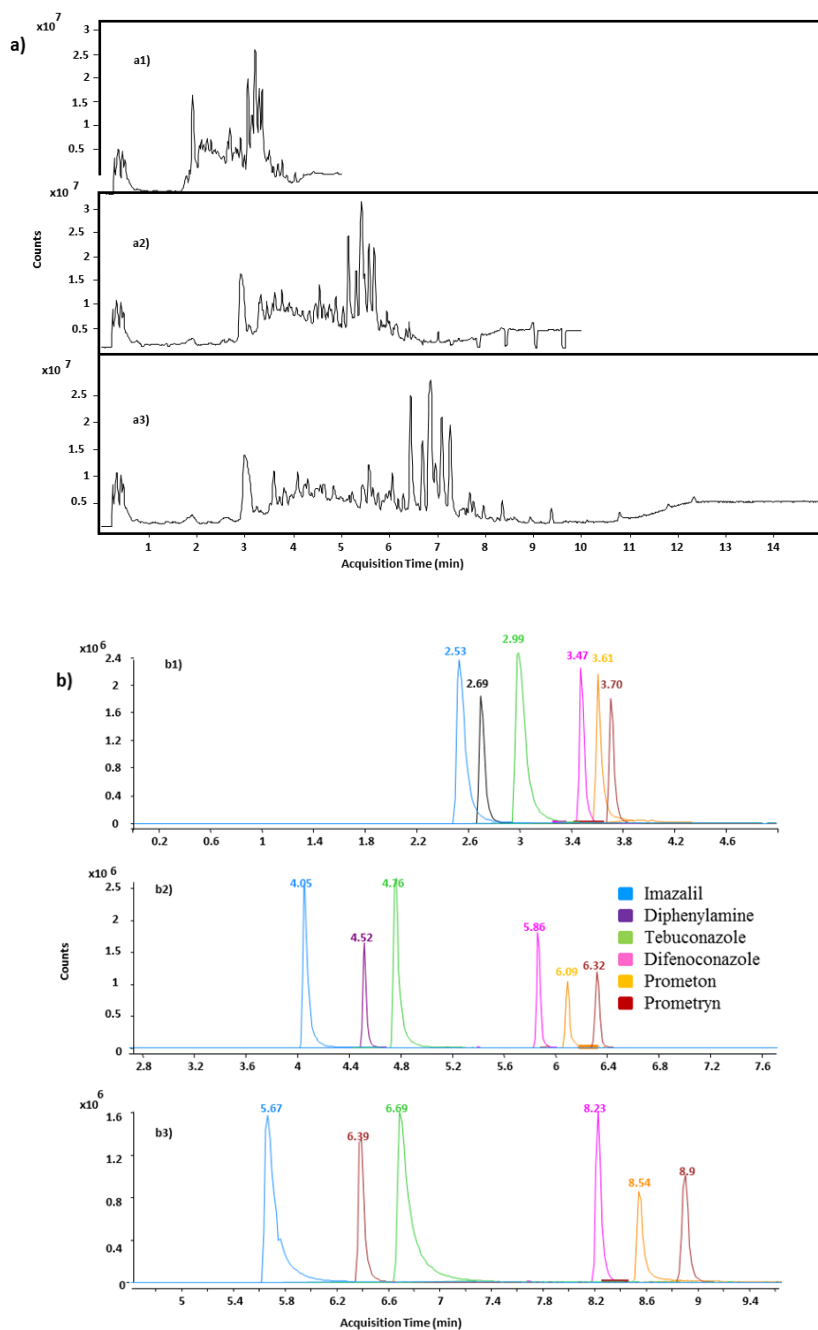


Figure 1 a) Total ion chromatograms (TICs) of a pesticide mixture ($100 \mu\text{g Kg}^{-1}$) in orange using elution gradients A (figure a1), B (figure a2) and C (figure a3). b) Extracted ion chromatograms (EICs) of some database compounds (imazalil, diphenylamine, tebuconazole, difenoconazole, prometon and prometryn ($100 \mu\text{g L}^{-1}$)) in orange with elution gradients A (figure b1), B (figure b2) and C (figure b3).

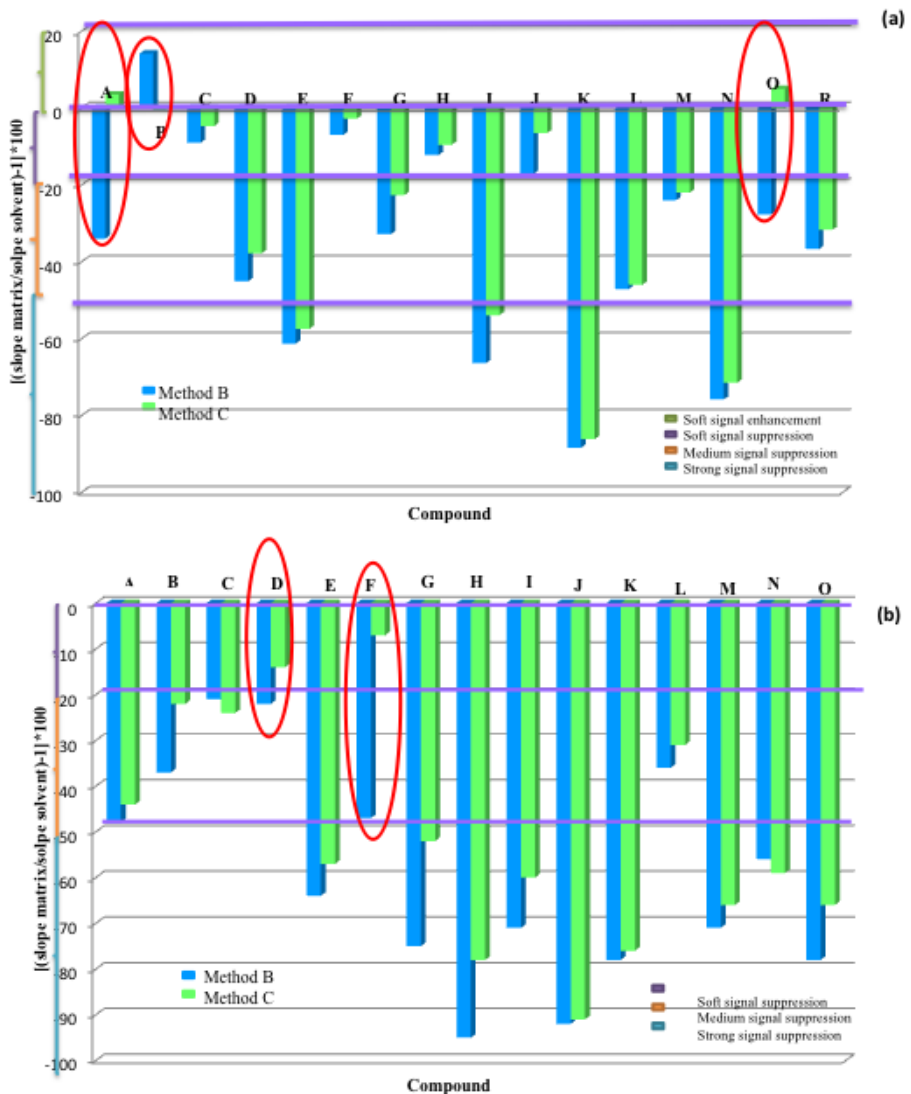


Figure 2 a) Percentages of signal suppression or enhancement for selected compounds in tomato (A: aflatoxin B₁; B: azoxystrobin; C: buprofezin; D: carbendazim; E: cyromazine; F: DEET; G: diuron; H: imazalil; I: imidacloprid; J: prochloraz; K: sarafloxacin; L: sulfamethoxazole; M: tebuconazole; N: tetracycline; O: thiabendazole; R: thiacloprid); (b) Percentages of signal suppression or enhancement for selected compounds in orange (A: aflatoxin B₁; B: azoxystrobin; C: buprofezin; D: carbendazim; E: cyromazine; F: DEET; G: Diuron; H: imidacloprid; I: prochloraz; J: sarafloxacin; K: sulfamethoxazole; L: tebuconazole; M: tetracycline; N: thiabendazole; O: thiacloprid).

Besides, the matrix components separation, a study of matrix effects using 15 representative analytes (including pesticides, veterinary drugs and mycotoxins) was also conducted in tomato and oranges with the two remaining methods (B and C). Matrix effects were calculated as follows: $[(\text{calibration curve slope in matrix} / \text{calibration curve in solvent}) - 1] \times 100$. Positive values indicate signal enhancement while negative signal involves values suppression (the more common phenomenon). Depending on this percentage, matrix effect was classified in different categories, according to previous literature [7,44]. A percentage between -20% and 20% was considered as mild matrix effect, as the slope ratios matrix/solvent would be approaching the unit. A medium matrix effect occurred when this percentage was from -50% to -20% or from +20% to +50%. Strong matrix effect would be produced when this percentage was below -50% or above +50%. The overall results for the two matrices tested are summarized in **Figure 2**.

As shown in **Figure 2(a)**, all the selected compounds showed signal suppression in tomato with both elution gradients B and C, with the exception of aflatoxin B₁, thiabendazole and azoxystrobin. The extent of matrix effects is not significantly different between the two gradients (B and C). In the case of orange (**Figure 2(b)**), all tested compounds showed signal suppression with both elution gradients assayed, although in general the matrix effects are slightly less intense in the case of the longer method. This is consistent with the fact that there is more time to separate species, thus minimizing the potential coelutions and the associated ionization competition and subsequent matrix suppression. As the main objective was to develop a screening method which separate and identify the most number of compounds

in a single run in the shortest period of time, elution gradient B was selected.

Identification of the targeted species by UHPLC-electrospray-time-of-flight mass spectrometry. For mass spectrometric detection of the studied species, a generic full-scan acquisition method with default source parameters was used. Default values were set for drying and nitrogen flow rates, vaporizer and drying gas temperatures considering the LC flow rate and mobile phase composition.

The identification of the target species was carried out using retention time values and accurate mass measurements of the (de)protonated molecules in most cases. Exceptionally, either sodium or ammonium adducts were identified as the most abundant ion for a few compounds (4 %). In general, 90% of compounds were detected in positive ion mode and only 10% of targeted compounds were identified in negative ionization mode. Additionally, it was found that, for *ca.* 20 % of the species, fragments generated from in-source CID were more abundant than the corresponding (de)protonated molecules. Fragmentor voltage was set at 190 V, a mild value to provide and balance between sensitivity for effective detection and additional mass spectrum information for confirmation purposes. Additionally, another method including two different fragmentor voltages (190 and 230 V) acquired in the same run was also tested (using 400 milliseconds for each experiment). This enabled the identification with two ions (typically the (de)protonated molecule and a second fragment ion) for nearly 85 % of the species tested (see Supplementary data, **Table S2**). In contrast, this second approach has the disadvantage of a reduced sensitivity as the acquisition time is reduced from 1.5 spectra per second to 1.25 spectra per second. For some of the compounds (*ca.* 50), only one ion was attained

so that the criteria of screening methods established by DG SANCO Document could not be meet [45].

For this purpose, an UHPLC-QTOF-MS instrument was used with “all ion mode” acquisition mode. This consists on the use of CID fragmentation in a collision cell without previous precursor isolation, so that all ions entering the mass spectrometer are subjected to thorough fragmentation, thus avoiding restrictions on the number of coeluting compounds subjected to MS/MS and also previous information required information to conduct the MS/MS experiments such as retention time windows or precursor ion masses. The acquisition method proposed consisted on two full-scan experiments with the collision cell different collision energies: 0 V (no fragmentation) and 20 V (fragmentation), using an acquisition time of 400 milliseconds for each experiment. With such experiments, at least two ions were obtained for identification/purposes in most cases with the exception of low molecular weight molecules, difficult to fragment. The detailed information including detected ion, elemental composition, retention time, theoretical m/z (exact mass) and experimental measured accurate masses with the relative mass error (expressed in ppm) are shown in **Table 1**, where compounds are grouped according to their class (pesticides, veterinary drugs, mycotoxins, perfluorinated compounds, food packaging contaminants, nitrosamines and sweeteners).

Piperophos	C ₁₄ H ₂₈ NO ₃ PS ₂	6.76	[M+H] ⁺	354.1321	354.1324	0.85
Pirimicarb	C ₁₁ H ₁₈ N ₄ O ₂	3.51	[M+H] ⁺	239.1503	239.1503	0.00
Pirimiphos Methyl	C ₁₁ H ₂₀ N ₃ O ₃ PS	6.41	[M+H] ⁺	306.1036	306.1034	-0.65
Pretilachlor Isomer 1	C ₁₇ H ₂₆ ClNO ₂	6.81	[M+H] ⁺	312.1725	312.1723	-0.64
Pretilachlor Isomer 2	C ₁₇ H ₂₆ ClNO ₂	6.73	[M+H] ⁺	312.1725	312.1723	-0.64
Prochloraz	C ₁₅ H ₁₆ Cl ₃ N ₃ O ₂	5.4	C ₁₂ H ₁₃ Cl ₃ NO ₂ ⁺	308.0006	308.0008	0.65
Procymidone	C ₁₃ H ₁₁ Cl ₂ NO ₂	6.09	[M+H] ⁺	284.024	284.0242	0.70
Profenofos	C ₁₁ H ₁₅ BrClO ₃ PS	6.79	[M+H] ⁺	372.9424	372.9424	0.00
Prohexadione	C ₁₀ H ₁₂ O ₅	4.09	[M-H] ⁻	211.0612	211.0613	0.47
Promecarb	C ₁₂ H ₁₇ NO ₂	5.69	C ₁₀ H ₁₅ O ⁺	151.1117	151.1118	0.66
Prometon	C ₁₀ H ₁₉ N ₅ O	4.05	[M+H] ⁺	226.1662	226.1659	-1.33
Prometryn	C ₁₀ H ₁₉ N ₅ S	4.76	[M+H] ⁺	242.1434	242.1437	1.24
Propachlor	C ₁₁ H ₁₄ ClNO	5.27	[M+H] ⁺	212.0837	212.0836	-0.47
Propamocarb	C ₉ H ₂₀ N ₂ O ₂	1.14	[M+H] ⁺	189.1598	189.1599	0.53
Propanil	C ₉ H ₉ Cl ₂ NO	5.47	[M+H] ⁺	218.0134	218.0132	-0.92
Propaquizafop	C ₂₂ H ₂₂ ClN ₃ O ₅	6.93	[M+H] ⁺	444.1321	444.1321	0.00
Propargite	C ₁₉ H ₂₆ O ₄ S	7.40	[M+Na] ⁺	373.1444	373.1446	0.54
Propazine	C ₉ H ₁₆ ClN ₅	5.41	[M+H] ⁺	230.1167	230.1169	0.87
Propetamphos	C ₁₀ H ₂₀ NO ₄ PS	6.16	C ₃ H ₁₁ NO ₂ PS ⁺	156.0243	156.0245	1.28
Propham	C ₁₀ H ₁₃ NO ₂	5.30	C ₇ H ₈ NO ₂ ⁺	138.055	138.056	7.24
Propiconazole	C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	6.13	[M+H] ⁺	342.0771	342.0771	0.00
Propisochlor	C ₁₅ H ₂₂ ClNO ₂	6.4	C ₁₀ H ₁₅ N ⁺	148.1121	148.1122	0.68
Propoxur	C ₁₁ H ₁₅ NO ₃	4.75	[M+H] ⁺	232.0944	232.0944	0.00
Propylene thiourea	C ₄ H ₈ N ₂ S	0.53	[M+H] ⁺	117.0481	117.0481	0.00
Propyzamid	C ₁₂ H ₁₁ Cl ₂ NO	5.89	C ₇ H ₆ Cl ₂ NO ⁺	189.9821	189.9824	1.58
Proquinazid	C ₁₄ H ₁₇ IN ₂ O ₂	7.51	[M+H] ⁺	373.0407	373.0405	-0.54
Prosulfocarb	C ₁₄ H ₂₁ NOS	6.91	[M+H] ⁺	252.1417	252.1418	0.40
Prosulfuron	C ₁₅ H ₁₆ F ₃ N ₅ O ₄ S	5.64	[M+H] ⁺	420.0948	420.0946	-0.48
Pymetrozin	C ₁₀ H ₁₁ N ₅ O	0.70	[M+H] ⁺	218.1036	218.1036	0.00
Pyracarbolid	C ₁₃ H ₁₅ NO ₂	4.89	[M+H] ⁺	218.1176	218.1176	0.00
Pyraclostrobin	C ₁₉ H ₁₈ ClN ₃ O ₄	6.6	[M+H] ⁺	388.1059	388.1056	-0.77
Pyranocoumarin	C ₂₀ H ₁₈ O ₄	6.47	[M+H] ⁺	323.1278	323.1277	-0.31
Pyrazophos	C ₁₄ H ₂₀ N ₃ O ₅ PS	6.51	[M+H] ⁺	374.0934	374.0935	0.27
Pyridaben	C ₁₉ H ₂₅ ClN ₂ OS	7.61	[M+H] ⁺	365.1449	365.1451	0.55
Pyridaphenthion	C ₁₄ H ₁₇ N ₂ O ₄ PS	5.86	[M+H] ⁺	341.0719	341.0719	0.00
Pyrifenox Isomer 1	C ₁₄ H ₁₂ Cl ₂ N ₂ O	4.57	[M+H] ⁺	295.0399	295.039	-3.05
Pyrifenox Isomer 2	C ₁₄ H ₁₂ Cl ₂ N ₂ O	4.65	[M+H] ⁺	295.0399	295.0397	-0.68
Pyrimethanil	C ₁₂ H ₁₃ N ₃	4.54	[M+H] ⁺	200.1182	200.1179	-1.50
Pyriproxifen	C ₂₀ H ₁₉ NO ₃	7.10	[M+H] ⁺	322.1438	322.144	0.62
Pyroquilon	C ₁₁ H ₁₁ NO	4.28	[M+H] ⁺	174.0913	174.0912	-0.57
Quinalphos	C ₁₂ H ₁₅ N ₂ O ₃ PS	6.35	[M+H] ⁺	299.0614	299.0615	0.33
Quinmerac	C ₁₁ H ₈ ClNO ₂	3.67	C ₁₁ H ₇ ClNO ⁺	204.0211	204.0212	0.44
Quinoclamine	C ₁₀ H ₆ ClNO ₂	4.59	[M+H] ⁺	208.016	208.0159	-0.48
Quinoxifen	C ₁₅ H ₈ Cl ₂ FNO	6.75	[M+H] ⁺	308.004	308.0043	0.97
Quizalofop-P-Ethyl	C ₁₉ H ₁₇ ClN ₂ O ₄	6.85	[M+H] ⁺	373.095	373.0949	-0.27
Resmethrin (R+S isomers)	C ₂₂ H ₂₆ O ₃	7.73	[M+H] ⁺	339.1955	339.1948	-2.06
Rimsulfuron	C ₁₄ H ₁₇ N ₅ O ₇ S ₂	4.96	[M+H] ⁺	432.0642	432.0631	-2.55
Rotenone	C ₂₃ H ₂₂ O ₆	6.15	[M+H] ⁺	395.1489	395.1487	-0.51
Secbumeton	C ₁₀ H ₁₉ N ₅ O	4.05	[M+H] ⁺	226.1662	226.1663	0.44
Sethoxydim	C ₁₇ H ₂₉ NO ₃ S	7.13	[M+H] ⁺	328.1941	328.1942	0.30
Siduron	C ₁₄ H ₂₀ N ₂ O	5.51	[M+H] ⁺	233.1648	233.1648	0.00
Simazine	C ₇ H ₁₂ ClN ₅	4.44	[M+H] ⁺	202.0854	202.0856	0.99
Spinosyn A	C ₄₁ H ₆₅ NO ₁₀	5.37	[M+H] ⁺	732.4681	732.4677	-0.55
Spinosyn D	C ₄₂ H ₆₇ NO ₁₀	5.54	[M+H] ⁺	746.4838	746.4832	-0.80
Spiromesifen	C ₂₃ H ₃₀ O ₄	7.62	C ₁₇ H ₂₂ O ₃ ⁺	273.1485	273.149	-1.83
Spirotetramat	C ₂₁ H ₂₇ NO ₅	5.60	[M+H] ⁺	374.1962	374.1961	-0.27
Spiroxamine	C ₁₈ H ₃₅ NO ₂	4.91	[M+H] ⁺	298.2741	298.274	-0.34

Sulcotrione	C ₁₄ H ₁₃ ClO ₅ S	4.86	[M+H] ⁺	329.0245	329.0245	0.00
Sulfaquinoxaline	C ₁₄ H ₁₂ N ₄ O ₂ S	4.38	[M+H] ⁺	301.0754	301.0752	-0.66
Sulfometuron Methyl	C ₁₅ H ₁₆ N ₄ O ₅ S	4.87	[M+H] ⁺	365.0914	365.0913	-0.27
Sulfotep	C ₈ H ₂₀ O ₅ P ₂ S ₂	6.65	[M+H] ⁺	323.03	323.0299	-0.31
Sulprofos	C ₁₂ H ₁₉ O ₂ PS ₃	7.31	[M+H] ⁺	323.0358	323.0358	0.00
Tcpp	C ₉ H ₁₈ Cl ₃ O ₄ P	5.65	C ₄ H ₉ Cl ₂ O ₃ ⁺	174.9923	174.9922	-0.57
Tebuconazole	C ₁₆ H ₂₂ ClN ₃ O	5.86	[M+H] ⁺	308.1524	308.1522	-0.65
Tebufenpyrad	C ₁₈ H ₂₄ ClN ₃ O	6.85	[M+H] ⁺	334.1681	334.1683	0.60
Tebutam	C ₁₅ H ₂₃ NO	6.05	[M+H] ⁺	234.1852	234.1854	0.85
Tebuthiuron	C ₉ H ₁₆ N ₄ OS	4.27	[M+H] ⁺	229.1118	229.112	0.87
Teflubenzuron	C ₁₄ H ₆ Cl ₂ F ₄ N ₂ O ₂	6.68	[M-H] ⁻	378.9670	378.9673	0.79
Tembotrione	C ₁₇ H ₁₆ ClF ₃ O ₆ S	5.76	C ₁₅ H ₁₄ ClO ₅ S ⁺	341.0245	341.0250	1.47
Temephos	C ₁₆ H ₂₀ O ₆ P ₂ S ₃	7.18	[M+H] ⁺	466.997	466.9971	0.21
Tepraloxym Isomer 1	C ₁₇ H ₂₄ ClNO ₄	5.84	[M+H] ⁺	342.1467	342.1467	0.00
Tepraloxym Isomer 2	C ₁₇ H ₂₄ ClNO ₄	4.65	[M+H] ⁺	342.1467	342.1462	-1.46
Terbacil	C ₉ H ₁₃ ClN ₂ O ₂	4.50	[M-H] ⁻	215.0593	215.0585	-3.72
Terbufos	C ₉ H ₂₁ O ₂ PS ₃	7.13	C ₄ H ₁₃ O ₂ PS ₂ ⁺	187.0011	187.0017	3.21
Terbumeton	C ₁₀ H ₁₉ N ₅ O	4.10	[M+H] ⁺	226.1662	226.1662	0.00
Terbutylazine	C ₉ H ₁₆ ClN ₅	5.54	[M+H] ⁺	230.1167	230.1171	1.30
Terbutryn	C ₁₀ H ₁₉ N ₅ S	4.79	[M+H] ⁺	242.1434	242.1435	0.41
Tetrachovinphos	C ₁₀ H ₉ Cl ₄ O ₄ P	6.08	C ₈ H ₃ Cl ₄ ⁺	127.0155	127.0154	-0.79
Thiabendazole	C ₁₀ H ₇ N ₃ S	2.98	[M+H] ⁺	202.0433	202.0437	1.98
Thiacloprid	C ₁₀ H ₉ ClN ₄ S	4.30	[M+H] ⁺	253.0309	253.0309	0.00
Thiamethoxam	C ₈ H ₁₀ ClN ₅ O ₂ S	3.43	C ₈ H ₁₁ N ₄ OS ⁺	211.0648	211.0647	-1.03
Thidiazuron	C ₉ H ₈ N ₄ OS	4.50	[M+H] ⁺	221.0492	221.0488	-1.81
Thifensulfuron methyl	C ₁₂ H ₁₃ N ₅ O ₆ S ₂	4.68	[M+H] ⁺	388.038	388.0375	-1.29
Thiocyclam	C ₅ H ₁₁ NS ₃	0.78	C ₅ H ₅ S ₃ ⁺	136.9548	136.9551	2.19
Thiodicarb	C ₁₀ H ₁₈ N ₄ O ₄ S ₃	4.77	[M+Na] ⁺	377.0382	377.0379	-0.80
Thiofanox	C ₉ H ₁₈ N ₂ O ₂ S	4.99	[M+Na] ⁺	241.0981	241.0983	0.83
Thiophanate Methyl	C ₁₂ H ₁₄ N ₄ O ₄ S ₂	4.72	[M+H] ⁺	343.0529	343.0528	-0.29
Tolclofos Methyl	C ₉ H ₁₁ Cl ₂ O ₃ PS	6.67	[M+H] ⁺	300.9616	300.9615	-0.33
Tralkoxidym	C ₂₀ H ₂₇ NO ₃	7.24	[M+H] ⁺	330.2064	330.2064	0.00
Transfluthrin	C ₁₅ H ₁₂ Cl ₂ F ₄ O ₂	7.36	C ₇ H ₃ F ₄ ⁺	163.0165	163.0166	0.61
Triadimefon	C ₁₄ H ₁₆ ClN ₃ O ₂	5.80	[M+H] ⁺	294.1004	294.1007	1.02
Triadimenol isomer 1	C ₁₄ H ₁₈ ClN ₃ O ₂	5.43	C ₂ H ₄ N ₃ ⁺	70.0399	70.0400	1.43
Triadimenol isomer 2	C ₁₄ H ₁₈ ClN ₃ O ₂	5.53	C ₂ H ₄ N ₃ ⁺	70.0399	70.0400	1.43
Triallat	C ₁₀ H ₁₆ Cl ₃ NOS	7.41	[M+H] ⁺	304.0091	304.0092	0.33
Triasulfuron	C ₁₄ H ₁₆ ClN ₅ O ₅ S	4.91	[M+H] ⁺	402.0633	402.063	-0.75
Triazophos	C ₁₂ H ₁₆ N ₃ O ₃ PS	6.11	[M+H] ⁺	314.0723	314.0726	0.96
Triazoxide	C ₁₀ H ₆ ClN ₅ O	4.14	[M+H] ⁺	248.0334	248.0333	-0.40
Trichlorfon	C ₄ H ₈ Cl ₃ O ₄ P	3.52	[M+H] ⁺	256.9299	256.9302	1.17
Triclocarban	C ₁₃ H ₉ Cl ₃ ON ₂	6.63	[M+H] ⁺	314.9853	314.985	-0.95
Tridemorph	C ₁₉ H ₃₉ NO	5.44	[M+H] ⁺	298.3105	298.3105	0.00
Trietazine	C ₉ H ₁₆ ClN ₅	5.95	[M+H] ⁺	230.1167	230.117	1.30
Triethanolamine	C ₆ H ₁₅ NO ₃	0.28	[M+H] ⁺	150.1125	150.112	-3.33
Trifloxystrobin	C ₂₀ H ₁₉ F ₃ N ₂ O ₄	6.81	[M+H] ⁺	409.137	409.1368	-0.49
Trifloxysulfuron	C ₁₄ H ₁₃ F ₃ N ₅ O ₆ S	5.12	[M+H] ⁺	438.069	438.0685	-1.14
Triflumizole	C ₁₅ H ₁₅ ClF ₃ N ₃ O	5.88	C ₁₂ H ₁₂ ClF ₃ NO ⁺	278.0554	278.0555	0.36
Triflururon	C ₁₅ H ₁₀ ClF ₃ N ₂ O ₃	6.38	[M-H] ⁻	357.0259	357.0265	1.68
Trifluralin	C ₁₃ H ₁₆ F ₃ N ₃ O ₄	7.27	[M+H] ⁺	336.1166	336.1176	2.98
Triforine	C ₁₀ H ₁₄ Cl ₆ N ₄ O ₂	5.16	C ₉ H ₁₂ Cl ₆ N ₃ O ⁺	387.9106	387.9102	-1.03
Trimethylsulfonium	C ₃ H ₈ S	0.26	[M+H] ⁺	77.0425	77.0423	-2.60
Trinexapac-Ethyl	C ₁₃ H ₁₆ O ₅	5.35	[M+H] ⁺	253.1071	253.1072	0.40
Triticonazole	C ₁₇ H ₂₀ ClN ₃ O	5.53	[M+H] ⁺	318.1368	318.1366	-0.63
Vamidothion	C ₈ H ₁₈ NO ₄ PS ₂	3.65	C ₆ H ₁₂ NOS ⁺	146.0634	146.0637	2.05
Vinclozolin	C ₁₂ H ₉ Cl ₂ NO ₃	6.27	C ₁₁ H ₁₀ Cl ₂ NO ⁺	242.0134	242.0128	-2.48
Zoxamide	C ₁₄ H ₁₆ Cl ₃ NO ₂	6.51	[M+H] ⁺	336.0319	336.0316	-0.89

Veterinary drugs						
Albendazole sulfone	C ₁₂ H ₁₅ N ₃ O ₄ S	3.97	[M+H] ⁺	298.0856	298.0863	2.95
Albendazole sulfoxide	C ₁₂ H ₁₅ N ₃ O ₅ S	3.51	[M+H] ⁺	282.0907	282.0911	1.42
Amoxicillin	C ₁₆ H ₁₉ N ₃ O ₅ S	0.93	C ₁₆ H ₁₇ N ₂ O ₅ S ⁺	349.0853	349.0857	1.15
Ampicillin	C ₁₆ H ₁₉ N ₃ O ₄ S	3.17	[M+H] ⁺	350.1169	350.1164	-1.43
Benzothiazole	C ₇ H ₅ NS	4.35	[M+H] ⁺	136.0215	136.0213	-1.47
Benzydamine	C ₁₉ H ₂₃ N ₃ O	4.47	[M+H] ⁺	310.1914	310.1914	0.00
Caffeine	C ₈ H ₁₀ N ₄ O ₂	3.04	[M+H] ⁺	195.0877	195.0875	-1.03
Carbadox	C ₁₁ H ₁₀ N ₄ O ₄	3.40	[M+H] ⁺	263.0775	263.0775	0.00
Carbamazepine	C ₁₅ H ₁₂ N ₂ O	4.65	[M+H] ⁺	237.1022	237.102	-0.84
Chloramphenicol	C ₁₁ H ₁₂ O ₅ N ₂ Cl ₂	4.14	[M-H] ⁻	321.0051	321.0052	0.31
Chlorotetracycline iso. 1	C ₂₂ H ₂₃ ClN ₂ O ₈	3.62	[M+H] ⁺	479.1216	479.1210	-1.25
Chlortetracycline iso. 2	C ₂₂ H ₂₃ ClN ₂ O ₈	3.87	[M+H] ⁺	479.1216	479.1206	-2.09
Ciprofloxacin	C ₁₇ H ₁₈ FN ₃ O ₃	3.46	[M+H] ⁺	332.1405	332.1401	-1.20
Clarithromycin	C ₃₈ H ₆₉ NO ₁₃	4.67	[M+H] ⁺	748.4842	748.4823	-2.54
Clenbuterol	C ₁₂ H ₁₈ Cl ₂ N ₂ O	3.61	[M+H] ⁺	277.0869	277.087	0.36
Clofibric Acid	C ₁₀ H ₁₁ O ₃ Cl	5.24	C ₆ H ₄ ClO ⁻	126.9951	126.9951	0.00
Cloxacillin	C ₁₉ H ₁₈ ClN ₃ O ₅ S	5.17	[M+CH ₄ OH] ⁺	468.0991	468.0995	0.85
Cotinine	C ₁₀ H ₁₂ N ₂ O	0.41	[M+H] ⁺	177.1022	177.1022	0.00
Danofloxacin	C ₁₉ H ₂₀ FN ₃ O ₃	3.48	[M+H] ⁺	358.1561	358.1563	0.56
Demeclocycline isomer 1	C ₂₁ H ₂₁ ClN ₂ O ₈	3.64	[M+H] ⁺	465.1059	465.1069	2.15
Demeclocycline isomer 2	C ₂₁ H ₂₁ ClN ₂ O ₈	3.46	[M+H] ⁺	465.1059	46.1041	-3.87
Diclofenac	C ₁₄ H ₁₁ Cl ₂ NO ₂	5.89	C ₁₃ H ₈ Cl ₂ N ⁺	250.0196	250.0210	5.60
Dicloxacillin isomer 1	C ₁₉ H ₁₇ N ₃ Cl ₂ O ₅ S	5.34	[M+CH ₄ OH] ⁺	502.0601	502.0606	1.00
Dicloxacillin isomer 2	C ₁₉ H ₁₇ N ₃ Cl ₂ O ₅ S	5.45	[M+CH ₄ OH] ⁺	502.0601	502.0609	1.59
Difloxacin	C ₂₁ H ₁₉ F ₂ N ₃ O ₃	3.72	[M+H] ⁺	400.1467	400.1466	-0.25
Digoxin	C ₄₁ H ₆₄ O ₁₄	4.45	C ₃₅ H ₅₅ O ₁₁ ⁺	651.3739	651.3733	-0.92
Dimetridazole	C ₅ H ₇ N ₃ O ₂	1.29	[M+H] ⁺	142.0611	142.0611	0.00
Diphenhydramine	C ₁₇ H ₂₁ NO	4.3	C ₁₃ H ₁₁ ⁺	167.0855	167.0856	0.60
Doramectin	C ₅₀ H ₇₄ O ₁₄	7.99	C ₂₁ H ₃₁ O ₃ ⁺	331.2268	331.2272	1.21
Doxicycline	C ₂₂ H ₂₄ N ₂ O ₈	3.98	[M+H] ⁺	445.1605	445.1608	0.67
Enoxacin	C ₁₅ H ₁₇ FN ₄ O ₃	3.33	[M+H] ⁺	321.1357	321.1357	0.00
Enrofloxacin	C ₁₉ H ₂₂ FN ₃ O ₃	3.54	[M+H] ⁺	360.1718	360.172	0.56
Eprinomectin B _{1a}	C ₅₀ H ₇₅ NO ₁₄	7.14	[M+Na] ⁺	936.5080	936.5093	1.39
Eprinomectin B _{1b}	C ₄₉ H ₇₃ NO ₁₄	7.14	[M+Na] ⁺	922.4923	922.4902	-2.28
Erythromycin	C ₃₉ H ₆₇ NO ₁₃	4.32	[M+H] ⁺	734.4685	734.4671	-1.91
Estrone	C ₁₈ H ₂₂ O ₂	5.47	[M+H] ⁺	271.1693	271.1693	0.00
Febantel ₁	C ₁₆ H ₁₈ N ₄ O ₂ S	4.16	[M+H] ⁺	331.1223	331.1231	2.72
Febantel ₂	C ₁₈ H ₂₀ N ₄ O ₄ S	4.29	[M+H] ⁺	389.1278	389.1271	-1.80
Fleroxacin	C ₁₇ H ₁₈ F ₃ N ₃ O ₃	3.31	[M+H] ⁺	370.1373	370.1378	0.14
Flufenamic Acid	C ₁₄ H ₁₀ F ₃ NO ₂	6.22	C ₁₄ H ₉ F ₃ NO ⁺	264.0631	264.0628	-1.14
Flumequine	C ₁₄ H ₁₂ FNO ₃	4.75	[M+H] ⁺	262.0874	262.0871	-1.14
Fluoxetine	C ₁₇ H ₁₈ F ₃ NO	4.75	[M+H] ⁺	310.1413	310.1416	0.97
Furosemide	C ₁₂ H ₁₁ ClN ₂ O ₂ S	4.70	[M-H] ⁻	329.004	329.0033	-2.13
Gemfibrozil	C ₁₅ H ₂₂ O ₃	6.33	C ₇ H ₁₃ O ₂ ⁺	129.091	129.0912	1.55
Hydrochlorothiazide	C ₇ H ₈ ClN ₃ O ₄ S ₂	2.64	[M-H] ⁻	295.9572	295.9568	-1.69
Hydroflumethiazide	C ₈ H ₈ F ₃ N ₃ O ₄ S ₂	3.58	C ₈ H ₆ F ₃ N ₂ O ₄ S ₂ ⁺	314.9716	314.972	1.27
Ibuprofen	C ₁₃ H ₁₈ O ₂	5.97	C ₁₂ H ₁₇ ⁺	161.1325	161.1325	0.00
Indomethacine	C ₁₉ H ₁₆ ClNO ₄	5.90	[M+H] ⁺	358.0841	358.0838	-0.84
Irgasan	C ₁₂ H ₇ Cl ₃ O ₂	6.69	C ₆ H ₃ Cl ₂ O ⁺	160.9555	160.9559	2.49
Josamycin	C ₄₂ H ₆₉ NO ₁₅	4.93	[M+H] ⁺	828.474	828.4739	-0.12
Ketoprofen	C ₁₆ H ₁₄ O ₃	5.24	[M+H] ⁺	255.1016	255.1008	-3.14
Leucomalachite Green	C ₂₃ H ₂₆ N ₂	4.88	[M+H] ⁺	331.2169	331.2171	0.60
Levamisole	C ₁₁ H ₁₂ N ₂ S	1.98	[M+H] ⁺	205.0794	205.079	-1.95
Lincomycin	C ₁₈ H ₃₄ N ₂ O ₆ S	2.94	[M+H] ⁺	407.221	407.2206	-0.98
Lomefloxacin	C ₁₇ H ₁₉ F ₂ N ₃ O ₃	3.47	[M+H] ⁺	352.1467	352.1462	-1.42

Malachite Green	C ₂₃ H ₂₄ N ₂	5.06	[M+H] ⁺	329.2012	329.2013	0.30
Marbofloxacin	C ₁₇ H ₁₉ FN ₄ O ₄	3.30	[M+H] ⁺	363.1463	363.1466	0.83
Mebendazole	C ₁₆ H ₁₃ N ₃ O ₃	4.42	[M+H] ⁺	296.103	296.1025	-1.69
Meclofenamic Acid	C ₁₄ H ₁₁ Cl ₂ NO ₂	6.26	C ₁₄ H ₁₀ Cl ₂ NO ⁺	278.0134	278.0138	1.44
Mefenamic Acid	C ₁₅ H ₁₅ NO ₂	6.25	C ₁₅ H ₁₄ NO ⁺	224.107	224.1071	0.45
Menadione	C ₁₁ H ₁₀ O ₅ S	3.16	[M-H] ⁻	253.0171	253.0171	0.00
Metformin	C ₄ H ₁₁ N ₅	0.27	[M+H] ⁺	130.1087	130.1086	-0.77
Metronidazole	C ₆ H ₉ N ₃ O ₃	1.06	C ₆ H ₈ N ₃ O ₂ ⁺	128.0456	128.0455	-0.08
Miconazole	C ₁₈ H ₁₄ Cl ₄ N ₂ O	5.35	[M+H] ⁺	414.9933	414.9934	0.24
Minocycline	C ₂₃ H ₂₇ N ₃ O ₇	3.06	[M+H] ⁺	458.1922	458.1921	-0.22
Monensin	C ₃₆ H ₆₂ O ₁₁	8.94	[M+Na] ⁺	693.4184	693.4207	3.46
Naproxen	C ₁₄ H ₁₄ O ₃	5.27	C ₁₃ H ₁₃ O ⁺	185.0961	185.096	-0.54
Natamycin	C ₃₃ H ₄₇ NO ₁₃	4.37	[M+H] ⁺	666.312	666.3115	-0.75
Nicotine	C ₁₀ H ₁₄ N ₂	0.40	[M+H] ⁺	163.123	163.1231	0.61
Nifuroxazide	C ₁₂ H ₉ N ₃ O ₅	4.20	[M+H] ⁺	276.0615	276.0623	2.90
Norfloxacin	C ₁₆ H ₁₈ FN ₃ O ₃	3.38	[M+H] ⁺	320.1405	320.1406	0.31
Orbifloxacin	C ₁₉ H ₂₀ F ₃ N ₃ O ₃	3.58	[M+H] ⁺	396.153	396.1532	0.50
Oxacillin isomer 1	C ₁₉ H ₁₉ N ₃ O ₅ S	4.96	[M+CH ₄ OH] ⁺	434.1380	434.1383	0.69
Oxacillin isomer 2	C ₁₉ H ₁₉ N ₃ O ₅ S	5.04	[M+CH ₄ OH] ⁺	434.1380	434.1379	-0.23
Oxolinic Acid	C ₁₃ H ₁₁ NO ₅	4.19	[M+H] ⁺	262.071	262.0713	1.14
Oxybendazole	C ₁₂ H ₁₅ N ₃ O ₃	3.99	[M+H] ⁺	250.1186	250.1186	0.00
Oxytetracycline	C ₂₂ H ₂₄ N ₂ O ₉	3.36	[M+H] ⁺	461.1555	461.1559	0.87
Penicillin G isomer 1	C ₁₆ H ₁₈ N ₂ O ₄ S	4.50	[M+H] ⁺	335.1060	335.1060	0.00
Penicillin G isomer 2	C ₁₆ H ₁₈ N ₂ O ₄ S	4.56	[M+H] ⁺	335.1060	335.1061	0.30
Penicillin V Isomer 1	C ₁₇ H ₂₂ N ₂ O ₆ S	4.73	[M+CH ₄ OH] ⁺	383.1271	383.1277	1.57
Penicillin V Isomer 2	C ₁₆ H ₁₈ N ₂ O ₆ S	4.87	[M+CH ₄ OH] ⁺	383.1271	383.1271	0.00
Pentylentetrazole	C ₆ H ₁₀ N ₄	2.43	[M+H] ⁺	139.0978	139.0976	-0.14
Phenylbutazone	C ₁₉ H ₂₀ N ₂ O ₂	6.12	[M+H] ⁺	309.1598	309.1595	-0.97
Pravastatin	C ₂₃ H ₃₆ O ₇	4.54	[M-H] ⁻	423.2388	423.2399	2.60
Prednisolone	C ₂₁ H ₂₈ O ₅	4.36	[M+H] ⁺	361.201	361.1996	-3.88
Promethazine	C ₁₇ H ₂₀ N ₂ S	4.45	[M+H] ⁺	285.142	285.142	0.00
Propranolol	C ₁₆ H ₂₁ O ₂ N	4.15	[M+H] ⁺	260.1645	260.1647	0.77
Ranitidine	C ₁₃ H ₂₂ N ₄ O ₃ S	1.44	[M+H] ⁺	315.1485	315.1485	0.00
Robenidine	C ₁₈ H ₂₃ NO ₃	3.43	[M+H] ⁺	302.1751	302.1748	-0.99
Ronidazole	C ₆ H ₈ N ₄ O ₄	1.55	C ₅ H ₆ N ₃ O ₂ ⁺	140.0455	140.0454	-0.71
Roxithromycin	C ₄₁ H ₇₆ N ₂ O ₁₅	4.74	[M+H] ⁺	837.5318	837.5299	-2.27
Salbutamol	C ₁₃ H ₂₁ NO ₃	1.01	[M+H] ⁺	240.1594	240.1596	0.83
Sarafloxacin	C ₂₀ H ₁₇ F ₂ N ₃ O ₃	3.69	[M+H] ⁺	386.1311	386.1306	-1.29
Spiramycin	C ₄₃ H ₇₄ N ₂ O ₁₄	3.79	[M+H] ⁺	843.5213	843.5215	0.24
Streptomycin	C ₂₁ H ₃₉ N ₇ O ₁₂	0.24	C ₈ H ₁₉ N ₆ O ₄ ⁺	263.1462	263.1466	1.52
Sulfabenzamide	C ₁₃ H ₁₂ N ₂ O ₃ S	4.30	C ₆ H ₆ NO ₂ S ⁺	156.0114	156.0108	-3.85
Sulfacetamide	C ₈ H ₁₀ N ₂ O ₃ S	1.33	C ₆ H ₆ NO ₂ S ⁺	156.0114	156.0114	0.00
Sulfachloropyridazine	C ₁₀ H ₉ ClN ₄ O ₂ S	3.8	[M+H] ⁺	285.0208	285.021	0.07
Sulfadiazine	C ₁₀ H ₁₀ N ₄ O ₂ S	1.63	[M+H] ⁺	251.0597	251.0597	0.00
Sulfadimethoxyn	C ₁₂ H ₁₄ N ₄ O ₄ S	4.39	[M+H] ⁺	311.0809	311.0805	-0.13
Sulfadoxine	C ₁₂ H ₁₄ N ₄ O ₄ S	3.94	[M+H] ⁺	311.0809	311.0812	0.96
Sulfaguanidine	C ₇ H ₁₀ N ₄ O ₂ S	0.47	[M+H] ⁺	215.0597	215.0596	-0.46
Sulfamerazine	C ₁₁ H ₁₂ N ₄ O ₂ S	2.9	[M+H] ⁺	265.0754	265.0754	0.00
Sulfameter	C ₁₁ H ₁₂ N ₄ O ₃ S	3.51	[M+H] ⁺	281.0703	281.0701	-0.71
Sulfamethazine	C ₁₂ H ₁₄ N ₄ O ₂ S	3.32	[M+H] ⁺	279.091	279.0911	0.36
Sulfamethizole	C ₉ H ₁₀ N ₄ O ₂ S ₂	3.49	[M+H] ⁺	271.0318	271.0318	0.00
Sulfamethoxazole	C ₁₀ H ₁₁ N ₃ O ₃ S	3.97	[M+H] ⁺	254.0594	254.0594	0.00
Sulfamethoxypyridazine	C ₁₁ H ₁₂ N ₄ O ₃ S	3.53	[M+H] ⁺	281.0703	281.0703	0.00
Sulfamonomethoxine	C ₁₁ H ₁₂ N ₄ O ₃ S	3.74	[M+H] ⁺	281.0703	281.0703	0.00
Sulfanilamide	C ₆ H ₈ N ₂ O ₂ S	0.54	[M+H] ⁺	173.0379	173.038	0.58
Sulfapyridine	C ₁₁ H ₁₁ N ₃ O ₂ S	2.68	[M+H] ⁺	250.0645	250.0646	0.40
Sulfathiazole	C ₉ H ₉ N ₃ O ₂ S ₂	2.51	[M+H] ⁺	256.0209	256.021	0.39

Sulfisoxazol	C ₁₁ H ₁₃ N ₃ O ₃ S	4.14	[M+H] ⁺	268.075	268.075	0.00
Sulindac	C ₂₀ H ₁₇ FO ₃ S	4.93	[M+H] ⁺	357.0955	357.0957	0.00
Tetracycline	C ₂₂ H ₂₄ N ₂ O ₈	3.46	[M+H] ⁺	445.1605	445.1601	-0.90
Theobromine	C ₇ H ₈ N ₄ O ₂	1.08	[M+H] ⁺	181.072	181.0719	-0.55
Theophylline	C ₇ H ₈ N ₄ O ₂	1.87	[M+H] ⁺	181.072	181.0721	0.55
Thiamphenicol	C ₁₂ H ₁₅ Cl ₂ NO ₅ S	3.32	[M-H] ⁻	353.9975	353.9964	-3.11
Tilmicosin	C ₄₆ H ₈₀ N ₂ O ₁₃	4.02	[M+2H] ²⁺	435.2903	435.2901	-0.46
Tolfenamic Acid	C ₁₄ H ₁₂ ClNO ₂	6.39	[M+H] ⁺	262.0629	262.0633	1.53
Tolmetin	C ₁₅ H ₁₅ NO ₃	5.13	[M+H] ⁺	258.1125	258.1121	-1.55
Trimethoprim	C ₁₄ H ₁₈ N ₄ O ₃	3.22	[M+H] ⁺	291.1452	291.1451	-0.34
Tylosin	C ₄₆ H ₇₇ NO ₁₇	4.43	[M+H] ⁺	916.5264	916.5257	-0.76
β-Estradiol	C ₁₈ H ₂₄ O ₂	5.16	C ₁₈ H ₂₃ O ⁺	255.1743	255.1748	1.96
Food packaging contaminants						
1,3-Phenylenediamine	C ₆ H ₈ N ₂	0.29	[M+H] ⁺	109.0760	109.0757	-2.75
1,6-Phenylenediamine	C ₆ H ₈ N ₂	0.28	[M+H] ⁺	109.0760	109.0761	0.92
² 2-EHDP	C ₂₀ H ₂₇ O ₄ P	7.55	C ₁₂ H ₁₂ O ₄ P ⁺	251.0468	251.0476	3.19
2-Methoxy-5-methylalanine	C ₈ H ₁₁ ON	1.70	[M+H] ⁺	138.0913	138.0912	-0.72
2,4-Diaminoanisole	C ₇ H ₁₀ N ₂ O	0.41	[M+H] ⁺	139.0866	139.0867	0.72
2,4-Diaminotoluene	C ₇ H ₁₀ N ₂	0.40	[M+H] ⁺	123.0917	123.092	2.44
2,4-Dimethylaniline	C ₈ H ₁₁ N	1.72	[M+H] ⁺	122.0964	122.0963	-0.82
2,4,5-Trimethylaniline	C ₉ H ₁₃ N	3.27	[M+H] ⁺	136.1121	136.112	-2.18
2,6-Diaminotoluene	C ₇ H ₁₀ N ₂	0.40	[M+H] ⁺	123.0917	123.0915	0.81
4-Aminobiphenyl	C ₁₂ H ₁₁ N	4.16	[M+H] ⁺	170.0964	170.0962	-1.18
4-Chloroaniline	C ₆ H ₆ ClN	1.60	[M+H] ⁺	128.0262	128.0261	-0.78
4-Hexylresorcinol	C ₁₂ H ₁₈ O ₂	5.77	[M+H] ⁺	195.138	195.1395	7.69
Aniline	C ₆ H ₅ NH ₂	0.44	[M+H] ⁺	94.0651	94.0655	4.25
Benzyl butyl phthalate	C ₁₉ H ₂₀ O ₄	6.88	C ₇ H ₇ ⁺	91.0542	91.0547	5.49
Bisphenol A	C ₁₅ H ₁₆ O ₂	5.10	[M-H] ⁻	227.1078	227.1079	0.44
³ BA(2,3-DHP)GE	C ₂₁ H ₂₆ O ₅	5.25	[M+NH ₄] ⁺	376.2118	376.2119	0.27
⁴ BA(3Cl,2HP)(2,3DHP)E	C ₂₁ H ₂₇ ClO ₅	5.22	[M+COOH] ⁻	439.1529	439.1529	0.00
⁵ BA(3Cl2HP)GE isomer 1	C ₂₁ H ₂₅ ClO ₄	6.22	[M+NH ₄] ⁺	394.178	394.1774	-1.52
BA(3Cl2HP)GE isomer 2	C ₂₁ H ₂₅ ClO ₄	6.41	[M+NH ₄] ⁺	394.1780	394.1785	1.27
⁶ BAB(2,3DHP)E	C ₂₁ H ₂₈ O ₆	4.44	C ₁₂ H ₁₇ O ₃ ⁺	209.1172	209.1171	-0.48
Bisphenol A diglycidyl ether	C ₂₁ H ₂₄ O ₄	6.31	[M+NH ₄] ⁺	358.2013	358.2011	-0.56
Butyl p-hydroxybenzoate	C ₁₁ H ₁₄ O ₃	5.45	[M-H] ⁻	193.087	193.0868	-1.04
Di (2-ethylhexyl)adipate	C ₂₂ H ₄₂ O ₄	8.77	[M+Na] ⁺	393.2975	393.298	1.27
Dibutyl sebacate	C ₁₈ H ₃₄ O ₄	7.95	[M+H] ⁺	315.253	315.2536	1.90
Dicyclohexyl phthalate	C ₂₀ H ₂₆ O ₄	7.64	C ₈ H ₅ O ₃ ⁺	149.0233	149.0230	0.67
Diethyl phthalate	C ₁₂ H ₁₄ O ₄	5.50	C ₈ H ₅ O ₃ ⁺	149.0233	149.0240	4.70
Diisodecyl phthalate	C ₂₈ H ₄₆ O ₄	9.65	[M+H] ⁺	447.3469	447.3479	2.24
Diisononyl phthalate	C ₂₆ H ₄₂ O ₄	8.96	[M+H] ⁺	419.3156	419.3156	0.00
Dimethyl phthalate	C ₁₀ H ₁₀ O ₄	4.71	C ₉ H ₇ O ₃ ⁺	163.039	163.0391	0.61
Di-N-butyl phthalate	C ₁₆ H ₂₂ O ₄	6.97	C ₈ H ₅ O ₃ ⁺	149.0233	149.2040	4.70
Di N-octyl phthalate iso. 1	C ₂₄ H ₃₈ O ₄	8.88	[M+H] ⁺	391.2843	391.2843	0.00
Di N-octyl phthalate iso. 2	C ₂₄ H ₃₈ O ₄	8.94	[M+H] ⁺	391.2843	391.2847	1.02
Dipropyl phthalate	C ₁₄ H ₁₈ O ₄	6.29	C ₈ H ₅ O ₃ ⁺	149.0233	149.0236	2.01
Ethyl 4-hydroxybenzoate	C ₉ H ₁₀ O ₃	4.58	[M-H] ⁻	165.0557	165.0556	-0.61
Melamine	C ₃ H ₆ N ₆	0.26	[M+H] ⁺	127.0727	127.0733	4.72
Methyl paraben	C ₈ H ₈ O ₃	4.08	[M-H] ⁻	151.0401	151.0413	7.94
⁷ N,N-DEHA	C ₄ H ₁₁ NO	0.41	[M+H] ⁺	90.0913	90.0912	-1.11

² 2-EHDP: 2-Ethylhexyl diphenyl phosphate³ 2-EHDP: 2-Ethylhexyl diphenyl phosphate⁴ BA(3Cl2HP)GE: Bisphenol A (3-Chloro,2-hydroxypropyl)glycidyl ether⁵ BA(3Cl2HP)GE: Bisphenol A (3-Chloro,2-hydroxypropyl)glycidyl ether⁶ BAB (2,3DHP)E: Bisphenol A (2,3-dihydroxypropyl) ether

Nordihydroguaiaretic acid	C ₁₈ H ₂₂ O ₄	5.17	[M-H] ⁻	301.1445	301.1462	5.65
o-Anisidine	C ₇ H ₉ ON	0.65	C ₆ H ₇ NO ⁺	109.0522	109.0525	2.75
o-Toluidine	C ₇ H ₉ N	0.79	[M+H] ⁺	108.0808	108.0811	2.78
Propyl 4-hydroxybenzoate	C ₁₀ H ₁₂ O ₃	5.06	[M-H] ⁻	179.0714	179.071	-2.23
Tributyl o-acetylcitrate	C ₂₀ H ₃₄ O ₈	7.38	[M+H] ⁺	403.2326	403.2333	1.79
Tributyl phosphate	C ₁₂ H ₂₇ PO ₄	6.43	H ₄ PO ₄ ⁺	98.9842	98.9847	5.05
Triethyl phosphate	C ₆ H ₁₅ O ₄ P	4.03	H ₄ PO ₄ ⁺	98.9842	98.9847	5.05
Mycotoxins						
3-Acetyldeoxynivalenol	C ₁₇ H ₂₂ O ₇	3.84	[M+H] ⁺	339.1438	339.1447	2.65
Aflatoxin B1	C ₁₇ H ₁₂ O ₆	4.66	[M+H] ⁺	313.0707	313.0704	-0.96
Aflatoxin B2	C ₁₇ H ₁₄ O ₆	4.49	[M+H] ⁺	315.0863	315.0861	-0.63
Aflatoxin G1	C ₁₇ H ₁₂ O ₇	4.51	[M+H] ⁺	329.0656	329.0656	0.00
Aflatoxin G2	C ₁₇ H ₁₄ O ₇	4.32	[M+H] ⁺	331.0812	331.0813	0.30
Aflatoxin M1	C ₁₇ H ₁₂ O ₇	4.18	[M+H] ⁺	329.0656	329.0657	0.30
Alfa zearalenol	C ₁₈ H ₂₄ O ₅	5.22	C ₁₈ H ₂₃ O ₄ ⁺	303.1591	303.1593	0.66
Citrinin	C ₁₃ H ₁₄ O ₅	5.03	[M+H] ⁺	251.0914	251.0915	0.40
Cyclopiazonic acid	C ₂₀ H ₂₀ N ₂ O ₃	6.11	[M+H] ⁺	337.1547	337.1549	0.59
Deoxynivalenol	C ₁₅ H ₂₀ O ₆	2.37	[M+H] ⁺	297.1333	297.1340	2.36
Diacetoxyscirpenol	C ₁₉ H ₂₆ O ₇	4.56	[M+Na] ⁺	389.1571	389.1571	0.00
Ergocornine isomer 1	C ₃₁ H ₃₉ N ₅ O ₅	4.30	[M+H] ⁺	562.3024	562.3016	-1.42
Ergocornine isomer 2	C ₃₁ H ₃₉ N ₅ O ₅	4.40	[M+H] ⁺	562.3024	562.3017	-1.24
Fumonisin B ₁	C ₃₄ H ₅₉ NO ₁₅	4.41	[M+H] ⁺	722.3957	722.3934	-3.18
Fumonisin B ₂	C ₃₄ H ₅₉ NO ₁₄	4.78	[M+H] ⁺	706.4008	706.3995	-1.84
Gliotoxin	C ₁₃ H ₁₄ N ₂ O ₄ S ₂	4.45	C ₁₃ H ₁₅ N ₂ O ₄ ⁺	263.1026	263.1030	1.52
HT-2 toxin	C ₂₂ H ₃₂ O ₈	4.77	[M+H] ⁺	425.2170	425.2169	-0.24
Ochratoxin A	C ₂₀ H ₁₈ ClNO ₆	5.63	[M+H] ⁺	404.0895	404.089	-1.24
Patulin	C ₇ H ₆ O ₄	1.09	[M+H] ⁺	155.0339	155.0341	1.29
Sterigmatocystin	C ₁₈ H ₁₂ O ₆	5.81	[M+H] ⁺	325.0707	325.0704	-0.92
T2-Toxin	C ₂₄ H ₃₄ O ₉	5.40	[M+Na] ⁺	489.2095	489.2096	0.20
Zearalenone	C ₁₈ H ₂₂ O ₅	5.66	[M+H] ⁺	319.154	319.1539	-0.31
Perfluorinated compounds						
C ₃ pentafluoropropionic acid	C ₃ F ₅ HO ₂	0.81	C ₂ F ₅ ⁻	118.9926	118.9927	0.84
C ₄ Perfluorobutyric acid	C ₄ F ₇ HO ₂	2.96	C ₃ F ₇ ⁻	168.9894	168.9898	2.37
C ₅ Perfluoropentanoic acid	C ₅ HO ₂ F ₉	4.09	C ₄ F ₉ ⁻	218.9862	218.9867	2.28
C ₇ Perfluoroheptanoic acid	C ₇ HO ₂ F ₁₃	5.05	C ₆ F ₁₃ ⁻	318.9798	318.9814	5.02
C ₈ Perfluorooctanoic acid	C ₈ F ₁₅ O ₂ H	5.47	C ₇ F ₁₅ ⁻	368.9766	368.9781	4.07
C ₉ Perfluorononanoic acid	C ₉ F ₁₇ O ₂ H	5.89	C ₈ F ₁₇ ⁻	418.9734	418.9755	5.01
C ₁₀ Perfluorodecanoic acid	C ₁₀ F ₁₉ O ₂ H	6.33	C ₉ F ₁₉ ⁻	468.9702	468.9714	2.56
C ₁₁ Perfluoroundecanoic acid	C ₁₁ F ₂₁ O ₂ H	6.81	C ₁₀ F ₂₁ ⁻	518.967	518.9682	2.31
C ₁₂ Perfluorododecanoic acid	C ₁₂ F ₂₃ O ₂ H	7.35	C ₁₁ F ₂₃ ⁻	568.9638	568.9629	-1.58
Heptadecafluorooctane sulfonic acid	C ₈ HSO ₃ F ₁₇	6.66	[M-H] ⁻	498.9302	498.9327	5.01
Nitrosamines						
N-nitrosodiethylamine	C ₄ H ₁₀ N ₂ O	2.24	[M+H] ⁺	103.0866	103.0862	3.88
N-nitrosodimethylamine	C ₂ N ₂ H ₆ O	0.51	[M+H] ⁺	75.0553	75.0556	4.00
N-nitrosodi-n-dibutylamine	C ₈ H ₁₈ N ₂ O	5.75	[M+H] ⁺	159.1492	159.1494	1.26
N-nitrosodi-n-dipropylamine	C ₆ H ₁₄ N ₂ O	4.62	[M+H] ⁺	131.1174	131.1177	-1.53
N-nitrosomethylethylamine	C ₃ H ₈ N ₂ O	0.89	[M+H] ⁺	89.0709	89.0715	6.74
N-nitrosomorpholine	C ₄ H ₈ N ₂ O ₂	0.75	[M+H] ⁺	117.0659	117.066	0.85
N-nitroso-n-diphenylamine	C ₁₂ H ₁₀ N ₂ O	5.94	C ₉ H ₁₁ N ⁺	169.0886	169.0885	-0.94
N-nitrosopiperidine	C ₅ H ₁₀ N ₂ O	2.96	[M+H] ⁺	115.0866	115.0866	0.00

⁷ N,N-diethylhydroxylamine

N-nitrosopyrrolidine	C ₄ H ₈ N ₂ O	0.96	[M+H] ⁺	101.0709	101.071	0.99
Sweeteners						
Aspartame	C ₁₄ H ₁₈ N ₂ O ₅	3.38	[M-H] ⁻	293.1143	293.1152	3.07
Acesulfame	C ₄ H ₅ NO ₄ S	0.63	[M-H] ⁻	161.9867	161.9871	2.47
Saccharin	C ₇ H ₅ NO ₃ S	1.25	[M-H] ⁻	181.9917	181.9921	2.20
Sucralose	C ₁₂ H ₁₉ Cl ₃ O ₈	3.40	[M-H] ⁻	395.0073	395.0091	4.56
Cyclamate	C ₆ H ₁₂ NO ₃ S	1.45	[M-H] ⁻	178.0538	178.0538	0.00

Study of search parameters for automated screening. A snapshot of the software application used (Find by Formula tool, Agilent MassHunter Qualitative Analysis (version B.04.00)) is shown in **Figure 3** along with the main information included in the database. This software was used to build the database, identifying compounds with retention time and mass accurate measurements for the main ion of each one.

Automatic search of compounds in food samples could be done using this software. The main search parameters (accurate mass tolerance and retention time (RT) window) affecting the performance of the automated search using *Find by Formula* tool, were carefully examined. Different experiments were assayed varying RT windows (± 0.05 , ± 0.1 , ± 0.25 , ± 0.5 min) with two fixed accurate mass tolerances (± 5 or ± 10 ppm). Default settings of peak filtering were used to remove background and mobile phase ions and contribution. In these experiments, the database (630 compounds) was applied to 16 synthetic mixtures of pesticides ($100 \mu\text{g L}^{-1}$) with 30 compounds each. The number of false positives and negatives, average score (%) and success rate (%) were evaluated for each mixture. The term false positive meant that a compound was reported, but it was not present in the actual sample. On the other hand, a compound, which was present in the synthetic mixture but not reported by the software after the automated search was a false negative. In most cases, false negatives were due to either detector saturation (high concentrations of compounds or high sensitive compounds) with a low score (lower than 60%), relatively high to accurate mass errors

and not statistically representative mass spectrum, or because of being compounds with very low sensitivity (those which do not really perform properly mainly because of poor electrospray ionization).

a)

Elemental Composition	RT	Mass (M)	Compound	Comments
C25H24F6N4	6.02	494.1905	Hydramethylnon	pesticide
C14H14Cl2N2O	4.52	296.0483	Imazalil	pesticide
C9H10Cl2N2O	3.69	256.017	Imazalil Metabolite	pesticide
C16H20N2O3	4.11	288.1474	Imazamethabenz-Methyl	pesticide
C15H19N3O4	3.82	305.1376	Imazamox	pesticide
C13H15N3O3	3.41	261.1113	Imazapyr	pesticide
C17H17N3O3	4.56	311.127	Imazaquin	pesticide
C9H10CN5O2	3.81	255.0523	Imidacloprid	pesticide
C22H17ClF3N3O7	6.79	527.0707	Indoxacarb	pesticide
C7H3I2NO	5.41	370.8304	Ioxinil	pesticide
C13H13N3Cl2O3	6.6	329.0334	Iprodione	pesticide
C9H10	5.68	118.0783	Iprovalicarb F1	pesticide
C9H17N3O3PS	6.27	313.0417	Isazophos	pesticide
C15H24NO4PS	5.54	229.9803	Isocarbofos F1	pesticide
C15H23NO4	6.84	344.1085	Isufenphos fl	pesticide
C6H6O	5.18	94.0419	Isoprocarb F1	pesticide
C6H4O3S2	6.09	187.9602	Isoprothiolane F1	pesticide
C12H18N2O	5.04	206.1419	Isoproturon	pesticide

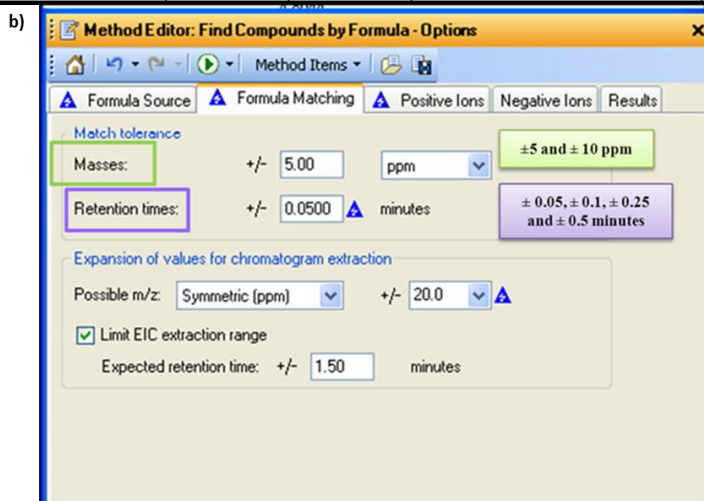


Figure 3. a) Csv file with relevant information (elemental composition, retention time, exact mass, compound name for the main ion of each compound) for the automatic search of compounds with Agilent MassHunter Qualitative Analysis software; b) Selection of mass error tolerance and retention time window for the automatic search using the specific software.

No significant differences were found in terms of the number of false negatives, average score and success rate for each mixture using the experiments at different retention time and mass bias. In contrast, significant differences were found in the number of false negatives, when different retention time windows were employed with 5 and 10 ppm as mass error tolerance.

The results in terms of false positive rates obtained for each of the synthetic mixtures tested (using 5 and 10 ppm as mass error tolerance) are shown in **Figure 4**. The results are expressed in percentage of false positive (%) related to the number of compounds expected (30 in each experiment). Thus, a value of 20 % of false errors means that 6 compounds (out of 630) not originally included in the synthetic samples were reported as positive with the automated search.

The percentages of false positives reported by the software using different retention time windows were compared. The data collected concluded that wider retention time windows yielded a higher value of false positives. The highest number of compounds was reported when 0.5 minutes was used, and the lowest, with 0.05 minutes. Those results did not depend heavily on the mass error tolerance employed. In this sense, it should be kept in mind that complex food extracts may shift the retention times so that these results may be affected, particularly in the case of early eluting compounds (more affected by matrix, pH and/or composition). For this reason, the narrowest retention time tolerance (0.05 minutes) was discarded. On the other hand, the results obtained using 0.1 and 0.25 minutes tolerances were relatively similar with minor differences in the number of false positives. Both tolerances could be adopted although in order to prevent false negatives due to retention time shifts for polar compounds, 0.25 minutes and 10 ppm were selected as the most appropriate retention time window

and mass error tolerance for screening step. Eventually, a second additional step would involve confirmation of the findings be accurate mass measurements of ions and fragments for each tentative compound detected.

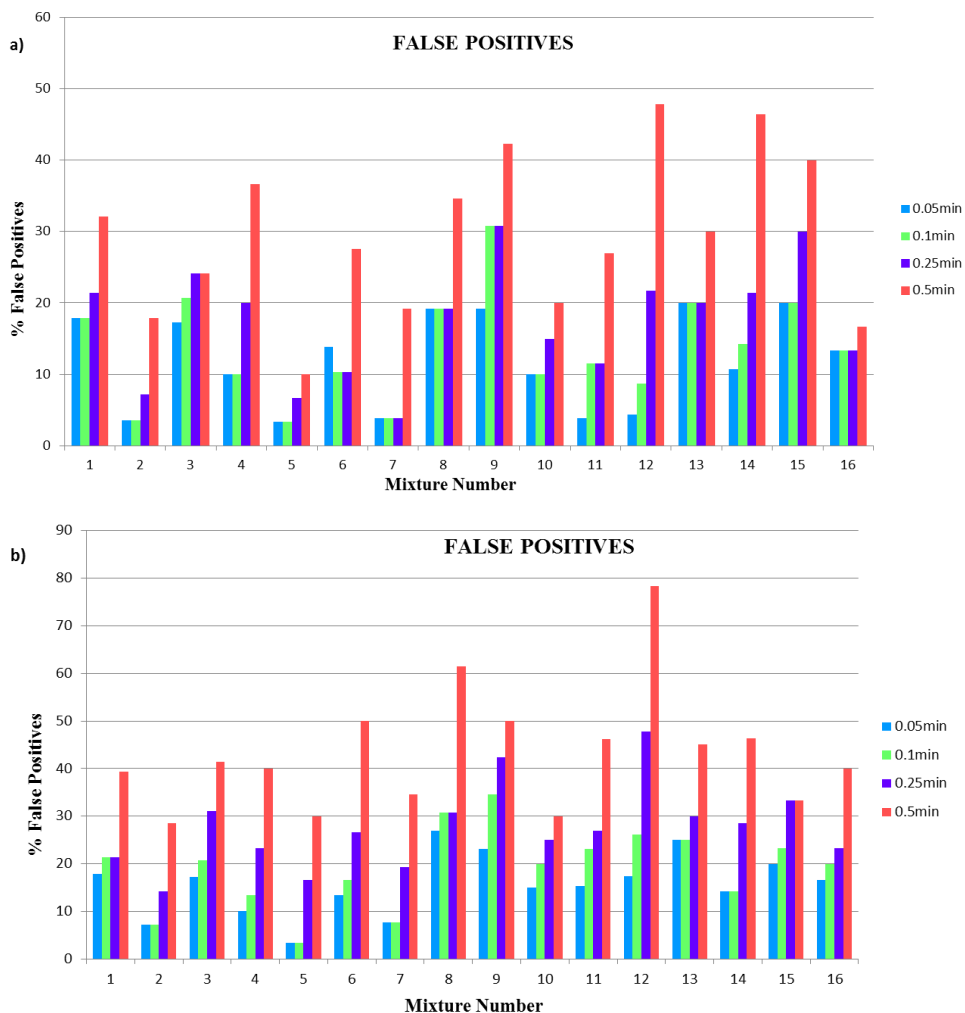


Figure 4 a) Number of false positives reported by the software when retention time windows varied from 0.05 to 0.5 minutes, using 5 ppm as mass error tolerance; (b) Number of false positives reported by the software when retention time windows varied from 0.05 to 0.5 minutes, using 10 ppm as mass error tolerance. Percentage of false positives calculated with respect to the 30 compounds included in each experiment.

Analytical performance. Three representative food matrices (tomato, orange and baby food) were employed to evaluate the performance of the proposed screening method in terms of linearity, matrix effect and limits of quantification (LOQs). In order to avoid coelutions between analytes that could shift the actual performance in terms of matrix effects, mixtures of selected compounds, containing approximately 30 compounds each one, were used to prepare the calibration curves in the concentration range from 1 to 1000 $\mu\text{g Kg}^{-1}$ (1, 10, 50, 100, 200, 500 and 1000) in solvent standards (20% methanol), tomato, orange and baby food extracts. Limits of quantification (LOQs) were estimated as the minimum concentration of analyte corresponding to a signal-to-noise ratio (S/N) = 10:1. This was experimentally calculated from the injection of matrix-matched standard solutions at low concentration levels, using the more abundant ion for each extracted ion chromatograms with narrow mass windows (± 20 ppm relative mass error).

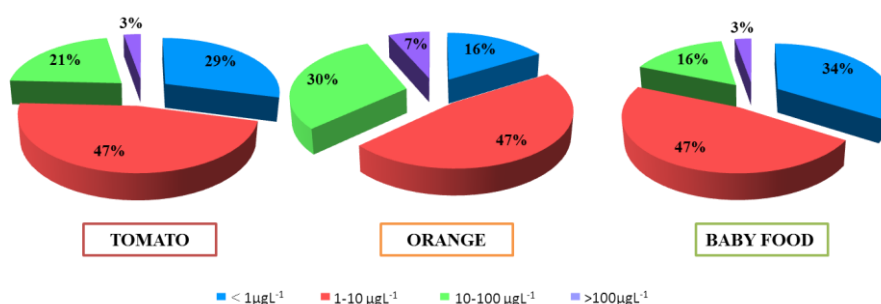


Figure 5. Percentage of database compounds classified according to their LOQs in tomato, orange and baby food.

Results are detailed in **Table 2**, along with the maximum residue level (MRLs) established for the pesticide/commodity combination tested, and they are also summarized in **Figure 5**, and the overall data of LOQs for each individual group of compounds is included as Supplementary material (**Figures S1-S2**). As shown in the different cake diagrams, most of pesticides and veterinary drugs showed limits of quantification from 1 to 10 $\mu\text{g Kg}^{-1}$ in tomato, orange

and baby food. The percentage of those compounds with $LOQs < 1 \mu g Kg^{-1}$ was higher in baby food and tomato than in orange. On the other hand, 65% of food packaging contaminants displayed $LOQs < 10 \mu g Kg^{-1}$ in baby food. In tomato and orange, most of those compounds had $LOQs$ from 10 to $100 \mu g Kg^{-1}$. For the rest of compound classes tested (food packaging contaminants, mycotoxins and perfluorinated compounds), the highest percentage of compounds with $LOQs > 10 \mu g Kg^{-1}$ was obtained in orange extracts. This can be attributed to the complexity of the orange matrix (and the extent of matrix effects therein) compared to both tomato and baby food matrices, as clearly illustrated in **Figure 6**.

An example of compounds detected in incurred food samples are shown in **Figure 7**, where the extracted ion chromatograms and mass spectra of tebuconazole and imazalil detected in peach jam and oranges, respectively, are shown. The $LOQs$ obtained were contrasted with the MRLs for the pesticide/commodity combinations available. Considering the default MRLs for pesticides in babyfood set at $10 \mu g Kg^{-1}$, over 85 % of the compounds fulfilled this threshold, being 58 above the value set. In most cases, the compounds are low sensitive due to poor ionization with electrospray. As has been reported by other authors, there is always a percentage in the range of 10 %, which does not yield good response factors due to its features not compatible to electrospray [29,32], even when using more sensitive instrumentation such as a newer UHPLC-QTOFMS which was also used (data not shown). In the case of tomato, despite 75 compounds (18 % out of 411 pesticides included) did not achieved the $10 \mu g Kg^{-1}$ sensitivity, only 35 were above the MRL value set (8.5 %). Finally, in the case of orange, around 30 % was above the $10 \mu g Kg^{-1}$ threshold, with 89 compounds (21 %) not fulfilling the MRL requirements. These results evidence one of the limitations of this type of screening approaches. The sensitivity is yet an issue, and this is

more evident as the matrix complexity increases. With the use of state-of-the-art instrumentation, using heated electrospray source providing a remarkable sensitivity increase, there will always be a percentage of “difficult to ionize” compounds, that would not be amenable to include in the screening method.

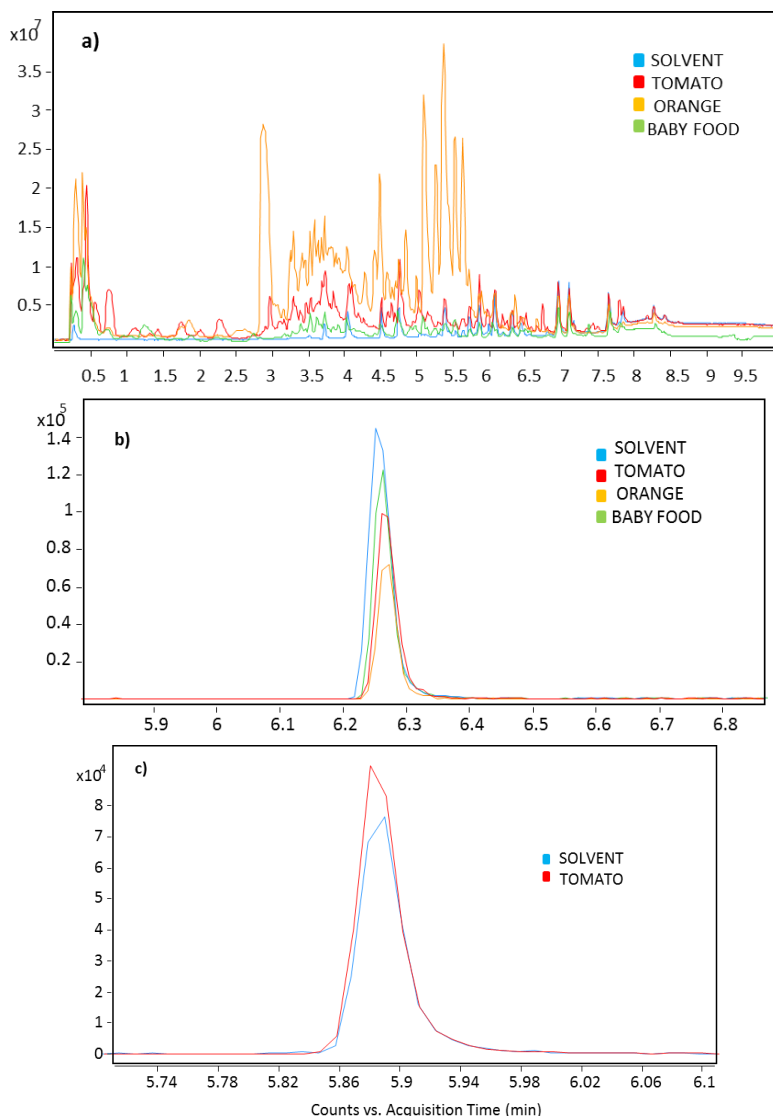


Figure 6 a) Overlapped total ion chromatograms (TICs) of a pesticide mixture (100 µg L⁻¹) in solvent, tomato, orange and baby food; b) Overlapped extracted ion chromatograms (EICs) of metribuzin (100 µg Kg⁻¹) in solvent, tomato, orange and baby food; c) Overlapped extracted ion chromatograms (EICs) of fluquinconazole (200 µg Kg⁻¹) in solvent and tomato.

Table 2. Limits of quantification (LOQs) in tomato, orange and baby food for the most abundant ion of each compound and their MRLs in tomato and orange.

Compound	LOQ tomato ($\mu\text{g Kg}^{-1}$)	MRL tomato (mg Kg^{-1})	LOQ orange ($\mu\text{g Kg}^{-1}$)	MRL orange (mg Kg^{-1})	LOQ baby food ($\mu\text{g Kg}^{-1}$)
Pesticides					
1-Naphtalene-Acetamide	2.80	0.05	17.36	0.05	2.51
2,4-Dichlorophenoxyacetic acid	13.55	0.05	9.09	1	15.63
2,4-Dinitrophenol	1.05	-	4.13	-	1.18
3,3-Dichlorobenzidine	0.97	-	5.36	-	0.30
3,5-Dichloroaniline	1.52	-	4.05	-	1.77
4-Chloro-2-methylphenol	71.43	-	166.67	-	153.85
4-Chloro-O-toloxoacetic acid	1.45	-	1.83	-	1.22
Acephate F ₁	11.9	0.01	7.93	0.01	7.14
Acetamiprid	2.38	0.2	7.47	0.9	1.93
⁸ Acibenzolar S-Methyl	11.9	1	42.55	0.02	4.27
Aclonifen	7.09	0.05	10.87	0.05	4.82
Alachlor	7.37	0.01	6.21	0.01	6.14
Albendazole	4.04	-	2.00	-	2.39
⁹ Aldicarb	7.94	0.02	83.33	0.02	7.2
Aldicarb Sulfone	5.03	-	6.94	-	5.38
Aldicarb Sulfoxide	25.6	-	15.7	-	12.98
Allethrin	20.33	-	25.25	-	11.26
Ametryne	1.33	-	1.30	-	0.98
Aminocarb	4.02	-	1.99	-	4.32
¹⁰ Amitraz	-	0.05	-	0.05	-
Amitrol	86.21	0.01	96.53	0.01	107.76
AMPA	102.56	-	194.17	-	307.69
Anilazine	8.62	0.01	14.08	0.01	12.66
Anilofos	0.33	-	0.35	-	0.34
Antimycin A	19.31	-	166.67	-	12.99
Asulam	48.54	0.5	81.97	0.5	34.28
Atrazine	0.27	0.05	0.48	0.05	0.13
Atrazine Desethyl	1.85	-	4.88	-	1.63
Atrazine Desisopropyl	1.83	-	3.05	-	1.68
Azaconazole	0.37	-	2.50	-	0.27
Azamethiphos	0.85	-	4.74	-	0.2
Azinphos-Ethyl	12.35	0.02	14.53	0.02	8.82
Azinphos Methyl	9.17	0.05	41.67	0.05	9.96
Azobenzene	42.52	-	130.20	-	48.54
¹¹ Azocyclotin	4.72	0.01	3.73	0.2	3.23
Azoxystrobin	0.30	3	140.85	15	0.18
Barban F ₁	23.42	0.05	46.5	0.05	25.51
¹² Benalaxyl	8.77	0.5	0.56	0.05	8.23
Bendiocarb	6.13	-	17.85	-	5.46

⁸ Sum of acibenzolar s-methyl and acibenzolar acid

⁹ Sum of aldicarb, its sulfoxide and its sulfone

¹⁰ Including metabolites containing the 2,4-dimethylaniline

¹¹ Sum of azocyclotin and cyhexatin

¹² Including other mixtures of isomers

Benfluralin	14.03	0.05	23.8	0.05	13.28
Benfuracarb	-	0.02	-	0.02	-
Bensulfuron Methyl	0.93	-	33.33	-	0.57
Bensulide	2.10	-	4.24	-	2
¹³ Bentazone	0.37	0.1	0.87	0.1	0.57
Benzidine	15.53	-	24.75	-	9.41
¹⁴ Bifenazate	2.42	0.5	4.69	0.9	3.56
Bifenox F ₁	7.97	0.05	10.33	0.1	10.83
Bitertanol	2.50	0.01	1.85	0.01	12.21
Boscalid	0.75	3	2.04	2	0.62
Brodifacoum isomer 1	1.93	-	4.12	-	3.7
Brodifacoum isomer 2	3.60	-	5.56	-	5.43
Bromacil F ₁	1.47	-	11.49	-	0.99
Bromadiolone isomer 1	0.75	-	0.87	-	0.81
Bromadiolone isomer 2	2.92	-	4.67	-	4.03
Bromophos Methyl	34.72	-	33.71	-	16.16
¹⁵ Bromoxynil	3.18	0.05	2.32	0.05	1.79
¹⁶ Bromuconazole Isomer 1	0.57	0.05	0.05	0.05	0.50
Bromuconazole Isomer 2	5.38	-	1.58	-	5.17
Bupirimate	6.49	2	0.56	0.05	4.96
Buprofezin	0.57	1	0.66	1	0.70
Butachlor	13.51	-	14.93	-	10.12
Butocarboxim	11.23	-	32.52	-	5.11
Butoxycarboxim	20.83	-	24.15	-	41.32
Butralin	2.63	0.01	4.63	0.01	2.79
Buturon	4.20	-	12.05	-	4.69
Cadusafos	1.67	0.01	4.63	0.01	1.35
Carbaryl	2.17	0.01	11.23	0.01	3.01
¹⁷ Carbendazim	3.37	0.3	2.9	0.2	3.33
¹⁸ Carbofuran	4.80	0.01	12.35	0.5	3.89
Carbofuran 3-Hydroxy	7.35	-	21.83	-	3.32
Carbosulfan	-	0.01	-	0.1	-
Carboxine	1.67	0.1	1.67	0.05	1.24
Carfentazone Ethyl	3.38	0.01	12.79	0.01	3.72
Chlorbromuron	6.07	-	3.64	-	4.25
Chlordimeform	1.72	-	3.62	-	3.30
Chlorfenvinfos	0.70	0.01	0.89	0.01	0.68
Chlorfluazuron	7.19	-	5.98	-	4.78
Chloridazon	1.05	0.5	1.10	0.1	0.38
Chlormequat chloride	11.10	0.05	14.53	0.05	12.13
Chloropropham	4.44	0.01	26.46	0.01	1.13
Chlorotoluron	1.03	0.01	4.35	0.01	0.59
Chloroxuron	0.37	0.05	3.28	0.05	0.39
Chlorpyrifos	6.47	0.5	4.65	0.3	2.76
Chlorpyrifos Methyl	10.10	0.5	13.16	0.5	5.51
Chlorsulfuron	6.21	0.05	15.97	0.05	1.56
Cinosulfuron	0.56	-	0.44	-	0.55
¹⁹ Clethodim isomer E	1.73	1	3.40	0.1	3.13
Clethodim isomer Z	7.23	-	-	-	2.13

¹³ Sum of bentazone and the conjugates of 6-OH and 8-OH bentazone¹⁴ Sum of bifenazate and bifenazate-diazene¹⁵ Including its esters¹⁶ Sum of diastereoisomers¹⁷ Sum of benomyl and carbendazim¹⁸ Including any carbofuran generated by carbosulfan, benfuracarb o furathiocarb.¹⁹ Sum of sethoxydim and clethodim, including degradation products.

Clodinafop-Propargyl	0.59	-	1.15	-	1.12
Clofentezine F ₁	13.40	0.3	9.47	0.5	9.27
Clomazone	1.28	0.01	32.89	0.01	0.99
Clopyralid	80.65	0.5	123.45	0.5	62.11
⁴⁹ Clothianidin	18.18	0.05	16.89	0.1	13.09
Coumaphos	1.39	-	1.14	-	1.20
Cyanazine	0.82	-	5.49	-	0.70
Cyazofamid	7.82	0.6	5.13	0.01	5.24
Cycloate	2.11	-	2.56	-	1.57
Cycloheximid	14.37	-	27.62	-	13.40
²⁰ Cycloxydim isomer 1	4.55	1.5	1.72	0.05	2.89
Cycloxydim isomer 2	14.08	-	7.75	-	15.50
Cymoxanil	202.03	0.2	322.57	0.05	-
Cyphenothrin	69.93	-	78.74	-	83.00
Cyproconazole	0.33	0.05	5.29	0.05	0.24
Cyprodinil	0.32	1	0.49	0.05	0.23
Cyromazine	2.65	0.6	2.82	0.05	2.63
²¹ Daminozide	9.43	0.02	22.07	0.02	14.93
Dazomet	-	0.02	-	0.02	-
Deet	0.45	-	1.69	-	0.32
Demeton-S-Methyl	14.29	-	26.32	-	10.16
Desethyl Terbutylazine	3.70	-	5.49	-	2.92
Desmedipham	2.33	0.05	16.67	0.05	1.79
Desmetryn	0.83	-	1.52	-	1.29
Diafenthiuron	3.41	-	4.44	-	1.36
Diazinon	0.19	0.01	0.48	0.01	0.15
Dibrom	6.75	-	27.86	-	10.15
Dicamba	95.69	0.05	130.76	0.05	93.46
Dichlofenthion	20.04	-	11.45	-	15.55
Dichlofluanid	-	-	-	-	-
²² Dichlorprop	0.81	0.05	0.25	0.05	0.99
Dichlorvos	0.92	0.01	3.94	0.01	0.80
Dicloran	64.10	0.3	100	0.1	8.33
Dicrotophos	0.92	-	1.41	-	0.70
Diethanolamine	-	-	-	-	-
Diethofencarb	11.33	1	84.75	0.05	8.76
Difenacoum isomer 1	0.81	-	1.30	-	0.87
Difenacoum isomer 2	0.76	-	1.23	-	0.69
Difenoconazole	0.21	2	0.27	0.1	0.23
Difenoaxuron	0.49	-	2.68	-	0.40
Difenzoquat	0.83	-	0.76	-	0.21
Diflubenzuron	4.13	-	3.57	-	2.29
Diflufenican	0.70	0.05	6.33	0.05	0.34
Dimethametryn	0.74	-	0.26	-	0.55
Dimethenamid	0.92	-	4.35	-	0.82
²³ Dimethoate	16.33	0.02	14.33	0.02	15.93
²⁴ Dimethomorph Isomer 1	2.28	1	-	0.8	2.84
Dimethomorph Isomer 2	1.97	-	1.08	-	2.15
Diniconazole	0.17	0.01	0.18	0.01	1.48
Diphenylamine	1.81	0.05	3.80	0.05	2.06

²⁰ Including degradation and reaction products which can be determined as 3-(3-thianyl) glutaric acid S-dioxide and/or 3-hydroxy-3-(3-thianyl) glutaric acid S-dioxide or methyl esters.

²¹ Sum of daminozide and 1,1-dimethyl-hydrazine

²² Sum of dichlorprop and its conjugates

²³ Sum of dimethoate and omethoate

²⁴ Sum of isomers

Diquat dibromide	-	0.05	-	0.05	
Diuron	0.81	0.01	2.54	0.01	0.56
Dmst	54.95	-	59.52	-	30.64
DNOC	0.99	0.05	0.50	0.05	0.88
Edifenphos	0.39	-	0.48	-	0.27
²⁵ Emamectin isomer 1	5.18	0.02	9.80	0.01	2.44
Emamectin isomer 2	3.25	-	4.76	-	1.30
²⁶ Endosulfan sulfate	2.10	0.05	2.13	0.05	3.40
Epn	3.04	-	2.65	-	4.01
Epoxiconazole	0.27	0.05	0.93	0.05	0.19
Eptc	5.75	0.01	11.76	0.01	4.38
Etaconazol	0.50	-	1.95	-	0.41
Ethephon	-	1	-	0.05	-
Ethidimuron	3.57	-	10.94	-	3.94
Ethiofencarb	6.17	-	8	-	1.6
Ethiofencarb Sulfone	25.63	-	38.46	-	9.43
Ethiofencarb Sulfoxide	14.90	-	17.50	-	4.65
Ethion	9.97	0.01	6.46	0.01	6.97
Ethiprole	0.60	-	5.46	-	0.54
²⁷ Ethofumesate	7.70	0.05	17.57	0.05	5.29
Ethoprophos	0.51	0.02	0.74	0.02	0.35
Ethoxyquin	0.77	0.05	2.82	0.05	0.62
Ethylenethiourea	17.4	-	113.64	-	51.55
Etofenprox	7.65	1	8.81	1	7.25
Etoazole	0.64	0.1	1.43	0.1	0.42
Etrimphos	0.20	-	0.20	-	0.19
Famoxadone	13.37	1	11.82	0.2	11.11
Famphur	1.05	-	6.67	-	0.68
Fenamidone	0.24	0.5	0.37	0.02	0.17
²⁸ Fenamiphos	0.95	0.04	0.96	0.02	0.90
Fenamiphos Sulfone	0.80	-	7.41	-	0.37
Fenamiphos Sulfoxide	0.47	-	2.50	-	0.38
Fenarimol	0.30	0.02	1.85	0.02	0.30
Fenazaquin	0.26	0.5	0.39	0.5	0.23
Fenbendazole	0.27	-	0.33	-	0.21
Fenhexamid	0.13	1	1.26	0.05	0.12
Fenhexamid 4-O-Glucoside	0.64	-	60.24	-	0.58
Fenitrothion	5.03	0.01	4.47	0.01	4.22
Fenobucarb	5.38	-	53.19	-	4.61
Fenoxaprop P-Ethyl	0.31	0.1	0.47	0.1	0.34
Fenoxycarb	4.35	0.05	3.82	2	2.71
Fenpiclonil	2.04	-	11.90	-	1.52
Fenpropathrin	417	0.01	228	2	201
²⁹ Fenpropidine	0.08	0.01	0.37	0.01	0.06
Fenpropimorph	0.30	0.05	0.11	0.05	0.20
Fenpyroximate	0.24	0.2	0.22	0.5	0.23
Fensulfothion	0.43	-	0.93	-	0.32
³⁰ Fenthion	14.08	0.01	7.14	0.01	8.24
³¹ Fentin Chloride	1.79	0.05	1.93	0.05	1.34

²⁵ Emamectin B1a²⁶ Sum of alpha- and beta-isomers and endosulfan-sulphate²⁷ Sum of ethofumesate and its metabolite²⁸ Sum of fenamiphos and its sulfoxide and sulfone²⁹ Sum of fenpropidin and its salts³⁰ Fenthion and its oxigen analogue, their sulfoxides and sulfone³¹ Including its salts, expressed as triphenyltin cation

Fenuron	6.77	-	13.70	-	1.92
Fipronil	3.94	0.005	14.25	0.005	2.95
Fluazifop	5.75	-	6.36	-	0.64
Fluazifop-Butyl	0.15	0.3	0.31	0.1	0.10
Fluazinam	2.19	0.05	4.59	0.05	2.48
Fluchloralin	7.89	-	7.47	-	5.99
Flucythrinate	80.97	0.05	91.73	0.05	26.33
Fludioxonil	0.58	0.9	0.52	10	0.56
Flufenacet	1.39	0.05	7.46	0.05	1.08
Flufenoxuron	1.92	0.5	5.35	0.3	1.18
Fluomethuron	0.70	0.01	1.27	0.01	0.72
Fluquinconazole	2.20	0.05	5.43	0.05	2.67
³² Fluroxypyr	17.42	0.05	59.53	0.05	15.38
Flusilazole	0.29	0.02	0.15	0.1	0.29
Flutolanil	0.66	0.05	0.70	0.05	0.59
Flutriafol	1.10	0.3	0.58	0.2	0.78
Fomesafen	23.92	0.01	47.63	0.01	13.34
Fonofos	5	-	7.41	-	5.56
Foramsulfuron	1.27	0.01	4.83	0.01	1.1
Forchlorfenuron	0.63	0.01	1.69	0.01	0.54
³³ Formetanate	26.60	0.3	23.27	0.01	16.95
³⁴ Fosetyl	21.65	100	27.62	75	35.97
Fosthiazate	0.27	0.02	0.28	0.02	0.21
Fuberidazol	0.79	0.05	1.17	0.05	0.66
Furalaxyl	0.71	-	3.77	-	0.57
Furathiocarb	0.64	0.01	0.43	0.01	0.44
Furmecycloz	0.87	-	0.63	-	0.56
³⁵ Gibberellic acid	8.18	-	37.04	-	3.40
Glufosinate ammonium	320.51	0.1	510.2	0.1	331.96
Glufosinate N-acetyl	7.09	-	12.34	-	10.99
Glyphosate	-	0.1	-	0.5	-
Griseofulvin	1.20	-	17.87	-	0.92
Haloxypop	0.67	0.05	0.60	0.05	0.52
Hexaflumuron	8.72	-	15.57	-	13.02
Hexazinone	1.07	-	3.83	-	0.86
Hexythiazox	5.99	0.5	5.10	1	3.63
Hydramethylnon	0.79	-	2.43	-	1.20
Imazalil	0.64	0.5	0.64	5	0.58
Imazalil metabolite	0.13	-	0.03	-	0.07
Imazamethabenz-methyl	2.90	-	5.37	-	2.51
Imazamox	0.50	0.05	3.03	0.05	0.36
Imazapyr	2.04	-	11.50	-	1.23
Imazaquin	1.43	0.05	0.53	0.05	1.07
Imidacloprid	9.62	0.5	16.86	1	9.03
Indoxacarb	1.03	0.5	1.38	0.02	1.07
³⁶ Ioxynil	0.47	0.01	0.39	0.01	0.24
Iprodione	35.71	5	24.75	0.02	20.39
Iprovalicarb	0.57	0.7	8.98	0.01	0.45
Isazophos	0.37	-	0.79	-	0.31
Isocarbophos	0.57	-	2.73	-	0.59
Isofenphos	56.18	-	57.47	-	148.11

³² Including its esters³³ Sum of formetanate and its salts³⁴ Sum of fosetyl, phosphonic acid and their salts.³⁵ No MRL required³⁶ Sum of ioxynil, its salts and its esters.

Isoprocarb	11.31	-	34.97	-	8.35
Isoprothiolane	2.58	0.01	4.20	0.01	2.10
Isoproturon	4.69	0.01	1.31	0.01	3.21
Isoxaben	3.67	0.02	13.40	0.02	3.29
³⁷ Isoxaflutole	7.35	0.05	11.57	0.05	0.87
³⁸ Ivermectin	11.11	0.02	28.57	0.01	10.53
Karbutilate	1.53	-	1.43	-	1.15
Kresoxim Methyl	25.50	0.5	36.77	0.05	14.41
Lactofen	4.57	0.01	8.38	0.01	1.89
Lenacil	33.56	0.1	12.69	0.1	17.48
Linuron	1.43	0.05	10.90	0.05	0.80
Lufenuron	19.16	0.5	22.52	1	18.38
³⁹ Malaoxon	8.93	-	3.88	-	5.77
³⁹ Malathion	2.53	0.02	7.46	0.02	3.16
Maleic hydrazine	-	0.2	-	0.2	
Mecarbam	7.04	0.05	4.81	0.05	8.93
Mecoprop F ₁	0.92	0.05	0.87	0.05	1.19
Mefenacet	0.67	-	2.93	-	0.44
Mepanipyrim	0.28	0.8	1.04	0.01	0.25
Mephosfolam	0.48	-	6.80	-	0.41
⁴⁰ Mepiquat chloride isomer 1	2.01	0.05	1.43	0.05	1.90
³³ Mepiquat chloride isomer 2	11.76	-	8.33	-	13.29
Mepronil	0.65	0.01	0.75	0.01	0.60
⁴¹ Mesotrione	1.90	0.05	9.78	0.05	1.64
⁴² Metaflumizone	1.63	0.6	2.07	0.05	1.18
Metalaxyl	1.27	0.2	0.70	0.5	1.31
Metamitron	1.15	0.1	2.53	0.1	0.88
Metazachlor	1.10	0.3	6.80	0.1	1.03
Methabenzthiazuron	0.62	0.01	4.55	0.01	0.38
Methacrifos	10.63	0.05	113.00	0.05	1.33
Methamidophos	43.10	0.01	27.78	0.01	49.21
Methidathion	6.49	0.02	129.87	0.02	4.77
⁴³ Methiocarb	2.74	0.2	46.30	0.1	1.13
³⁶ Methiocarb Sulfoxide	4.93	-	11.19	-	3.45
⁴⁴ Methomyl	2.60	0.02	10.93	0.02	2.96
Methoprotryne	0.60	-	1.57	-	0.44
Methoxyfenozide	7.03	2	7.87	2	6.31
Metobromuron	2.77	-	3.98	-	2.03
⁴⁵ Metolachlor	1.32	0.05	1.20	0.05	1.31
Metolcarb	9.80	-	16.13	-	3.10
Metoxuron	1.27	-	2.46	-	0.98
Metribuzin	0.60	0.1	2.83	0.1	0.57
Metsulfuron Methyl	0.53	0.05	3.30	0.05	0.28
Mevinphos	15.15	0.01	15.02	0.01	12.27
Molinate	9.90	0.05	49.50	0.05	6.18
Monocrotophos	3.89	0.01	4.88	0.01	3.70
Monolinuron	2.64	0.05	6.92	0.05	1.78

³⁷ Sum of isoxaflutole and its metabolite³⁸ Sum of avermectin B1a, B1b and delta-8,9 isomer of avermectin B1a³⁹ Sum of malathion and malaoxon, expressed as malathion⁴⁰ Sum of both isomers⁴¹ Sum of mesotrione and MNBA⁴² Sum of isomers Z and E⁴³ Sum of methiocarb, methiocarb sulfone and sulfoxide⁴⁴ Sum of methomyl and thiodicarb, expressed as methomyl⁴⁵ Metolachlor y S-metolachlor

Monuron	0.97	0.01	4.22	0.01	0.87
Morpholin	-	-	-	-	-
Myclobutanil	2.26	0.3	0.91	3	1.49
Naptalam	12.22	-	58.14	-	3.15
Neburon	0.47	-	0.76	-	0.38
Nereistoxin isomer 1	232.56	-	250	-	196.08
Nereistoxin isomer 2	62.89	-	67.11	-	38.46
Nitenpyram	2.27	-	10.87	-	1.64
N-Methylcarbamate	11.24	-	13.33	-	9.13
N.N-Diethyl-2-Naphthoxypropamide	0.30	-	0.68	-	0.21
Norflurazone	1.44	-	0.68	-	0.80
Novaluron	0.63	1	0.97	0.01	1.98
Nuarimol	1.05	-	0.37	-	0.86
Ofurace	1.22	-	66.67	-	0.88
⁴⁶ Omethoate	3.57	-	5.43	-	3.93
Orbencarb	1.29	-	2.35	-	1.18
Oryzalin	0.25	0.01	0.28	0.01	0.35
Oxadiazon	1.64	0.05	6.88	0.05	1.37
Oxadixyl	8.85	0.01	20.16	0.01	9.32
Oxamyl	8.93	0.01	12.50	0.01	6.91
Oxfendazole	0.47	-	3.92	-	0.45
Oxyfluorfen	7.30	0.05	3.00	0.05	2.78
Paclobutrazol	0.44	0.02	1.18	0.5	0.46
⁴⁷ Paraoxon methyl	0.97	-	0.22	-	0.79
Paraquat dichloride	-	0.02	-	0.02	
Parathion	8.00	0.05	5.43	0.05	6.09
⁴⁸ Parathion-Methyl	3.32	0.01	7.52	0.01	2.51
Pebulate	1.67	-	2.54	-	0.63
Penconazole	0.23	0.1	0.28	0.05	0.14
Pencycuron	0.53	0.05	1.22	0.05	0.42
Pendimethalin	4.31	0.05	3.61	0.05	4.30
Phenmedipham	4.33	0.05	28.25	0.05	1.97
Phenothrin	50.00	0.05	88.55	0.05	92.31
Phenthoate	15.63	-	15.87	-	12.47
Phosalone	10.87	0.01	16.67	0.01	5.66
⁴⁹ Phosmet	45.05	0.05	84.73	0.5	9.81
Phosphamidon	0.38	0.01	0.77	0.01	0.45
Phosphonic acid	1.64	-	4.83	-	2.00
Picloram	7.55	0.01	27.03	0.01	5.24
Picolinafen	4.12	0.05	3.28	0.05	2.31
Piperonyl Butoxide	0.88	-	0.76	-	0.09
Piperophos	0.18	-	0.23	-	0.16
Pirimicarb	1.33	1	4.33	3	0.58
Pirimiphos Methyl	0.16	1	0.29	1	0.09
Pretilachlor Isomer 1	2.76	-	3.58	-	2.06
Pretilachlor Isomer 2	10.87	-	14.08	-	7.34
⁵⁰ Prochloraz	2.03	0.05	3.37	10	1.72
Procymidone	7.23	0.01	6.27	0.01	5.93
Profenofos	1.10	10	1.59	0.01	0.72
⁵¹ Prohexadione	9.26	0.05	10.00	0.05	7.14

⁴⁶ Expressed as dimethoate⁴⁷ Expressed as parathion-methyl⁴⁸ Sum of parathion-methyl and paraoxon-methyl⁴⁹ Sum of Phosmet and phosmet oxon⁵⁰ Sum of prochloraz and its metabolites

Promecarb	16.67	-	21.01	-	13.76
Prometon	0.89	-	2.82	-	0.84
Prometryn	1.25	-	2.54	-	1.10
Propachlor	3.15	0.02	6.24	0.02	2.45
⁵² Propamocarb	0.56	4	0.70	0.01	0.79
Propanil	1.18	0.1	4.08	0.1	0.89
Propaquizafop	0.40	0.05	0.87	0.05	0.32
Propargite	12.65	2	50	3	9.52
Propazine	0.34	-	1.40	-	0.28
Propetamphos	14.25	-	10.85	-	5.78
Propham	11.63	0.05	17.42	0.05	3.88
Propiconazole	0.22	0.05	0.31	6	0.19
Propisochlor	14.10	0.01	16.57	0.01	13.65
Propoxur	6.67	0.05	36.76	0.05	6.04
Propylene thiourea	27.62	-	31.65	-	11.76
Propyzamid	1.67	0.02	1.62	0.02	1.45
Proquinazid	0.17	0.15	0.50	0.02	0.12
Prosulfocarb	0.57	0.01	2.51	0.01	0.53
Prosulfuron	0.78	0.02	6.67	0.02	0.64
Pymetrozin	8.47	0.5	2.83	0.3	6.03
Pyracarbolid	1.11	-	2.98	-	1.00
Pyraclostrobin	0.33	0.3	0.69	2	0.40
Pyranocoumarin	1.12	-	0.77	-	1.28
Pyrazophos	0.03	0.05	0.41	0.05	0.34
Pyridaben	1.56	0.3	1.72	0.5	1.25
Pyridaphenthion	0.31	-	0.43	-	0.22
Pyrifenox Isomer 1	1.28	-	3.34	-	0.84
Pyrifenox Isomer 2	0.76	-	2.02	-	0.61
Pyrimethanil	0.88	1	0.32	8	0.71
Pyriproxifen	0.35	1	0.21	0.6	0.30
Pyroquilon	1.61	-	3.47	-	0.96
Quinalphos	1.49	0.05	2.54	0.05	1.39
Quinmerac	2.11	0.1	1.75	0.1	1.51
Quinoclamine	4.46	-	11.76	-	2.88
Quinoxifen	0.67	0.02	0.56	0.02	0.21
Quizalofop-P-Ethyl	4.72	0.4	8.38	0.05	3.76
Resmethrin (R+S Stereoisomers)	9.17	0.1	25.25	0.1	8.07
Rimsulfuron	21.78	0.05	-	0.05	-
Rotenone	2.23	0.01	7.14	0.01	1.55
Secbumeton	0.25	-	1.35	-	0.19
¹² Sethoxydim	1.54	-	2.11	-	1.71
Siduron	1.08	-	3.92	-	0.64
Simazine	0.68	0.01	2.85	0.01	0.60
⁵³ Spinosyn A	0.92	1	6.25	0.3	0.84
Spinosyn D	5.88	-	8.55	-	5.86
Spiromesifen	2.15	1	4.74	0.02	0.84
Spirotetramat	0.90	2	0.63	1	0.62
Spiroxamine	0.66	0.05	0.36	0.05	0.46
Sulcotrione	1.37	0.05	10.06	0.05	0.83
Sulfaquinoxaline	1.96	-	13.33	-	0.76
Sulfometuron methyl	0.92	-	3.83	-	0.53
Sulfotep	1.43	-	1.65	-	0.84

⁵¹ Prohexadione acid and its salts⁵² Sum of propamocarb and its salts⁵³ Sum of spinosyn A y D, expressed as spinosad

Sulprofos	8.47	-	3.67	-	5.96
Tcpp	1.75	-	23.47	-	1.44
Tebuconazole	0.10	0.9	1.09	0.9	0.12
Tebufenpyrad	0.34	0.5	0.27	0.5	0.22
Tebutam	0.24	-	0.91	-	0.17
Tebuthiuron	0.77	-	4.22	-	0.71
Teflubenzuron	1.43	1.5	1.47	0.05	2.23
Tembotrione	2.70	0.02	24.75	0.02	1.63
Temephos	2.74	-	3.68	-	4.64
⁵⁴ Tepraloxdim isomer 1	4.13	0.1	6.77	0.1	4.57
Tepraloxdim isomer 2	9.30	48	8.20	48	6.96
Terbacil	9.43	-	27.03	-	2.61
Terbufos	-	0.01	-	0.01	-
Terbumeton	0.83	-	0.98	-	0.63
Terbuthylazine	0.54	0.05	3.33	0.1	0.36
Terbutryn	1.28	-	2.11	-	0.88
Tetrachoviphos	1.67	-	2.73	-	1.08
Thiabendazole	0.47	0.05	0.31	5	0.20
Thiacloprid	2.28	0.5	2.92	0.02	2.02
⁵⁵ Thiamethoxam	6.03	0.2	9.33	0.5	2.70
Thidiazuron	0.23	-	1.02	-	0.19
Thifensulfuron methyl	1.56	0.05	7.52	0.05	0.53
Thiocyclam	23.81	-	7.54	-	18.66
³⁸ Thiodicarb	1.72	-	7.63	-	1.01
Thiofanox	20.08	-	56.81	-	16.57
Thiophanate Methyl	21.73	1	98.33	6	22.34
Tolclofos Methyl	9.09	1	9.71	0.05	6.16
Tralkoxidym	1.61	0.02	1.58	0.02	1.31
Transfluthrin	12.22	-	16.65	-	6.03
⁵⁶ Triadimefon	0.74	1	1.28	0.1	0.47
⁴⁹ Triadimenol isomer 1	31.25	-	151.52	-	7.06
⁴⁹ Triadimenol isomer 2	86.21	-	847.46	-	35.21
Triallat	3.00	-	2.75	-	2.28
Triasulfuron	0.48	0.05	4.42	0.05	0.38
Triazophos	0.27	0.01	0.63	0.01	0.18
Triazoxide	0.29	-	0.31	-	0.19
Trichlorfon	1.93	0.01	3.07	0.01	3.96
Triclocarban	1.74	-	2.54	-	1.49
Tridemorph	2.86	0.01	1.89	0.01	2.44
Trietazine	0.29	-	0.20	-	0.18
Triethanolamine	-	-	-	-	-
Trifloxystrobin	0.67	0.5	0.89	0.3	0.43
Trifloxysulfuron	0.33	-	13.89	-	0.22
⁵⁷ Triflumizole	3.64	1	25.64	0.1	1.90
Triflumuron	0.78	0.05	1.04	1	1.14
Trifluralin	14.03	0.01	13.74	0.01	14.14
Triforine	7.14	0.01	13.15	0.01	2.14
Trimethylsulfonium	51.55	0.05	45.45	0.5	11.24
⁵⁸ Trinexapac-Ethyl	5.78	0.01	16.45	0.01	3.87
Triticonazole	0.72	0.01	4.93	0.01	0.61
Vamidothion	0.95	-	25.64	-	2.05

⁵⁴ Sum of tepraloxdim and its metabolites⁵⁵ Sum of thiamethoxam and clothiadinin⁵⁶ Sum of triadimefon and triadimenol⁵⁷ Triflumizole and its metabolite⁵⁸ Sum of trinexapac and its salts

Vinclozolin	0.77	0.05	0.40	0.05	
Zoxamide	3.50	0.5	5.26	0.02	2.48
Veterinary Drugs					
Albendazole sulfone	0.34	-	5.00	-	0.41
Albendazole sulfoxide	0.35	-	1.28	-	0.29
Amoxicillin	153.85	-	42.37	-	85.47
Ampicillin	-	-	-	-	-
B-Estradiol	56.18	-	41.49	-	25.13
Benzothiazole	75.56	-	81.97	-	29.24
Benzydamide	0.17	-	0.41	-	0.38
Caffeine	1.02	-	5.46	-	1.23
Carbadox	1.09	-	4.46	-	2.04
Carbamazepine	0.49	-	4.82	-	0.59
Chloramphenicol	2.84	-	2.29	-	1.49
Chlortetracycline isomer 1	31.85	-	30.68	-	23.15
Chlortetracycline isomer 2	5.59	-	6.04	-	2.54
Ciprofloxacin	1.63	-	3.70	-	1.50
Clarithromycin	0.84	-	1.90	-	0.60
Clenbuterol	3.79	-	3.11	-	1.35
Clofibrac acid	2.99	-	7.87	-	2.67
Cloxacillin	0.84	-	7.52	-	2.00
Cotinine	1.16	-	3.41	-	6.62
Danofloxacin	1.62	-	1.93	-	0.75
Demeclocycline isomer 1	2.13	-	7.7	-	3.85
Demeclocycline isomer 2	27.17	-	35.78	-	31.25
Diclofenac	15.15	-	8.70	-	6.06
Dicloxacillin isomer 1	4.03	-	16.67	-	8.26
Dicloxacillin isomer 2	0.38	-	1.53	-	0.77
Difloxacin	3.75	-	1.74	-	4.15
Digoxin F ₁	10.34	-	102.04	-	10.75
Dimetridazole	2.01	-	3.83	-	3.87
Diphenhydramine	0.97	-	4.83	-	0.27
Doramectin	55.25	-	109.89	-	64.10
Doxycycline	8.62	-	40.98	-	5.24
Enoxacin	5.99	-	7.87	-	3.72
Enrofloxacin	4.85	-	4.31	-	2.53
Eprinomectin B _{1a}	31.06	-	51.02	-	4.65
Eprinomectin B _{1b}	83.33	-	78.12	-	53.19
Erythromycin	16.72	-	21.93	-	7.24
Estrone	16.39	-	65.79	-	8.36
Febantel (1)	5.36	-	5.10	-	2.80
Febantel (2)	3.13	-	3.70	-	0.55
Fleroxacin	-	-	-	-	-
Flufenamic acid	1.39	-	2.07	-	5.24
Flumequine	1.58	-	6.25	-	2.55
Fluoxetine	0.69	-	6.36	-	0.69
Furosemide	7.01	-	27.78	-	7.30
Gemfibrozil	25.25	-	42.37	-	9.80
Hydrochlorothiazide	7.35	-	10.53	-	10.99
Hydroflumethiazide	5.04	-	-	-	39.37
Ibuprofen	10.73	-	47.17	-	14.95
Indomethazine	3.94	-	29.41	-	1.82
Irgasan	100	-	106.38	-	61.73
Josamycin	2.99	-	12.82	-	3.06
Ketoprofen	3.52	-	14.36	-	1.18
Leucomalachite green	2.17	-	4.01	-	4.13

Levamisole	4.15	-	5.68	-	3.98
Lincomycin	0.64	-	1.28	-	0.42
Lomefloxacin	1.32	-	3.15	-	0.41
Malachite Green	0.12	-	0.50	-	0.53
Marbofloxacin	1.44	-	6.25	-	0.86
Meclofenamic acid	6.13	-	9.71	-	3.95
Mefenamic acid	3.94	-	4.76	-	4.20
Metformin	15.53	-	2.79	-	60.97
Miconazole	0.33	-	5.41	-	0.47
Minocycline	11.93	-	48.54	-	17.99
Naproxen	20.83	-	333.33	-	28.25
Natamycin	4.46	-	12.66	-	5.05
Nicotine isomer 1	83.33	-	119.05	-	50.51
Nicotine isomer 2	23.15	-	67.57	-	32.68
Nifuroxazide	23.70	-	357.14	-	12.99
Norfloxacin	3.48	-	2.47	-	2.28
Orbifloxacin	1.58	-	1.80	-	0.20
Oxacillin isomer 1	12.66	-	56.18	-	57.53
Oxacillin isomer 2	0.84	-	9.52	-	6.14
Oxolinic acid	1.92	-	1.70	-	2.58
Oxybendazole	0.82	-	2.62	-	0.30
Oxytetracycline	2.07	-	4.37	-	1.31
Penicillin G (mix isomers)	2.44	-	4.31	-	2.70
Penicillin V isomer1	13.89	-	47.17	-	6.21
Penicillin V isomer2	9.17	-	49.02	-	3.32
Pentylentetrazole	-	-	-	-	-
Phenylbutazone	5.37	-	15.38	-	12.66
Pravastatin	10.82	-	57.47	-	3.48
Prednisolone	13.70	-	18.66	-	2.93
Promethazine	0.46	-	1.54	-	2.56
Propranolol	1.30	-	1.52	-	0.35
Ranitidine	5.29	-	5.32	-	4.18
Robenidine	4.22	-	4.73	-	0.56
Ronidazole	59.52	-	27.32	-	22.12
Roxithromycin	0.99	-	3.18	-	0.42
Salbutamol	5.29	-	7.46	-	4.12
Sarafloxacin	1.63	-	10.99	-	1.11
Spiramycin	3.22	-	7.14	-	3.65
Streptomycin	-	-	-	-	-
Sulfabenzamide	16.72	-	23.92	-	3.22
Sulfacetamide	61.73	-	50.51	-	50.51
Sulfachloropyridazine	4.15	-	11.24	-	2.07
Sulfadiazine	19.76	-	24.39	-	5.59
Sulfadimethoxyn	1.07	-	10.00	-	0.47
Sulfadoxine	3.55	-	4.52	-	0.85
Sulfaguanidine	41.32	-	35.21	-	30.67
Sulfamerazine	1.16	-	3.22	-	1.58
Sulfameter	1.53	-	1.73	-	0.67
Sulfamethazine	2.35	-	3.79	-	0.78
Sulfamethizole	4.12	-	4.46	-	1.70
Sulfamethoxazole	2.31	-	3.19	-	1.28
Sulfamethoxypyridazine	1.22	-	0.96	-	1.82
Sulfamonomethoxine	4.05	-	5.41	-	1.93
Sulfanilamide	52.08	-	25.77	-	56.82
Sulfapyridine	8.20	-	8.26	-	2.97
Sulfathiazole	8.93	-	10.75	-	2.36
Sulfisoxazol	9.43	-	41.32	-	2.59

Sulindac	1.13	-	7.17	-	0.85
Tetracycline	2.26	-	2.87	-	1.45
Theobromine	83.33	-	58.82	-	14.66
Theophylline	60.98	-	54.35	-	17.92
Thiamphenicol	1.87	-	4.41	-	1.74
Tilmicosin	0.67	-	3.12	-	0.41
Tolfenamic acid	3.07	-	8.77	-	2.18
Tolmetin	5.88	-	29.94	-	2.94
Trimethoprim	0.56	-	0.49	-	0.25
Tylosin	0.64	-	3.39	-	1.83
Food Packaging contaminants					
1,3-Phenylendiamine	60.24	-	147.05	-	15.8
1,6-Phenylendiamine	434.78	-	-	-	435
2-Ethylhexyl diphenyl phosphate	0.19	-	0.27	-	0.21
2-Methoxy-5-methylalanine	0.33	-	4.78	-	4.13
2,4-Diaminoanisole	15.92	-	16.18	-	67.57
2,4-Diaminotoluene	2.32	-	5.71	-	14.23
2,4-Dimethylaniline	3.61	-	2.67	-	10.53
2,4,5-Trimethylaniline	-	-	-	-	-
2,6-Diaminotoluene	53.19	-	196.08	-	15.63
4-Aminobiphenyl	1.21	-	1.54	-	3.07
4-Chloroaniline	2.61	-	3.65	-	6.41
4-Hexylresorcinol	64.93	-	409.84	-	161.29
Aniline	6.74	-	2.72	-	3.07
Benzyl butyl phthalate	13.16	-	16.67	-	3.69
Bisphenol A	-	-	-	-	-
BA (2,3-DHP) G	36.50	-	-	-	6.40
BA (3Cl,2HP)(2,3DHP) E	42.02	-	40.54	-	7.69
BA (3Cl,2HP)GE	47.16	-	59.52	-	18.66
BAB (2,3DHP)E	12.14	-	83.33	-	32.25
Bisphenol A diglycidyl ether	17.12	-	19.68	-	2.22
Butyl p-hydroxybenzoate	14.58	-	23.64	-	0.84
DEHA	-	-	-	-	-
Dibutyl sebacate	1.30	-	1.10	-	0.78
Dicyclohexyl phthalate	2.86	-	4.18	-	12.2
Diethyl phthalate	5.32	-	16.34	-	6.02
Diisodecyl phthalate	-	-	-	-	2.36
Diisononyl phthalate	52.08	-	63.29	-	64.10
Dimethyl phthalate	14.53	-	19.01	-	0.71
Di N-butyl phthalate	-	-	-	-	0.51
Di-n-octyl phthalate	40	-	48.09	-	4.93
Dipropyl phthalate	31.25	-	33.56	-	3.13
Ethyl 4-hydroxybenzoate	27.62	-	52.63	-	12.66
Melamine	150.38	-	186.92	-	83.33
Methylparaben	48.08	-	119.05	-	1.50
N,N-diethylhydroxylamine	396.83	-	625	-	675.68
Nordihydroguaiaretic acid	-	-	-	-	1.69
o-Anisidine	0.93	-	0.45	-	2.86
o-Toluidine	0.41	-	0.32	-	5.68
Propyl 4-hydroxybenzoate	8.88	-	9.32	-	1.35
Tributyl o-acetylcitrate	0.16	-	1.00	-	0.03
Tributyl phosphate	0.85	-	0.15	-	1.06
Mycotoxins					
3-Acetyldeoxynivalenol	94.34	-	-	-	62.5
Aflatoxin B ₁	7.46	-	15.06	-	0.53

Aflatoxin B ₂	0.51	-	17.12	-	0.19
Aflatoxin G ₁	0.81	-	53.19	-	0.42
Aflatoxin G ₂	1.10	-	12.11	-	0.26
Aflatoxin M ₁	2.30	-	6.88	-	0.36
Alfa zearalenol	25.25	-	55.56	-	11.68
Citrinin	-	-	-	-	-
Cyclopiazonic acid	47.17	-	65.79	-	5.18
Deoxynivalenol	83.33	-	166.67	-	166.67
Diacetoxyscirpenol	84.03	-	133.33	-	38.76
Ergocornine isomer 1	1.14	-	3.24	-	0.65
Ergocornine isomer 2	8.13	-	7.58	-	4.20
Fumonisin B ₁	0.05	-	0.06	-	0.05
Fumonisin B ₂	-	-	-	-	-
Gliotoxin	12.05	-	82.64	-	12.47
HT-2 toxin	144.93	-	151.06	-	9.94
Ochratoxin A	0.93	-	83.33	-	0.7
Patulin	431	-	595	-	833
Sterigmatocystin	0.51	-	0.31	-	0.14
T2-Toxin	10.44	-	-	-	3.65
Zearalenone	11.65	-	420.17	-	5.38
Perfluorinated compounds					
Pentafluoropropionic acid	5.32	-	19.61	-	19.61
Perfluorobutyric acid	0.68	-	0.85	-	8.70
Perfluoropentanoic acid	0.84	-	1.88	-	1.65
Perfluoroheptanoic acid	0.26	-	0.29	-	0.26
Perfluorooctanoic acid	4.42	-	1.81	-	5.46
Perfluorononanoic acid	0.22	-	0.31	-	0.27
Perfluorodecanoic acid	0.29	-	0.23	-	0.16
Perfluoroundecanoic acid	0.33	-	0.69	-	0.50
Perfluorododecanoic acid	0.38	-	0.35	-	0.54
Heptadecafluorooctane-sulfonic acid	0.16	-	0.16	-	0.10
Nitrosamines					
N-nitrosodiethylamine	357.14	-	877.19	-	833.33
N-nitrosodimethylamine	357.14	-	238.10	-	210.13
N-nitrosodi-n-dibutylamine	10.71	-	19.16	-	8.47
N-nitrosomethylethylamine	>1000	-	>1000	-	>1000
N-nitrosomorpholine	103.63	-	163.93	-	113.64
N-nitroso-n-diphenylamine	31.45	-	75.76	-	23.26
N-nitrosopiperidine	57.47	-	1.67	-	24.51
N-nitrosopyrrolidine	7.63	-	10.99	-	28.57
N-nitrosodi-n-dipropylamine	112.36	-	322.58	-	162.60
N-nitrosodiethylamine	357.14	-	877.19	-	833.33
Sweeteners					
Aspartame	1.94	-	13.44	-	5.56
Acesulfame-K	5.88	-	3.14	-	7.91
Saccharin	2.59	-	2.27	-	4.93
Sucralose	3.61	-	8.94	-	11.63
Cyclamate	1.80	-	3.15	-	6.80

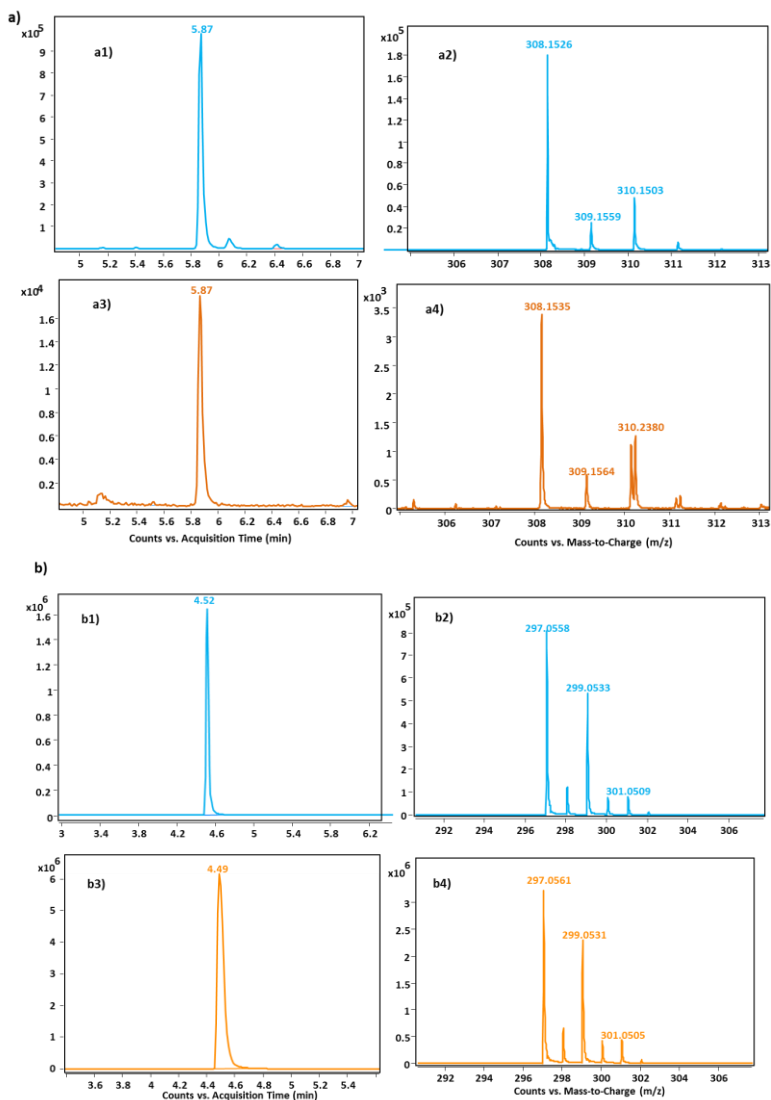


Figure 7(a). Extracted ion chromatogram (EIC) of tebuconazole in solvent (20% methanol) (figure a1); mass spectrum of tebuconazole in solvent (20% methanol) (figure a2); Extracted ion chromatogram (EIC) of tebuconazole in peach jam (figure a3); mass spectrum of tebuconazole in peach jam (figure a4); (b) Extracted ion chromatogram (EIC) of imazalil in solvent (20% methanol) (figure b1); mass spectrum of imazalil in solvent (20% methanol) (figure b2); Extracted ion chromatogram (EIC) of imazalil in orange (figure b3); mass spectrum of imazalil in orange (figure b4).

Besides the performance in terms of LOQs, matrix effects were also tested. Matrix effects usually occur during ionization step, where the matrix constituents influence the ionization of co-eluted analyte(s). Coelution with

matrix interferences or with compounds belonged to the same batch could produce signal suppression or enhancement of the target compounds. This fact also could cause mass measurement deviations from theoretical m/z values. As an example, **Figure 6(b)** includes the extracted ion chromatograms of a pesticide (metribuzin, $100 \mu\text{g Kg}^{-1}$) in solvent, tomato, orange and baby food. Signal suppression was observed in these three matrixes. Orange was the one that produced the highest signal suppression, followed by tomato and baby food. **Figure 6(c)** shows extracted ion chromatograms (EICs) for fluquinconazole in solvent and tomato. For this compound, signal enhancement was observed in matrix ($200 \mu\text{g Kg}^{-1}$) although this is not the standard behavior. The same criterion -described in section 3.1.1- was applied for matrix effects evaluation. Slope ratios matrix/solvent from 0.8 to 1 were considered as soft signal suppression, from 0.5 to 0.8, medium signal suppression and lower than 0.5, strong signal suppression. Signal enhancement could also be classified as soft (slope ratios matrix/solvent from 1 to 1.2), medium (slope ratios matrix/solvent from 1.2 to 1.5) and strong (slope ratios matrix/solvent from 1.5 to 2). **Table S3** and **Figure S2** (Supplementary data) includes the data from the matrix effects displayed by the different classes of compounds, being signal suppression the most common effect produced in tomato, orange and baby food. Medium signal suppression was the most common effect produced in tomato for pesticides, mycotoxins, veterinary drugs, food packaging contaminants and nitrosamines, with the exception of perfluoro organic compounds and sweeteners. However, strong signal suppression was the most common effect produced in orange in most cases compounds. Finally, soft signal suppression for pesticides, veterinary drugs, mycotoxins, food packaging contaminants and sweeteners was the most common effect produced in baby food. This is consistent with the complexity of each of the matrix revealed by the TIC profiles shown in **Figure 6**. In summary, signal

suppression were more often produced than signal enhancement. Orange was the matrix where compounds, in general, had strong signal suppression and baby food, soft signal suppression. Tomato often produced medium signal suppression.

Conclusions

A screening method using UHPLC-TOFMS has been developed for the examination of over 630 food contaminants, including pesticides, veterinary drugs, food packaging contaminants, mycotoxins, nitrosamines, perfluoroorganic compounds and sweeteners. The method was based on a database with retention time values and mass accurate measurements of the ions of interest. It was found that software parameters such as retention time window and mass error tolerance have a clear influence on the automatic search results. Taking into account the number of false positives and negatives reported by the software. 0.25 minutes as retention time window and 10 ppm (relative mass error) mass tolerance were selected. The proposed was also examined in terms of linearity, matrix effect and limits of quantification in three different matrixes: tomato, orange and baby food. For most of compounds, signal suppression was the most common matrix effect produced. In general, baby food and orange produced the lowest and the highest matrix effect, respectively. This clearly had an impact on the sensitivity of the method. Limits of quantification were also calculated for the 630 compounds included, and most of them were $< 10\mu\text{g Kg}^{-1}$ in tomato, orange and baby food. However, in the particular case of pesticides with relatively low response factors (ca. 10-20 % of the compounds depending on the complexity of the matrix) the detection was not fulfilling the MRL established for the tested pesticide/commodity combination. This is a drawback of the entire approach that may be partially solved with more

sensitive and updated instrumentation, except for the case of compounds not really amenable to electrospray ionization.

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III.2.3. Anexo

Table S1. Elution gradients assayed to develop the screening method.

Elution Gradient A		Elution Gradient B		Elution Gradient C	
Time	%B	Time	%B	Time	%B
0	0	0	5	0	5
1	5	2	5	2	5
4	100	8	100	12	100
5	100	10	100	15	100

Table S2. Fragmentation in all ion mode using LC-QTOFMS for compounds without fragments or whose relative abundance was lower than 10% when in-source CID fragmentation was used in LC-TOFMS at 220V.

Compound	Elemental Composition	Ion detected	Theoretical m/z	Relative Abundance (%)			
				0V	10V	20V	30V
Pesticides							
4-Chloro-2-methylphenol	C ₇ H ₇ OCl	[M-H] ⁻	141.0113	100	100	100	100
Acibenzolar S-methyl	C ₈ H ₆ N ₂ OS ₂	[M+H] ⁺	210.9994	100	100	100	14
Acibenzolar S-methyl F ₂		C ₆ H ₄ S ₂	139.9749	-	-	26	100
Acibenzolar S-methyl F ₁		C ₆ H ₄ N ₂ S	136.0090	-	-	19	35
Acibenzolar S-methyl F ₃		C ₇ H ₇	91.0542	-	-	43	38
Amitrol	C ₂ H ₄ N ₄	[M+H] ⁺	85.0509	100	100	100	100
Amitrol F ₁		C ₂ H ₅ N ₂	57.0447	-	-	-	-
AMPA	C ₇ H ₁₀ N ₂ O ₄	[M-H] ⁻	185.0568	ND	ND	ND	ND
Anilazine	C ₉ H ₅ Cl ₃ N ₄	[M-H] ⁻	272.9507	100	100	100	100
Brodifacoum	C ₃₁ H ₂₃ BrO ₃	[M-H] ⁻	521.0758	100	100	100	100
Bromadiolone	C ₃₀ H ₂₃ BrO ₄	[M-H] ⁻	525.0707	100	100	100	100
Bromophos methyl	C ₈ H ₈ BrCl ₂ O ₃ PS	[M+H] ⁺	364.8565	ND	ND	ND	ND
Bromoxynil	C ₇ H ₃ ONBr ₂	[M-H] ⁻	273.8509	100	100	100	100
Chlordimeform	C ₁₀ H ₁₃ ClN ₂	[M+H] ⁺	197.0840	100	100	100	-
Chlordimeform F ₁		C ₈ H ₇ ClN	152.0262	-	-	11	-
Chlordimeform F ₂		C ₇ H ₆ Cl	125.0153	-	-	-	15
Chlordimeform F ₃		C ₈ H ₇ N	117.0573	-	-	40	100
Chloridazon	C ₁₀ H ₈ ClN ₃ O	[M+H] ⁺	222.0429	100	100	100	100
Chloridazon F ₁		C ₄ H ₅ ClN ₃ O	146.0116	-	-	1	10
Chloridazon F ₂		C ₄ H ₂ ClN ₃ O	128.9850	-	-	2	7
Chloridazon F ₃		C ₆ H ₇ N	104.0495	-	-	-	-
Chloridazon F ₄		C ₃ H ₂ ClN ₂	100.9901	-	-	-	-
Chloridazon F ₅		C ₆ H ₆ N	92.0495	-	-	-	-
Chloridazon F ₆		C ₂ H ₃ N ₂	55.0291	-	-	-	-
Chloridazon	C ₁₀ H ₈ ClN ₃ O	[M+Na] ⁺	244.0248	-	-	-	-
Chlormequat chloride	C ₅ H ₁₃ ClN ⁺	[M+H] ⁺	122.0737	100	100	100	4
Chlormequat chloride F ₁		C ₃ H ₉ N	59.0730	-	3	95	39
Chlormequat chloride F ₂		C ₃ H ₈ N ⁺	58.0651	-	2	83	100
Chlorpyrifos methyl	C ₇ H ₇ Cl ₃ NO ₃ PS	[M+H] ⁺	321.9023	100	100	2	-
Chlorpyrifos methyl F ₁		C ₆ H ₄ Cl ₃ NO ₂ PS	289.8760	-	27	15	4
Chlorpyrifos methyl F ₂		C ₂ H ₆ O ₂ PS	124.9826	-	100	100	100
Chlorpyrifos methyl F ₃		CH ₄ PO ₂	78.9943	-	-	5	35
Cyprodinil	C ₁₄ H ₁₅ N ₃	[M+H] ⁺	226.1339	100	100	100	100
Cyprodinil F ₁		C ₃ H ₁₂ N ₃	210.1026	-	-	2	18
Cyprodinil F ₂		C ₁₀ H ₁₀ N	144.0808	-	-	1	13
Cyprodinil F ₃		C ₈ H ₉ N ₂	133.0760	-	-	2	19
Cyprodinil F ₄		C ₇ H ₇ N ₂	119.0604	-	-	1	22
Cyprodinil F ₅		C ₈ H ₆ N	116.0495	-	-	-	11
Cyprodinil F ₆		C ₈ H ₆ N	108.0808	-	-	3	42
Cyprodinil F ₇		C ₆ H ₇ N	93.0573	-	-	1	51
Cyprodinil F ₈		C ₆ H ₅	77.0386	-	-	-	7
Dazomet	C ₅ H ₁₀ N ₂ S ₂	[M+H] ⁺	163.0358	100	100	100	100
Dazomet F ₁		C ₃ H ₆ NS ₂	119.9936	-	100	-	-
Dicloran	C ₆ H ₄ Cl ₂ N ₂ O ₂	[M+H] ⁺	206.9723	100	100	100	100
Difenacoum	C ₃₁ H ₂₄ O ₃	[M+H] ⁺	445.1798	100	100	48	20

Difenacoum F ₁		C ₁₉ H ₁₅ O ₃	291.1012	-	4	15	11
Difenacoum F ₂		C ₂₁ H ₁₆	257.1325	-	7	64	42
Difenacoum F ₃		C ₁₉ H ₁₅ O ₃	189.0546	-	2	11	13
Difenacoum F ₄		C ₁₄ H ₁₁	179.0855	-	-	21	100
Difenacoum F ₅		C ₁₀ H ₇ O ₃	175.0390	-	-	10	26
Difenacoum F ₆		C ₃ H ₉	165.0699	-	-	-	11
Difenacoum	C ₃₁ H ₂₄ O ₃	[M+Na] ⁺	467.1618	-	12	32	56
Difenzoquat	C ₁₇ H ₁₇ N ₂	[M] ⁺	249.1392	100	100	100	100
Difenzoquat F ₁		C ₁₆ H ₁₄ N ₂	234.1151	-	-	1	21
Difenzoquat F ₂		C ₁₆ H ₁₃ N ₂	233.1073	-	-	1	25
Difenzoquat F ₃		C ₁₅ H ₁₄ N	208.1121	-	-	2	12
Difenzoquat F ₄		C ₁₄ H ₁₁ N	193.0886	-	-	4	79
Difenzoquat F ₅		C ₁₀ H ₁₂ N	146.0964	-	-	2	12
Difenzoquat F ₆		C ₉ H ₉ N	131.0730	-	-	2	64
Difenzoquat F ₇		C ₉ H ₈ N	130.0651	-	-	1	35
Difenzoquat F ₈		C ₈ H ₈ N	118.0651	-	-	3	60
Diflufenican	C ₁₉ H ₁₁ F ₅ N ₂ O ₂	[M+H] ⁺	395.0813	100	100	37	2
Diflufenican F ₁		C ₁₃ H ₇ F ₃ NO ₂	266.0423	-	7	100	100
Diflufenican F ₂		C ₁₆ H ₄ FNO	246.0350	-	-	5	10
Emamectin	C ₄₉ H ₇₅ NO ₁₃	[M+H] ⁺	886.5311	100	100	100	22
Emamectin F ₁		C ₁₅ H ₂₈ NO ₅	302.1962	-	-	-	6
Emamectin F ₂		C ₈ H ₁₆ NO ₂	158.1176	-	1	14	100
Emamectin F ₃		C ₇ H ₁₂ NO	126.0913	-	-	-	5
Epoxiconazole	C ₁₇ H ₁₃ ClFN ₃ O	[M+H] ⁺	330.0804	100	100	100	100
Ethiprole	C ₁₃ H ₉ Cl ₂ F ₃ N ₄ OS	[M+H] ⁺	396.9899	100	100	66	21
Ethiprole F ₁		C ₁₁ H ₄ Cl ₂ F ₃ N ₄ S	350.9480	-	6	100	100
Ethiprole F ₂		C ₈ H ₄ Cl ₂ F ₃ N ₂	254.9714	-	-	-	31
Ethoxyquin	C ₁₄ H ₁₉ NO	[M+H] ⁺	218.1539	100	100	100	12
Ethoxyquin F ₁		C ₁₃ H ₁₆ NO	202.1226	7	12	46	35
Ethoxyquin F ₂		C ₁₂ H ₁₆ NO	190.1226	-	1	32	12
Ethoxyquin F ₃		C ₁₂ H ₁₄ NO	188.1070	-	-	19	34
Ethoxyquin F ₄		C ₁₁ H ₁₂ NO	174.0913	-	-	27	100
Ethoxyquin F ₅		C ₁₀ H ₁₀ NO	160.0757	-	-	6	39
Ethoxyquin F ₆		C ₉ H ₁₀ NO	148.0757	-	-	32	43
Ethoxyquin F ₇		C ₈ H ₈ NO	134.0600	-	-	8	25
Ethoxyquin F ₈		C ₈ H ₁₀ N	120.0808	-	-	-	13
Etoazole	C ₂₁ H ₂₃ F ₂ NO ₂	[M+H] ⁺	360.1770	100	100	100	3
Etoazole F ₁		C ₇ H ₁₆ O	177.1274	-	-	39	21
Etoazole F ₂		C ₇ H ₃ F ₂ O	141.0156	-	-	72	100
Fenarimol	C ₁₇ H ₁₂ Cl ₂ N ₂ O	[M+H] ⁺	331.0399	100	100	100	31
Fenarimol F ₁		C ₇ H ₄ ClO	138.9945	-	-	3	34
Fenarimol F ₂		C ₄ H ₅ N ₂	81.0447	-	-	21	100
Fenhexamid	C ₁₄ H ₁₇ Cl ₂ NO ₂	[M+H] ⁺	302.0709	100	100	85	4
Fenhexamid F ₁		C ₇ H ₁₃	97.1011	-	4	100	100
Fenitrothion	C ₉ H ₁₂ NO ₅ PS	[M+H] ⁺	278.0247	100	100	-	-
Fenpropidine	C ₁₉ H ₃₁ N	[M+H] ⁺	274.2529	100	100	100	57
Fenpropidine F ₁		C ₁₁ H ₁₅	147.1168	-	-	5	100
Fenpropidine F ₂		C ₅ H ₁₂ N	86.0964	-	-	5	67
Fenpropimorph	C ₂₀ H ₃₄ NO	[M+H] ⁺	304.2640	100	100	100	100
Fenpropimorph F ₁		C ₇ H ₁₆ NO	130.1226	-	-	6	89
Fenpropimorph F ₂		C ₆ H ₁₄ NO	116.1070	-	-	4	59
Fenpropimorph F ₃		C ₆ H ₁₂ N	98.0964	-	-	-	76
Fenthion	C ₁₀ H ₁₅ O ₃ PS ₂	[M+H] ⁺	279.0273	100	59	-	-
Fenthion F ₁		C ₉ H ₁₂ O ₂ PS ₂	247.0011	-	100	26	-
Fenthion F ₂		C ₉ H ₁₂ O ₃ PS	231.0239	-	-	-	-
Fenthion F ₃		C ₉ H ₉ S ₂	169.0140	-	56	100	88
Fenthion F ₄		C ₈ H ₉ OS	153.0369	-	-	21	49
Fenthion F ₅		C ₂ H ₆ O ₂ PS	124.9821	-	6	36	100
Fentin	C ₁₈ H ₁₄ Sn	[M+H] ⁺	351.019	100	100	100	100

Terbufos F ₁		C ₅ H ₁₄ O ₂ PS ₃	232.9888	71	-	-	-
Terbufos F ₂		C ₄ H ₁₂ O ₂ PS ₂	187.0011	11	20	-	-
Terbufos F ₃		C ₅ H ₁₁ S	103.0576	100	100	100	100
Thiofanox	C ₉ H ₁₈ N ₂ O ₂ S	[M+H] ⁺	219.1162	-	-	-	-
Thiofanox F ₁		C ₇ H ₁₄ NS	144.0841	18	1	-	-
Thiofanox F ₂		C ₂ H ₆ NO ₂	76.0393	33	25	17	-
Thiofanox F ₃		C ₄ H ₉	57.0699	100	100	100	-
Thiofanox	C ₉ H ₁₈ N ₂ O ₂ S	[M+Na] ⁺	241.0981	8	7	5	-
Triazoxide	C ₁₀ H ₆ ClN ₅ O	[M+H] ⁺	248.0334	100	100	100	100
Triazoxide F ₁		C ₉ H ₆ ClN ₄ O	221.0225	-	-	1	5
Triazoxide F ₂		C ₉ HO	125.0022	-	-	-	12
Triazoxide F ₃		C ₃ H ₆ ClN	123.9949	-	-	1	20
Triazoxide F ₄		C ₄ H ₃ N ₂	95.0240	-	-	5	49
Trietazine	C ₉ H ₁₆ ClN ₅	[M+H] ⁺	230.1167	100	100	100	100
Trietazine F ₁		C ₇ H ₁₃ ClN ₅	202.0854	-	-	32	19
Trietazine F ₂		C ₄ H ₇ ClN ₃	132.0323	-	-	26	37
Trietazine F ₃		C ₆ H ₁₀ N ₃	124.0869	-	-	13	31
Trietazine F ₄		C ₂ H ₃ ClN ₃	104.0010	-	-	7	48
Trietazine F ₅		C ₅ H ₁₁ N ₂	99.0917	-	-	28	83
Trietazine F ₆		C ₃ H ₇ N ₂	71.0604	-	-	7	77
Trifluralin	C ₁₃ H ₁₆ F ₃ N ₃ O ₄	[M+H] ⁺	336.1166	100	100	100	100
Trimethylsulfonium	C ₃ H ₈ S	M ⁺	77.0425	100	100	100	100
Veterinary drugs							
Benzothiazole	C ₇ H ₅ NS	[M+H] ⁺	136.0215	100	100	100	100
Clarithromycin	C ₃₈ H ₆₉ NO ₁₃	[M+H] ⁺	748.4842	100	100	19	-
Clarithromycin F ₁		C ₃₀ H ₅₆ NO ₁₀	590.3899	1	23	72	4
Clarithromycin F ₂		C ₂₉ H ₅₂ NO ₉	558.3637	-	2	16	4
Clarithromycin F ₃		C ₈ H ₁₆ NO ₂	158.1176	-	4	100	100
Clarithromycin F ₄		C ₆ H ₁₄ NO	116.1070	-	-	9	13
Danofloxacin	C ₁₉ H ₂₀ FN ₃ O ₃	[M+H] ⁺	358.1561	100	100	100	100
Danofloxacin F ₁		C ₁₈ H ₂₀ FN ₃ O	314.1663	-	-	24	20
Danofloxacin F ₂		C ₁₇ H ₁₅ FN ₂ O	283.1241	-	-	9	60
Danofloxacin F ₃		C ₆ H ₉ N	96.0808	-	-	12	48
Erythromycin	C ₃₇ H ₆₇ NO ₁₃	[M+H] ⁺	734.4685	100	100	16	-
Erythromycin F ₁		C ₂₉ H ₅₃ NO ₁₀	576.3742	1	30	76	11
Erythromycin F ₂		C ₂₉ H ₅₂ NO ₉	558.3637	-	9	24	2
Erythromycin F ₃		C ₂₉ H ₄₈ NO ₇	522.3495	-	5	17	3
Erythromycin F ₄		C ₈ H ₁₆ NO ₂	158.1176	-	5	100	100
Erythromycin F ₅		C ₆ H ₁₄ NO	116.1070	-	-	10	16
Erythromycin F ₆		C ₅ H ₇ O	83.0491	4	-	-	11
Fluoxetine	C ₁₇ H ₁₈ F ₃ NO	[M+H] ⁺	310.1413	100	100	16	-
Fluoxetine F ₁		C ₁₀ H ₁₄ N	148.1121	1	30	76	11
Malachite green	C ₂₃ H ₂₄ N ₂	[M+H] ⁺	329.2012	100	100	100	100
Malachite green F ₁		C ₂₂ H ₂₁ N ₂	313.1699	-	-	-	17
Malachite green F ₂		C ₁₅ H ₁₄ N	208.1121	-	-	-	9
Minocycline	C ₂₃ H ₂₇ N ₃ O ₇	[M+H] ⁺	458.1922	53	30	56	100
Minocycline F ₁		C ₁₉ H ₈ N	250.0651	100	100	100	10
Minocycline F ₂		C ₂₃ H ₂₆ N ₂ O ₇	221.0865	16	43	61	45
Minocycline F ₃		C ₂₂ H ₂₃ N ₂ O ₇	213.5747	-	3	30	17
Promethazine	C ₁₂ H ₇ NS	[M+H] ⁺	198.0372	100	100	100	100
Promethazine F ₁		C ₁₁ H ₈ N	154.0651	-	-	-	-
Promethazine F ₂		C ₄ H ₉ N	71.0730	-	-	8	38
Roxithromycin	C ₄₁ H ₇₆ N ₂ O ₁₅	[M+H] ⁺	837.5318	100	100	19	-
Roxithromycin F ₁		C ₃₃ H ₆₃ N ₂ O ₁₂	679.4376	-	19	100	44
Roxithromycin F ₂		C ₈ H ₁₆ NO ₂	158.1176	-	5	21	100
Sulindac	C ₂₀ H ₁₇ FO ₃ S	[M+H] ⁺	357.0955	100	100	100	63
Sulindac F ₁		C ₂₀ H ₁₇ FO ₂ S	340.0928	7	9	88	50
Sulindac F ₄		C ₁₈ H ₁₄ FOS	297.0744	-	-	15	19

Sulindac F ₅		C ₁₉ H ₁₆ FS	295.0951	-	-	14	52
Sulindac F ₆		C ₁₈ H ₁₃ FS	280.0717	-	-	9	24
Sulindac F ₇		C ₁₈ H ₁₃ F	248.0996	-	6	21	66
Sulindac F ₈		C ₁₇ H ₁₀ F	233.0761	18	19	55	100
Tylosin	C ₄₆ H ₇₇ NO ₁₇	[M+H] ⁺	916.5264	100	100	100	100
Tylosin F ₁		C ₈ H ₁₆ NO ₃	174.1125	-	-	-	15
Tylosin F ₂		C ₇ H ₁₃ O ₃	145.0859	-	-	5	4
Tylosin F ₃		C ₅ H ₁₁ NO	101.0835	-	-	-	-
Tylosin F ₄		C ₅ H ₉ O ₂	101.0597	-	-	13	29
Mycotoxins							
Ergocornine	C ₃₁ H ₃₉ N ₅ O ₅	[M+H] ⁺	562.3024	100	100	100	25
Ergocornine F ₁		C ₃₁ H ₃₈ N ₅ O ₄	544.2918	1	30	73	13
Ergocornine F ₂		C ₂₆ H ₂₂ N	348.1747	-	-	17	25
Ergocornine F ₃		C ₂₀ H ₂₁ O	277.1587	-	-	10	41
Ergocornine F ₄		C ₁₆ H ₁₈ N ₃ O	268.1444	1	2	41	98
Ergocornine F ₅		C ₈ H ₁₉ N ₂ O ₅	223.1288	-	-	7	55
Fumonisin B ₁	C ₃₄ H ₅₉ NO ₁₅	[M+H] ⁺	722.3957	100	100	100	100
Fumonisin B ₁ F ₁		C ₃₄ H ₅₈ NO ₁₄	704.3852	-	-	-	29
Fumonisin B ₁ F ₂		C ₃₄ H ₅₆ NO ₁₃	686.3746	-	-	-	6
Fumonisin B ₁ F ₃		C ₂₈ H ₅₂ NO ₉	546.3637	-	-	-	6
Fumonisin B ₁ F ₄		C ₂₈ H ₅₀ NO ₈	528.3531	-	-	-	4
Fumonisin B ₁ F ₅		C ₂₂ H ₄₄ NO ₃	370.3316	-	-	-	5
Fumonisin B ₁ F ₆		C ₂₂ H ₄₂ NO ₂	352.3137	-	-	-	6
Fumonisin B ₂	C ₃₄ H ₅₉ NO ₁₄	[M+H] ⁺	706.4008	ND	ND	ND	ND

Table S3. Regression equations and regression coefficients in solvent (20% methanol) and relations between calibration curve slopes in matrix (tomato, orange and baby food) and solvent for database compounds.

Compound	Equation (solvent)	Linearity (r) (Solvent)	Matrix Effect (Matrix slope/Solvent slope)		
			Tomato	Orange	Baby food
Pesticides					
1-Naphtalene-Acetamide	6178x+63904	0.9963	0.74	0.40	0.83
2,4-Dichlorophenoxy-acetic acid	367x-10323	0.9960	0.95	1.22	1.01
2,4-Dinitrophenol	3760x+134327	0.9948	0.92	0.57	0.97
3,3-Dichlorobenzidine	26399x+5228	0.9996	0.36	0.19	1.15
3,5-Dichloroaniline	4214x+18887	0.9991	0.85	0.27	0.73
4-Chloro-2-methylphenol	88x+25	0.9914	0.67	0.59	0.86
4-Chloro-O-tolyoxyacetic acid F ₁	8907x+63647	0.9963	0.81	0.55	0.95
Acephate F ₁	5261x+109545	0.9997	0.90	0.98	0.76
Acetamiprid	8058x+2937	0.9998	0.57	0.29	0.71
Acibenzolar S-Methyl	977x+674	0.9995	0.67	0.19	0.80
Aclonifen	889x+13793	0.9991	0.68	0.48	1.0
Alachlor F ₁	8327x+182982	0.9963	0.75	0.49	0.90
Albendazole	50580x+48224	0.9995	0.55	0.32	0.94
Aldicarb	1474x+287221	0.9907	0.69	0.15	0.76
Aldicarb Sulfone	2512x+24265	0.9976	0.63	0.78	0.95
Aldicarb Sulfoxide F ₁	1067x+11181	0.9962	1.16	1.24	1.03
Allethrin	1317x-26538	0.9958	0.54	0.57	0.98
Ametryne	82864x+173793	0.9982	0.63	0.50	0.86
Aminocarb	14232x+152595	0.9951	0.87	0.85	0.81
Amitraz	154x-2595	0.9889	-	-	-
Amitrol	5632x+239670	0.9959	0.15	0.13	0.12
AMPA	302x-2993	0.9973	0.64	0.63	0.41
Anilazine	179x-2431	0.9975	1.23	1.47	1.45
Anilofos	7052x+76241	0.9966	0.97	0.92	0.93
Antimycin A	908x+1201	0.9992	0.86	0.57	1.63
Asulam	546x+30071	0.9971	0.64	0.64	0.91
Atrazine	54308x+39692	0.9997	0.41	0.47	0.85
Atrazine Desethyl	17537x+252915	0.9920	0.65	0.71	0.74
Atrazine Desisopropyl	8853x+51128	0.9998	0.84	0.60	0.91
Azaconazole	15010x-62008	0.9999	0.63	0.41	0.88
Azamethiphos	704x+21388	0.9963	1.87	0.84	2.02
Azinphos-Ethyl	417x+8005	0.9982	0.61	0.43	0.85
Azinphos Methyl F ₁	1946x+24913	0.9996	0.81	0.20	0.74
Azobenzene	816x+7858	0.9973	0.66	0.19	0.48
Azocyclotin	5874x+1262	0.9994	0.82	0.59	1.21
Azoxystrobin	19362x+92669	0.9958	0.55	0.42	0.94
Barban F ₁	197x+14158	0.9887	0.74	0.47	0.83
Benalaxyl	36048x+53296	0.9999	1.01	0.52	1.08
Bendiocarb F ₁	5142x+144862	0.9928	0.80	0.50	0.96
Benfluralin	257x-15784	0.9973	0.96	0.78	0.91
Benfuracarb	-	-	-	-	-
Bensulfuron Methyl	10757x+112528	0.9973	0.74	0.03	1.19
Bensulide	613x+53433	0.9979	0.82	0.67	0.86
Bentazone	12654x+104330	0.9915	0.92	0.48	0.96

Benzidine	7660x+79789	0.9977	0.27	0.10	0.44
Bifenazate F ₁	7083X+8501	0.9999	0.67	0.72	0.47
Bifenox F ₁	183x+13460	0.9944	0.95	0.74	0.97
Bitertanol	6208x+165487	0.9951	0.93	0.68	0.19
Boscalid	6372x+30943	0.9993	0.68	0.45	0.82
Brodifacoum iso 1	3874x+7729	0.9957	0.96	0.72	0.12
Brodifacoum iso 2	2823x+3724	0.9988	0.91	0.79	0.12
Bromacil F ₁	3279x+30568	0.9993	0.63	0.18	0.94
Bromadiolone iso 1	3831x+17488	0.9939	0.83	0.71	0.56
Bromadiolone iso 2	640x+7030	0.9936	0.97	0.87	0.64
Bromophos Methyl	64x-982	0.9989	0.83	0.70	0.83
Bromoxynil	3662x+282643	0.9983	0.71	0.67	0.91
Bromuconazole Iso 1	4555x+7115	0.9998	0.89	0.64	1.0
Bromuconazole Iso 2	4262x+22692	0.9994	0.92	0.42	0.96
Bupirimate	73056x+64088	0.9976	0.74	0.43	0.96
Buprofezin	53916x+350605	0.9902	0.92	0.69	0.74
Butachlor	3598x-47463	0.9974	0.70	0.52	0.94
Butocarboxim	3646x+5035	0.9997	0.31	0.09	0.67
Butoxycarboxim	1025x+10210	0.9945	0.57	0.61	0.84
Butralin	4188x+3636	0.9997	0.67	0.67	0.63
Buturon	5009x+45813	0.9988	0.99	0.18	0.89
Cadusafos	5478x+39790	0.9996	0.78	0.63	0.96
Carbaryl	10082x+203579	0.9905	0.76	0.57	0.96
Carbendazim	20236x+486086	0.9947	0.87	0.83	0.88
Carbofuran	5281x+111582	0.9963	0.78	0.54	0.96
Carbofuran 3-Hydroxy	2830x+5138	0.9974	0.32	0.11	0.71
Carbosulfan	15813x-872	0.9991	-	-	
Carboxine	9315x+116137	0.9971	0.67	0.53	0.90
Carfentazone Ethyl	264x+4206	0.9997	1.31	0.82	1.19
Chlorbromuron	1749x+6076	0.9993	0.73	0.38	1.04
Chlordimeform	2636x-31475	0.9997	2.39	1.78	1.24
Chlorfenvinfos	5535x+94082	0.9983	0.78	0.57	0.80
Chlorfluazuron	524x+6378	0.9973	0.54	0.64	0.73
Chloridazon	6637x+370356	0.9953	0.80	0.53	0.91
Chlormequat chloride	12894x+313235	0.9956	0.23	0.24	0.21
Chloroprotham	555x+3960	0.9992	0.91	0.30	0.93
Chlorotoluron	23458x+9650	0.9997	0.46	0.39	0.80
Chloroxuron	14075x+512419	0.9941	0.97	0.39	0.93
Chlorpyrifos	867x-756	0.9985	0.39	0.51	0.93
Chlorpyrifos Methyl	442x+727	0.9981	0.52	0.34	0.95
Chlorsulfuron	3837x+47945	0.9993	0.22	0.15	0.87
Cinosulfuron	12147x	0.9996	0.90	0.55	0.93
Clethodim isomer E	4464x-1720	0.9995	0.56	0.46	0.54
Clethodim isomer Z	636x-14581	0.9939	1.68	-	1.26
Clodinafop-Propargyl	1419x-16100	0.9910	2.02	1.63	1.06
Clofentezine	947x+1058	1.0000	0.65	0.53	0.94
Clomazone	7680x+129265	0.9982	0.77	0.10	1.0
Clopyralid	488x-4199	0.998	0.60	0.50	0.64
Clothianidin	639x+2212	0.9997	0.46	0.24	0.64
Coumaphos	5416x+25846	0.999	0.79	0.72	0.92
Cyanazine	22011x+84641	0.9989	0.71	0.40	0.83
Cyazofamid	348x+45073	0.9911	0.77	0.42	0.88
Cycloate	9857x-77	0.9991	0.70	0.51	0.94
Cycloheximid	1457x-2529	0.9992	0.75	0.44	0.81
Cycloxydim isomer 1	18042x+146625	0.9936	0.25	0.28	0.39
Cycloxydim isomer 2	2634x+58896	0.9995	0.84	0.60	0.76
Cymoxanil	3091x-35115	0.9995	0.01	0.01	-

Cyphenothrin	51x+2874	0.9921	0.82	0.71	0.21
Cyproconazole	56527x+76182	0.9943	0.72	0.17	0.99
Cyprodinil	111556x+324458	0.9924	0.72	0.47	0.97
Cyromazine	12911x+94531	0.9969	0.59	0.66	0.60
Daminozide	6037x+370145	0.9911	0.38	0.25	0.24
Dazomet	-	-	-	-	-
Deet	88533x+221475	0.9939	0.67	0.57	0.96
Demeton-S-Methyl	1087x+19715	0.9974	0.57	0.24	0.80
Desethyl Terbuthylazine	8840x+255260	0.9967	0.77	0.47	0.98
Desmedipham	1740x+33117	0.9979	1.52	0.34	2.03
Desmetryn	27907x+3317309	0.996	1.20	0.71	0.77
Diafenthion	18808x-109430	0.9931	0.28	0.38	0.64
Diazinon	67789x+205670	0.9889	0.42	0.53	0.81
Dibrom F ₁	1464x+71934	0.9993	0.75	0.35	0.87
Dicamba F ₁	143x-9716	0.9983	1.27	0.63	1.13
Dichlofenthion	158x+9228	0.9916	0.97	0.72	0.84
Dichlofluanid	-	-	-	-	-
Dichlorprop	3139x+13189	0.9999	0.97	0.53	1.08
Dichlorvos	3899x+57275	0.9985	0.81	0.55	0.93
Dicloran	100x+991	0.999	0.57	0.60	2.71
Dicrotophos	9207x+23295	0.9990	0.71	0.42	0.93
Diethanolamine	-	-	-	-	-
Diethofencarb	882x+14685	0.9959	0.77	0.16	0.99
Difenacoum isomer 1	9702x+6461	0.9997	0.67	0.33	0.87
Difenacoum isomer 2	10601x+15165	0.9982	0.53	0.31	0.69
Difenoconazole	24063x+329568	0.9924	0.90	0.75	0.82
Difenoخور	22093x+1470500	0.9974	0.80	0.40	0.99
Difenzoquat	46277x+68681	0.9921	0.80	0.57	1.10
Diflubenzuron	590x+26345	0.9915	0.96	0.80	1.17
Diflufenican	14979x-8356	0.9995	0.43	0.37	0.88
Dimethametryn	85913x+11502	0.9999	0.65	0.38	0.87
Dimethenamid	7584x+87578	0.9965	0.87	0.35	0.97
Dimethoate	818x+5068	0.9992	0.76	0.37	0.78
Dimethomorph Iso. 1	2754x+63212	0.9939	1.26	-	1.01
Dimethomorph Iso. 2	3933x+48868	0.9976	0.95	0.51	0.87
Diniconazole	28545x+40768	0.9998	0.82	0.44	0.10
Diphenylamine	16704x+672180	0.9929	1	0.89	0.88
Diquat dibromide	-	-	-	-	-
Diuron	9720x-30163	0.9972	0.54	0.25	0.78
Dmst	450x+5854	0.9969	0.42	0.47	0.75
DNOC	3489x+181888	0.9930	0.96	2.16	1.17
Edifenphos	9516x+183572	0.9977	0.91	1.02	1.28
Emamectin Benz iso. 1	4682x+25683	0.9993	1.07	0.49	0.88
Emamectin Benz.isomer 2	5726x+68188	0.9986	1.14	0.59	0.93
Endosulfan sulfate	1666x+22387	0.9978	0.81	0.79	0.84
Epn	1359x+156	0.9989	0.57	0.78	0.43
Epoxiconazole	40761x+34898	0.9994	0.64	0.52	0.88
Eptc	2947x-1808	0.9965	0.71	0.50	0.94
Etaconazol	30327x+50504	1	0.85	0.50	1.03
Ethephon	-	-	-	-	-
Ethidimuron	2558x+11639	0.9999	0.94	0.33	0.85
Ethiofencarb	27387x+22204	0.9992	0.36	0.35	0.46
Ethiofencarb Sulfone	856x-1360	0.9998	9.13	4.02	0.87
Ethiofencarb Sulfoxide	6295x+17342	0.9993	1.83	0.98	0.77
Ethion	435x+22856	0.9998	0.63	0.79	0.90

Ethiprole	4445x+83155	0.9976	0.89	0.34	0.99
Ethofumesate	945x+98222	0.9924	0.60	0.30	0.74
Ethoprophos	18312x+134462	0.9987	0.78	0.48	1.14
Ethoxyquin	29642x-188817	0.9986	0.72	0.41	0.89
Ethylenethiourea	775x+11523	0.9982	0.25	0.18	0.25
Etofenprox	984x+104612	0.9984	0.35	0.41	0.43
Etoxazole	161013x+37349	0.9997	0.15	0.07	0.22
Etrimphos	52354x+181394	0.9992	0.72	0.45	0.78
Famoxadone F ₁	364x+7033	0.9951	0.71	0.45	0.78
Famphur	4904x+30091	0.9981	0.61	0.15	0.94
Fenamidone	47213x-21584	0.9993	0.63	0.53	0.88
Fenamiphos	16374x+35829	0.9969	0.90	0.73	0.95
Fenamiphos Sulfone	15923x-13662	0.9996	0.42	0.61	0.92
Fenamiphos Sulfoxide	8375x+50522	0.9979	0.78	0.56	0.95
Fenarimol	10295x+618799	0.9970	0.99	0.30	0.98
Fenazaquin	55318x+164835	0.9979	0.43	0.47	0.79
Febendazole	58051x+20672	0.9998	0.68	0.50	0.88
Fenhexamid	5873x+119100	0.9973	0.91	0.62	1.03
Fenhexamid 4-O-Gluc.	393x+11039	0.9962	0.80	0.30	0.88
Fenitrothion	1038x+17604	0.9956	0.74	0.62	0.89
Fenobucarb	2973x+50898	0.9905	0.47	0.11	0.72
Fenoxaprop P-Ethyl	10140x-3402	1	0.59	0.43	0.54
Fenoxycarb	4970x+6676	0.9993	0.61	0.34	0.97
Fenpiclonil	1616x-12581	0.9997	0.74	0.22	0.99
Fenpropathrin	841x+20813	0.9985	0.38	0.38	0.79
Fenpropidine	98515x+325712	0.9932	0.77	0.40	1.04
Fenpropimorph	106072x+197029	0.9979	0.71	0.45	1.04
Fenpyroximate	41697X-45244	0.9938	0.78	0.6	0.76
Fensulfothion	16819x+16070	0.9995	0.73	0.48	0.97
Fenthion	1859x+13147	0.999	0.55	0.44	0.93
Fentin chloride	11141x+17413	0.9995	0.48	0.39	0.85
Fenuron	20420x+54985	0.9933	0.24	0.20	0.82
Fipronil	382x+3274	0.9937	0.71	0.56	0.95
Fluazifop	9920x+71342	0.9971	0.73	0.38	0.88
Fluazifop-Butyl	50197x+110515	0.9988	0.60	0.48	0.97
Fluazinam	926x-6753	0.9960	0.84	0.72	0.87
Fluchloralin	298x+1194	0.9988	0.67	0.94	0.88
Flucythrinate	65x-1290	0.9980	0.88	0.58	0.16
Fludioxonil	73156x-27344	0.9999	0.80	0.51	0.98
Flufenacet	3488x+21444	0.9985	0.75	0.53	0.96
Flufenoxuron	1781x-10734	0.9986	0.46	0.24	0.39
Fluomethuron	17219x+770661	0.9951	1.04	0.63	1.01
Fluquinconazole	613x-28130	0.9975	1.72	0.98	1.42
Fluroxypyr	153x-3363	0.9962	0.94	0.25	0.86
Flusilazole	46105x+126595	0.9910	0.92	0.52	0.93
Flutolanil	14615x+234702	0.9930	0.88	0.55	0.98
Flutriafol	12726x+60443	0.9971	0.42	0.40	0.67
Fomesafen	130x+7241	0.9976	0.44	0.29	0.78
Fonofos	274x+2989	0.9999	0.63	0.28	0.69
Foramsulfuron	1865x+17212	0.9993	0.85	0.59	0.84
Forchlorfenuron	15315x-30917	0.9998	0.73	0.54	0.86
Formetanate	272x+17789	0.9953	4.92	4.33	7.15
Fosetyl	3137x-83573	0.993	0.09	0.12	0.05
Fosthiazate	11557x+44719	0.9977	0.78	0.54	0.83
Fuberidazol	51693x+130978	0.9993	0.69	0.83	0.83
Furalaxyl	24849x+18489	0.9977	0.76	0.29	0.94
Furathiocarb	20348x-108720	0.9998	0.77	0.59	1.11

Furmecyclox	24864x+27809	0.9984	0.59	0.49	0.91
Gibberellic acid	4437x+33353	0.9993	0.58	0.15	0.90
Glufosinate ammonium	512x-5710	0.9969	0.29	0.32	0.28
Glufosinate N-acetyl	4437x+33353	0.9993	1.08	1.24	0.97
Glyphosate	-	-	-	-	-
Griseofulvin	8071x-2172	1	0.70	0.16	0.92
Haloxypop	6380x+83878	0.9951	0.73	0.43	0.94
Hexaflumuron	213x+3839	0.9982	0.67	0.46	0.71
Hexazinone	33685x+30862	0.9998	0.70	0.47	0.87
Hexythiazox	3252x+9581	0.9964	0.56	0.53	0.92
Hydramethylnon	26144x-122056	0.9907	0.75	0.51	0.26
Imazalil	30735x+122415	0.9957	0.76		0.84
Imazalil metabolite	23306x+17736	0.9992	0.50	0.36	0.86
Imazamethabenz-methyl	50110x+2080458	0.995	0.86	0.43	0.99
Imazamox	44739x+24207	0.9999	0.56	0.39	0.78
Imazapyr	28984x+62276	0.999	0.53	0.13	0.88
Imazaquin	39796x+234781	0.9935	0.72	0.53	0.95
Imidacloprid	2061x+11727	0.9995	0.69	0.19	0.74
Indoxacarb	4895x+7636	0.9992	0.82	0.74	0.79
Ioxynil	9335x+70448	0.9907	0.96	1.36	1.05
Iprodione	281x+4619	0.9932	0.53	0.47	0.94
Iprovalicarb	16443x-63406	0.9970	0.81	0.27	1.01
Isazophos	16756x-108279	0.9998	0.86	0.59	1.03
Isocarbophos	7233x+121576	0.9972	0.90	0.22	0.97
Isofenphos	113x+10650	0.9977	0.87	0.69	0.33
Isoprocab	2130x+102274	0.9969	0.71	0.44	0.96
Isoprothiolane	2049x+26488	0.9982	0.78	0.45	0.95
Isoproturon	48661x+160826	0.9986	0.56	0.51	0.82
Isoxaben	12834x+1000000	0.9963	0.83	0.60	0.93
Isoxaflutole	422x+2096	0.9965	1.12	0.49	0.86
Ivermectin	130x+18532	0.9938	1.08	0.98	1.14
Karbutilate	22140x+77410	0.9941	0.69	0.58	0.92
Kresoxim Methyl	3170x+12498	0.994	0.49	0.25	0.87
Lactofen	526x+1223	0.9984	0.46	0.38	1.10
Lenacil	3493x+82378	0.9955	0.50	0.54	0.96
Linuron	4130x+14151	0.9997	0.63	0.11	1.14
Lufenuron	182x+6439	0.998	0.71	0.62	0.78
Malaoxon	3494x-19572	0.9988	0.97	0.90	1.50
Malathion	999x+17140	0.9979	0.87	0.85	0.70
Maleic hydrazide	-	-	-	-	-
Mecarbam	205x+9310	0.9972	0.80	0.57	0.82
Mecoprop	3586x+50620	0.9978	0.89	0.60	0.52
Mefenacet	17736x+24907	0.9997	0.66	0.42	0.99
Mepanipyrim	105485x+65254	0.9998	0.81	0.37	0.90
Mephosfolam	18954x+74441	0.9958	0.81	0.35	0.95
Mepiquat isomer 1	31198x+63096	0.997	0.34	0.29	0.36
Mepiquat isomer 2	1571x+41174	0.9994	0.49	0.53	0.44
Mepronil	22145x-19694	0.9997	0.82	0.52	0.88
Mesotrione	1646x+191510	0.9997	0.69	0.50	0.80
Metaflumizone	3297x+2014	0.9908	0.68	0.32	0.51
Metalaxyl	11301x+1000000	0.9927	1.07	1.12	1.04
Metamitron	22489x+1385097	0.9956	0.68	0.57	0.90
Metazachlor	13313x+42757	0.9985	0.88	0.45	0.94
Methabenzthiazuron	22520x+29154	0.9984	0.57	0.32	0.92
Methacrifos	580x+13628	0.9953	0.83	0.05	0.82

Methamidophos	1856x+11725	0.9994	0.38	0.45	0.33
Methidathion	432x+37463	0.9955	0.58	0.10	0.78
Methiocarb F ₁	1432x+17917	0.9983	1.05	0.27	0.73
Methiocarb Sulfoxide	3473x+32319	0.9985	0.81	0.56	1.16
Methomyl	5058x+36099	0.9996	0.91	0.47	0.78
Methoprotryne	71034x-49821	0.9994	0.65	0.50	0.90
Methoxyfenozide	4686x+12224	0.9997	0.85	0.54	0.95
Metobromuron	2646x-5489	0.9993	0.72	0.45	0.98
Metolachlor	12382x+496891	0.9965	0.84	0.59	0.84
Metolcarb	9083x+167241	0.991	0.60	0.21	0.53
Metoxuron	19246x+40731	0.9991	0.64	0.44	0.83
Metribuzin	42605x+1967818	0.9972	0.92	0.52	0.96
Metsulfuron Methyl	9802x+10345	0.9967	0.48	0.32	0.91
Mevinphos	1517x-9243	0.9983	0.63	0.36	0.78
Molinate	7192x+132288	0.9989	0.77	0.46	1.24
Monocrotophos	1924x+11883	0.9996	0.90	0.80	0.95
Monolinuron	4433x+36871	0.9993	0.69	0.41	1.02
Monuron	10052x+247891	0.9929	0.87	0.46	0.97
Morpholin	1607x+136520	0.9936	0.25	0.16	0.28
Myclobutanil	8923x+45649	0.9973	0.46	0.48	0.71
Naptalam	3664x+36191	0.9950	0.13	0.04	0.24
Neburon	11180x+105647	0.9968	0.83	0.74	0.97
Nereistoxin isomer 1	884x+23678	0.9931	0.34	0.15	0.35
Nereistoxin isomer 2	503x+33105	0.9984	0.41	0.37	1.47
Nitenpyram	10157x+82642	0.9983	0.75	0.27	0.96
N-Methylcarbamate	5149x+132787	0.995	0.88	0.54	0.92
N,N-Diethyl-2-Naphtoloxypromamide	30874x+9344	0.9937	0.74	0.48	1.05
Norflurazone	14654x+36526	0.9966	0.57	0.30	0.97
Novaluron	2014x+67322	0.9904	0.76	0.70	0.37
Nuarimol	23353x+7531	0.9988	0.70	0.30	0.85
Ofurace	8710x+21359	0.9965	0.71	0.06	0.98
Omethoate	1565x+42950	0.9999	1.04	0.97	0.94
Orbencarb	4242x+12274	0.9955	0.86	0.79	0.94
Oryzalin	11005x+23285	0.9991	0.68	0.98	1.02
Oxadiazon	1582x+36245	0.9956	0.85	0.59	1.02
Oxadixyl	3595x+34935	0.9987	1.00	0.35	0.95
Oxamyl	1287x+9576	0.9993	0.94	1.02	1.22
Oxfendazole	17652x+479408	0.9957	0.93	0.46	0.97
Oxyfluorfen	1254x+2280	0.9942	0.35	0.45	0.93
Paclobutrazol	48240x+121355	0.9975	0.91	0.35	0.87
Paraoxon methyl	4947x+10391	0.9994	0.65	0.38	0.80
Paraquat	-	-	-	-	-
Parathion	576x+8523	0.9988	0.67	0.53	0.88
Parathion-Methyl	1034x+12306	0.9989	0.61	0.33	0.81
Pebulate	3701x-57815	0.999	0.93	0.77	0.91
Penconazole	51984x+52117	0.9972	0.63	0.49	1.01
Pencycuron	27063x-6473	0.999	0.73	0.52	0.93
Pendimethalin	4274x-7731	0.9958	0.94	0.73	0.94
Phenmedipham	2028x-10384	0.9978	1.27	0.08	2.80
Phenothrin	289x+15733	1	0.88	0.59	0.48
Phenthoate	310x+2684	0.9953	0.84	0.64	1.05
Phosalone	571x+170	0.9997	0.49	0.37	0.94
Phosmet	602x+5355	0.9981	0.95	0.22	4.38
Phosphamidon	22640x+1369037	0.997	1.13	0.85	0.96
Phosphonic acid	24719x-71408	0.9986	0.46	0.44	0.38
Picloram	452x-101	0.999	0.52	0.23	0.75

Picolinafen	3009x+37214	0.9983	0.52	0.54	0.92
Piperonyl Butoxide	17686x+14409	0.9991	0.87	0.72	0.86
Piperophos	25953x+305650	0.9992	0.85	0.75	0.99
Pirimicarb	51474x+103803	0.9978	0.42	0.34	0.97
Pirimiphos Methyl	106074x+202741	0.996	0.48	0.42	0.89
Pretilachlor Isomer 1	10909x+14014	0.9991	0.74	0.60	0.99
Pretilachlor Isomer 2	3952x-3981	0.9981	0.66	0.53	0.98
Prochloraz	4203x+91082	0.9952	0.91	0.23	0.81
Procymidone	849x+31052	0.9964	0.66	0.41	0.80
Profenofos	3445x+1472	0.995	0.73	0.62	1.12
Prohexadione	3507x-149323	0.9926	0.64	0.31	0.89
Promecarb	1511x+41408	0.9954	0.84	0.53	1.02
Prometon	78403x+31785	0.9982	0.76	0.55	0.80
Prometryn	87997x+14636	0.9991	0.72	0.57	0.82
Propachlor	13108x+15517	0.9991	0.71	0.20	0.92
Propamocarb	17193x+177480	0.9992	1.30	1.23	0.92
Propanil	4583x+14860	0.9998	0.66	0.23	0.87
Propaquizafofop	8549x+10397	0.9994	0.98	0.78	1.22
Propargite	421x+50376	0.9921	0.85	0.61	0.93
Propazine	61140x+309890	0.9954	0.74	0.21	0.88
Propetamphos	1055x-7853	0.9962	0.35	0.46	0.86
Propham	1408x-1149	0.9989	0.50	0.19	0.89
Propiconazole	6173x+213211	0.9959	0.80	0.62	0.94
Propisochlor	734x+45676	0.9994	0.86	0.74	0.89
Propoxur	1490x+177476	0.9901	0.49	0.28	0.55
Propylene thiourea	1821x+16124	0.9996	0.54	0.55	0.82
Propyzamid	2626x+28916	0.9968	0.80	0.46	0.92
Proquinazid	38189x+30866	0.999	0.57	0.58	0.86
Prosulfocarb	10528x+156527	0.996	0.87	0.60	0.95
Prosulfuron	6974x+182406	0.9951	0.60	0.11	0.73
Pymetrozin	13511x+41743	0.9996	0.41	0.41	0.58
Pyracarbolid	22031x+23291	0.9998	0.73	0.51	0.81
Pyraclostrobin	8381x+271047	0.9923	1.18	0.69	1.00
Pyranocoumarin	9606x+5420	0.9996	1.05	0.97	0.93
Pyrazophos	8653x+88118	0.9934	0.48	0.35	0.92
Pyridaben	6421x+14394	0.9960	0.57	0.52	0.97
Pyridaphenthion	16591x+683607	0.9973	0.73	0.50	1.01
PyrifenoX Isomer 1	7402x-14174	0.9998	0.64	0.75	0.97
PyrifenoX Isomer 2	15684x-15118	0.9999	0.73	0.47	0.92
Pyrimethanil	83467x+634239	0.9902	0.72	0.50	0.89
Pyriproxifen	711307x+57127	0.999	0.71	0.63	0.82
Pyroquilon	26088x+32607	0.9972	0.49	0.36	0.82
Quinalphos	12901x+147882	0.9975	0.90	0.73	0.97
Quinmerac	5466x+9818	0.9995	0.50	0.35	0.70
Quinoclamine	1995x+15278	0.9988	0.55	0.25	0.85
Quinoxifen	22328x-33998	0.9989	0.36	0.32	1.15
Quizalofop-P-Ethyl	11074x+224483	0.9925	0.73	0.62	0.91
Resmethrin (R+S Stereoisomers)	643x+1875	0.9991	0.87	0.74	0.41
Rimsulfuron	5321x+12093	0.9948	0.02	-	-
Rotenone	3941x+5361	0.9993	0.71	0.48	1.03
Secbumeton	69507x-49845	0.9992	0.68	0.50	0.89
Sethoxydim	31536x+294095	0.9998	0.39	0.33	0.35
Siduron	27763x-13166	0.9993	0.53	0.35	0.89
Simazine	21374x-54094	0.9994	0.92	0.40	0.61
Spinosyn A	18853x+281754	0.9930	0.84	0.14	0.91
Spinosyn D	4556x-51858	0.9986	0.93	0.22	0.93

Spiromesifen	2084x-11334	0.9810	0.45	0.43	1.15
Spirotetramat	8837x-269144	0.9974	1.47	0.81	2.14
Spiroxamine	78893x+68965	0.998	0.70	0.69	1.0
Sulcotrione	6157x-2611	0.9998	0.48	0.23	0.79
Sulfaquinoxaline	3461x+4471	0.9998	0.68	0.37	1.03
Sulfometuron Methyl	14320x+156825	0.9979	0.54	0.22	0.93
Sulfotep	3866x+2995	0.9986	0.58	0.50	0.98
Sulprofos	1455x-12763	0.9994	0.35	0.31	0.50
Tcpp	2283x+8635	0.9993	0.72	0.20	0.87
Tebuconazole	34181x+147175	0.9928	0.96	0.58	0.81
Tebufenpyrad	23175x+142860	0.9991	0.68	0.85	1.07
Tebutam	68610x-34994	0.999	0.67	0.63	0.97
Tebuthiuron	47253x+192334	0.9952	0.73	0.34	0.79
Teflubenzuron	874x+27003	0.9899	1	0.89	1.09
Tembotrione	1591x+72	0.9992	0.53	0.24	0.87
Temphos	926x+4145	0.9996	0.87	0.40	0.52
Tepraloxymid isomer 1	4773x+207479	0.9963	0.51	0.36	0.46
Tepraloxymid isomer 2	1438x-8169	0.9959	0.87	0.74	1.16
Terbacil	1653x+80812	0.991	0.95	0.25	0.97
Terbufos	-	-	-	-	-
Terbumeton	82884x+61211	0.9998	0.69	0.55	0.91
Terbutylazine	46239x+101460	0.9989	0.61	0.18	0.92
Terbutryn	882051x+280604	0.9972	0.58	0.54	0.84
Tetrachovinphos	2922x+3859	0.9991	0.61	0.34	0.93
Thiabendazole	27731x+149898	0.9946	0.50	0.37	0.99
Thiacloprid	4003x+37954	0.9996	0.84	0.43	0.94
Thiamethoxam	1335x+74807	0.9936	0.34	0.19	0.72
Thidiazuron	5651x+35852	0.9986	0.74	0.33	0.92
Thifensulfuron methyl	2823x-14250	0.9999	0.69	0.37	0.73
Thiocyclam	2208x-6463	0.9998	0.72	0.73	0.91
Thiodicarb	1575x+53172	0.9933	1.10	0.46	1.26
Thiofanox	760x+88565	0.9918	0.81	0.39	0.98
Thiophanate Methyl	688x-28381	0.9945	0.65	0.88	0.63
Tolclofos Methyl	1258x-25918	0.9969	0.61	0.38	0.90
Tralkoxidym	23830x-17419	0.9999	0.41	0.37	0.45
Transfluthrin	260x+534	0.9999	0.63	0.52	0.88
Triadimefon	25882x+101967	0.9964	0.60	0.34	0.94
Triadimenol isomer 1	625x+3369	0.9993	0.53	0.20	0.95
Triadimenol isomer 2	142x+5289	0.9980	0.49	0.19	0.94
Triallat	1452x+52745	0.9997	0.79	0.82	1.04
Triasulfuron	6744x+34588	0.9972	0.71	0.46	0.88
Triazophos	25175x+28640	0.9972	0.66	0.39	0.96
Triazoxide	27227x+22610	0.9986	0.58	0.41	0.90
Trichlorfon	244x-1383	0.9862	2.65	1.52	1.29
Triclocarban	1248x+3367	0.9989	0.95	0.62	0.69
Tridemorph	50510x+555498	0.9902	0.95	0.38	1.11
Trietazine	114288x+59644	0.9994	0.62	0.41	1.02
Triethanolamine	-	-	-	-	-
Trifloxystrobin	13179x+43534	0.9946	0.59	0.48	0.91
Trifloxysulfuron	12122x-4589	0.9998	0.62	0.05	0.94
Triflumizole	2996x+76224	0.9951	0.37	0.22	0.70
Triflumuron	2806x+21125	0.9977	1.05	0.90	1.40
Trifluralin	257x-15975	0.9972	0.96	0.78	0.91
Triforine	1032x-5610	0.9994	0.52	0.34	1.32
Trimethylsulfonium	798x+16917	0.9955	0.27	0.27	0.85
Trinexapac-Ethyl	3956x+17062	0.9995	0.50	0.10	0.74
Triticonazole	23552x+278603	0.9982	0.84	0.19	0.99

Vamidothion	1807x+97968	0.9934	0.73	0.39	0.42
Vinclozolin	47x-532	0.9993	0.77	0.40	-
Zoxamide	3975x+13702	0.9998	0.68	0.71	0.96
Veterinary Drugs					
Albendazole sulfone	19704x-15063	0.997	0.69	0.40	0.98
Albendazole sulfoxide	6887x+49737	0.9953	0.81	0.63	1.03
Amoxicillin	568x-11885	0.9987	0.59	0.70	0.73
Ampicillin	-	-	-	-	-
B-Estradiol	766x+5536	0.9999	0.65	0.57	0.81
Benzothiazole	513x-12380	0.9999	0.64	0.63	0.96
Benzydamide	32213x+170866	0.9936	0.90	0.67	0.90
Caffeine	19440x+40663	0.9972	0.58	0.46	0.88
Carbadox	2063x+14240	0.9999	0.79	0.52	0.84
Carbamazepine	22321x+166401	0.9945	0.60	0.57	0.89
Chloramphenicol	881x+75468	0.9891	0.86	0.43	0.84
Chlortetracycline iso.1	1633x-24055	0.9934	0.45	0.27	0.54
Chlortetracycline iso.2	2929x+67937	0.9879	0.64	0.35	0.84
Ciprofloxacin	6414x-18976	0.9937	0.86	0.67	0.86
Clarithromycin	24722x+277975	0.9951	0.69	0.05	0.87
Clenbuterol	5632x+103753	0.9973	0.84	0.62	0.73
Clofibric acid	2420x+9385	0.9986	0.70	0.39	0.74
Cloxacillin	19405x-61092	0.9988	0.73	0.29	0.78
Cotinine	24922x+37863	0.996	0.31	0.22	0.20
Danofloxacin	5573x+51348	0.998	0.79	0.39	0.88
Demeclocycline iso. 1	3118x+56562	0.9969	0.61	0.55	0.70
Demeclocycline iso. 2	204x+804	0.9987	3.24	2.50	1.94
Diclofenac	417x+7061	0.991	0.69	0.33	0.78
Dicloxacillin iso.1	483x+5588	0.9985	0.73	0.17	0.77
Dicloxacillin iso 2	3855x+13280	0.9997	0.55	0.27	0.59
Difloxacin	12292x-197783	0.9988	0.58	0.45	0.72
Digoxin	1212x+16457	0.998	0.67	0.19	0.51
Dimetridazole	11542x+25076	0.9952	0.80	0.78	0.84
Diphenhydramine F ₁	95612x+93259	0.9992	0.71	0.52	0.90
Doramectin F ₁	142x+16168	0.9989	0.86	0.91	0.87
Doxycycline	5071X+52887	0.9983	0.65	0.39	0.59
Enoxacin	7401x-89237	0.9965	0.81	0.42	0.83
Enrofloxacin	8983x+67933	0.9959	0.65	0.46	0.75
Eprinomectin B _{1a}	388x-2086	0.9997	0.76	0.67	1.00
Eprinomectin B _{1b}	117x-4294	0.9946	0.91	0.84	1.34
Erythromycin	10570x+92450	0.9945	0.03	0.02	0.05
Estrone	1157x+12786	0.9992	0.79	0.23	0.64
Febantel (1)	3129X+36443	0.9987	0.72	0.60	0.78
Febantel (2)	7114x+32698	0.9982	0.58	0.74	0.86
Fleroxacin	-	-	-	-	-
Flufenamic acid	5837x+52312	0.9978	0.67	0.46	0.71
Flumequine	4826x+91023	0.9928	0.77	0.37	0.61
Fluoxetine	16607x+49634	0.9947	0.66	0.46	0.71
Furosemide	1188x-26399	0.9988	0.75	0.15	0.73
Gemfibrozil	835x+33975	0.991	0.82	0.43	0.87
Hydrochlorothiazide	984x+23489	0.9953	1.10	0.94	0.95
Hydroflumethiazide	128x-1602	0.9963	0.46	-	0.80
Ibuprofen	1008x+38230	0.9945	0.75	0.42	1.04
Indomethazine	1273x-2766	0.9998	0.84	0.25	1.03
Irgasan	64x+1153	0.9986	0.83	0.56	1.00
Josamycin	17663x+28667	0.9981	0.48	0.42	0.58

Ketoprofen	3095x+6671	0.9998	1.07	0.34	0.65
Leucomalachite green	7923x-5763	0.9977	0.79	0.55	0.31
Levamisole	23694x-91463	0.9972	0.86	0.90	0.84
Lincomycin	9705x+27756	0.9997	1.00	0.54	0.97
Lomefloxacin	12442x-101451	0.9999	0.71	0.54	0.74
Malachite Green	50180x+162945	0.997	0.72	0.69	0.86
Marbofloxacin	7691x+76901	0.9947	0.72	0.28	0.86
Mebendazole	-	-	-	-	-
Meclofenamic acid	625x+726	0.9956	0.64	0.51	0.77
Mefenamic acid	2269x+22435	0.9932	0.75	0.52	0.83
Menadione	-	-	-	-	-
Metformin	3960x+256922	0.9926	0.25	0.44	0.06
Miconazole	11018x+109815	0.9915	0.73	0.41	1.03
Minocycline	2013x-69542	0.9949	0.668	0.28	0.69
Monensin	-	-	-	-	-
Naproxen F ₁	564x+4749	0.9996	0.50	0.07	0.69
Natamycin	4317x-18406	0.9999	0.72	0.25	0.54
Nicotine isomer 1	2434x+115588	0.9937	0.27	0.15	0.39
Nifuroxazide	315x+7339	0.9975	0.88	0.47	0.52
Norfloxacin	5061x+6760	0.9991	0.75	0.34	0.81
Orbifloxacin	12979X+10133	0.9957	0.78	0.62	0.82
Oxacillin isomer 1	279x-4700	0.9945	5.26	3.52	5.75
Oxacillin aisomer 2	6466x+69139	0.996	1.17	0.42	0.61
Oxolinic acid	5083x+50250	0.9964	0.51	0.43	0.51
Oxybendazole	32796x+62518	0.999	0.60	0.37	0.71
Oxytetracycline	2393x+142332	0.9921	0.79	0.71	0.82
Penicillin G (mix isom.)	1846x+23826	0.9947	0.78	0.42	0.80
Penicillin V isomer1	2331x-9907	1	0.95	0.62	0.91
Penicillin V isomer2	2882x-14959	0.9998	0.81	0.40	0.75
Pentylene tetrazole	-	-	-	-	-
Phenylbutazone	4230x+75838	0.9969	0.70	0.42	0.31
Pravastatin	2113x+22035	0.9915	0.53	0.25	0.60
Prednisolone	1887x+11242	0.9991	0.67	0.33	0.83
Promethazine	23359x+110584	0.9948	0.66	0.56	0.20
Propranolol	34367x+108269	0.9977	0.86	0.52	0.87
Ranitidine	8111x+161888	0.9985	0.98	0.98	0.80
Robenidine	9193x+76036	0.9985	0.84	0.61	0.86
Ronidazole	1700x+5642	0.9989	0.80	0.67	0.77
Roxithromycin	18679x+24349	0.9984	0.51	0.45	0.71
Salbutamol	9660x+129771	0.9996	0.97	0.96	0.91
Sarafloxacin	10602x-142884	0.9992	0.57	0.40	0.69
Spiramycin	4446x+20914	0.9992	0.68	0.45	0.85
Sulfabenzamide	1374x-783	1.000	0.91	0.30	0.80
Sulfacetamide	1271x+11583	0.9977	0.78	0.89	0.79
Sulfachloropyridazine	1876x-12722	0.999	0.78	0.23	0.58
Sulfadiazine	2282x-21048	0.9984	0.94	0.86	0.69
Sulfadimethoxyn	8571x+96905	0.9979	0.96	0.61	0.97
Sulfadoxine	5510x+92162	0.9963	0.83	0.63	0.80
Sulfaguanidine	1982x-24354	0.9987	0.39	0.30	0.12
Sulfamerazine	4445x+186458	0.9934	1.17	1.00	0.99
Sulfameter	3648x+137526	0.9916	0.92	0.73	0.97
Sulfamethazine	6784x+20329	0.9988	0.87	0.68	0.77
Sulfamethizole	2436x-9080	0.9999	0.69	0.64	0.86
Sulfamethoxazole	4266x+2230	0.9999	0.83	0.43	0.73
Sulfamethoxy pyridazine	6118x+56484	0.9915	0.69	0.61	0.84
Sulfamonomethoxine	5095x+18666	0.9998	0.70	0.68	0.90
Sulfanilamide	581x-10134	0.9977	0.43	0.30	0.33

Sulfapyridine	4636x-55723	0.9990	0.71	0.84	1.05
Sulfathiazole	2134x-35032	0.9973	0.82	0.78	0.75
Sulfisoxazol	4446x+20914	0.9992	0.68	0.45	0.85
Sulindac	4642x+28261	0.9922	0.62	0.40	0.67
Streptomycin	-	-	-	-	-
Tetracycline	5828X+6575	0.9972	0.63	0.56	0.62
Theobromine	1977x-20619	0.9993	0.79	0.91	0.41
Theophylline	2434x-9891	0.9998	0.89	0.79	0.59
Thiamphenicol	1016x+14997	0.9916	0.91	0.51	0.91
Tilmicosin	3286x-104308	0.995	0.96	0.52	0.88
Tolfenamic acid	2299x+50673	0.9976	0.69	0.53	0.92
Tolmetin	3055x+11913	0.9997	0.74	0.21	0.83
Trimethoprim	23853x+79912	0.9973	0.66	0.74	0.70
Tylosin	12965x+106850	0.9972	0.51	0.56	0.40
Food Packaging contaminants					
1,3-Phenylenediamine	4722x-112386	0.9973	0.22	0.21	0.20
1,6-Phenylenediamine	783x-21714	1	0.12	-	0.32
2-Ethylhexyl diphenyl phosphate	10034x+68634	0.9984	0.78	0.78	0.81
2-Methoxy-5-methylalanine	51118x-7117	0.9995	1.00	0.80	0.85
2,4-Diaminoanisoole	572x+42792	0.9898	0.59	0.59	0.29
2,4-Diaminotoluene	1322x+13999	0.9967	1.07	0.81	-
2,4-Dimethylaniline	31714x-140108	0.9961	0.70	0.72	0.79
2,4,5-Trimethylaniline	-	-	-	-	-
2,6-Diaminotoluene	6451x-149132	0.9989	0.27	0.10	0.17
4-Aminobiphenyl	63763x-2936	0.9962	0.46	0.34	0.88
4-Chloroaniline	10271x-48663	0.9998	0.93	0.69	0.67
4-Hexylresorcinol	349x-8292	0.9998	0.71	-	0.83
Aniline	47375x+251178	0.9904	0.30	0.40	0.81
Benzyl butyl phthalate	569x-18613	0.9987	0.91	0.75	0.64
Bisphenol A	-	-	-	-	-
¹ BA 2,3-DHP GE	512x-16262	0.9966	0.58	-	0.80
¹ BA (3-Cl,2-HP) (2,3-DHP)E	249x+4296	0.9994	0.69	0.27	0.88
¹ BA (3-Cl,2-HP) GE	267x+6623	0.998	0.28	0.15	1.16
¹ BAB (2,3-DHP) E	1445x-59092	0.9945	0.60	0.07	0.89
Bisphenol A diglycidyl ether	260x-4997	0.9992	0.80	0.64	0.59
Butyl p-hydroxybenzoate	598x+16027	0.9986	0.80	0.57	0.84
Di (2-ethylhexil)adipate	-	-	-	-	-
Dibutyl secabate	1984x+24314	0.9942	0.95	0.71	0.96
Dicyclohexyl phthalate	1648x+19954	0.9989	0.93	0.85	0.98
Diethyl phthalate	1167x+34117	0.9983	0.82	0.17	0.58
Diisodecyl phthalate	-	-	-	-	-
Diisononyl phthalate	730x+71198	0.9984	0.75	0.56	0.86
Dimethyl phthalate	4663x+32760	0.9994	0.60	0.28	0.55
Di N-butyl phthalate	71x+32901	0.989	0.90	0.59	0.86
Di N-octyl phthalate	1124x+12493	0.9806	0.73	0.48	0.33
Dipropyl phthalate	109x+6099	0.9922	0.78	0.51	0.85
Ethyl 4-hydroxybenzoate	373x-8344	0.9991	0.61	0.30	0.96
Melamine	2021x+207308	0.9898	0.12	0.07	0.17
Methyl paraben	168x-13374	0.9954	0.45	0.15	0.88
N,N-diethylhydroxylamine	106x-5208	0.9924	0.30	0.28	0.24

Nordihydroguaiaretic acid	-	-	-	-	-
o-Anisidine	41638x+53134	0.9989	1.07	0.72	0.84
o-Toluidine	53050x+20111	0.9989	0.55	0.73	0.88
Propyl 4-hydroxybenzoate	544x+10329	0.999	0.70	0.59	0.86
Tributyl-o-acetylcitrate	3961x+91319	0.9957	0.90	0.70	0.90
Tributyl phosphate	7925x+428759	0.9983	1.21	0.99	0.64
Triethyl phosphate	6107x+2716	0.9993	0.86	0.44	0.77
Mycotoxins					
3-Acetyl deoxynivalenol	144x-1741	0.9992	0.42	-	0.46
Aflatoxin B1	3113x+46773	0.9974	0.66	0.39	0.77
Aflatoxin B2	5103x+119591	0.9977	0.91	0.32	0.77
Aflatoxin G1	4675x-5550	0.9979	0.91	0.19	0.98
Aflatoxin G2	5490x+23627	0.9984	0.94	0.53	0.91
Aflatoxin M1	3938x-4790	0.9996	0.87	0.35	1.18
Alfa zearalenol	640x-10829	0.9967	0.60	0.18	0.70
Citrinin	-	-	-	-	-
Cyclopiazonic acid	3165x-90756	0.9965	0.31	0.05	0.67
Deoxynivalenol	312x-5048	0.9919	0.75	0.49	1.19
Diacetoxyscirpenol	272x-5501	0.9938	0.80	0.27	0.91
Ergocornine isomer 1	18094x-26699	0.9965	0.73	0.59	0.65
Ergocornine isomer 2	3546x-89996	0.9967	0.78	0.44	0.88
Fumonisin B1	58184x-96822	0.9995	0.93	0.32	0.83
Fumonisin B2	-	-	-	-	-
Glitoxin F1	508x-4880	0.9956	0.72	0.14	0.75
HT-2 toxin	475x-14057	0.9924	0.12	0.08	0.50
Ochratoxin A	2937x-55884	0.9946	0.90	0.04*	0.96
Patulin	71x-168	0.9999	0.68	-	0.48
Sterigmatocystin	16867x-1841	0.9999	1.01	0.36	0.73
T2-Toxin	905x+11013	0.9983	0.57	-	0.83
Zearalenone	993x-21054	0.9960	0.64	0.03	0.83
Perfluorinated compounds					
Pentafluoropropionic acid	1675x+23654	0.9987	1.33	1.30	1.23
Perfluorobutyric acid	2917x-58916	0.9906	1.27	1.15	0.91
Perfluoropentanoic acid	2848x+9270	0.9999	1.22	0.96	1.21
Perfluoroheptanoic acid	20778x+37478	0.9991	1.12	0.97	1.05
Perfluorooctanoic acid	1329x+15133	0.9997	0.78	0.70	0.66
Perfluorononanoic acid	53415x+44747	0.9984	0.60	0.34	0.52
Perfluorodecanoic acid	94384x-3533	1	0.26	0.22	0.23
Perfluoroundecanoic acid	82328x+89188	0.9977	0.21	0.15	0.41
Perfluorododecanoic acid	122835x+362680	0.9919	0.16	0.28	0.39
Heptadecafluoro-octane sulfonic acid	116468x+91192	0.999	0.40	0.39	0.28
Nitrosamines					
N-nitrosodiethylamine	51x+436	0.9997	1.16	1.04	0.80
N-nitrosodimethylamine	44x-394	0.9953	0.73	0.70	0.59
N-nitrosodi-n-dibutylamine	2562x-31309	0.9956	0.74	0.34	0.68
N-nitrosomethylethylamine	43x-1999	0.9992	0.65	0.72	0.74
N-nitrosomorpholine	1401x+29838	0.999	0.63	0.60	0.52
N-nitroso-n-diphenylamine	512x-7678	0.9966	0.36	0.19	0.41

N-nitrosopiperidine	1384x+6753	0.9997	0.75	0.50	0.67
N-nitrosopyrrolidine	4982x+153317	0.9983	0.85	0.80	0.60
N-nitrosodi-n-dipropylamine	134x-3348	0.9972	0.66	0.85	0.78
N-nitrosodiethylamine	51x+436	0.9997	1.16	1.04	0.80
Sweeteners					
Aspartame	1280x+21748	0.9969	0.93	0.49	1.24
Acesulfame-K	816x+7531	0.9999	1.96	2.35	1.90
Saccharin	4464x-21786	0.9996	1.05	1.13	1.00
Sucralose	462x+9301	0.9979	0.85	0.52	0.89
Cyclamate	7584x-132661	0.9975	0.75	0.97	0.99
Aspartame	1280x+21748	0.9969	0.93	0.49	1.24

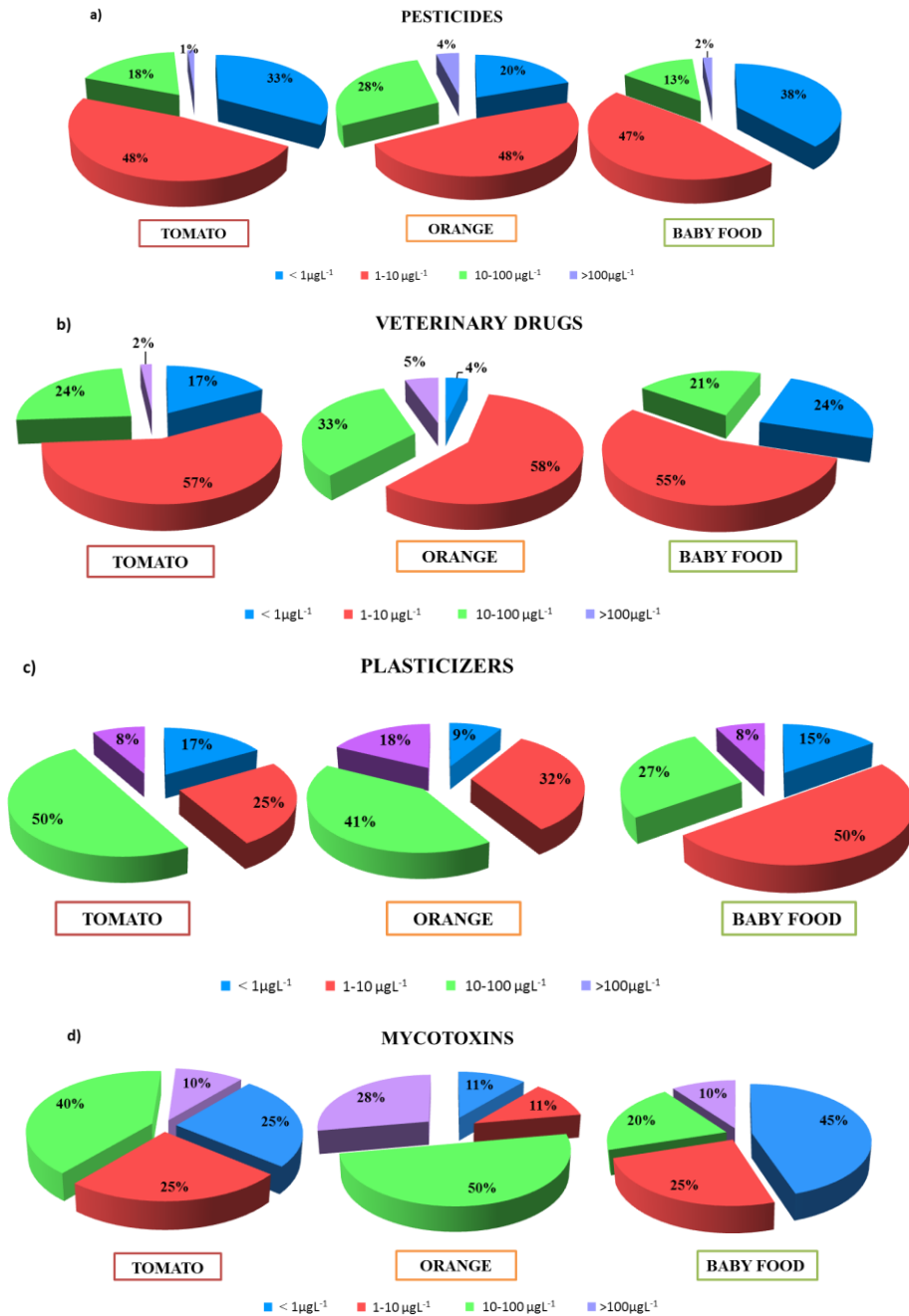


Figure S1. Percentage of a) pesticides; b) veterinary drugs; c) plasticizers; d) mycotoxins; e) nitrosamines; f) perfluorinated compounds; g) sweeteners, according to their limits of quantification (LOQs) in tomato, orange and baby food.

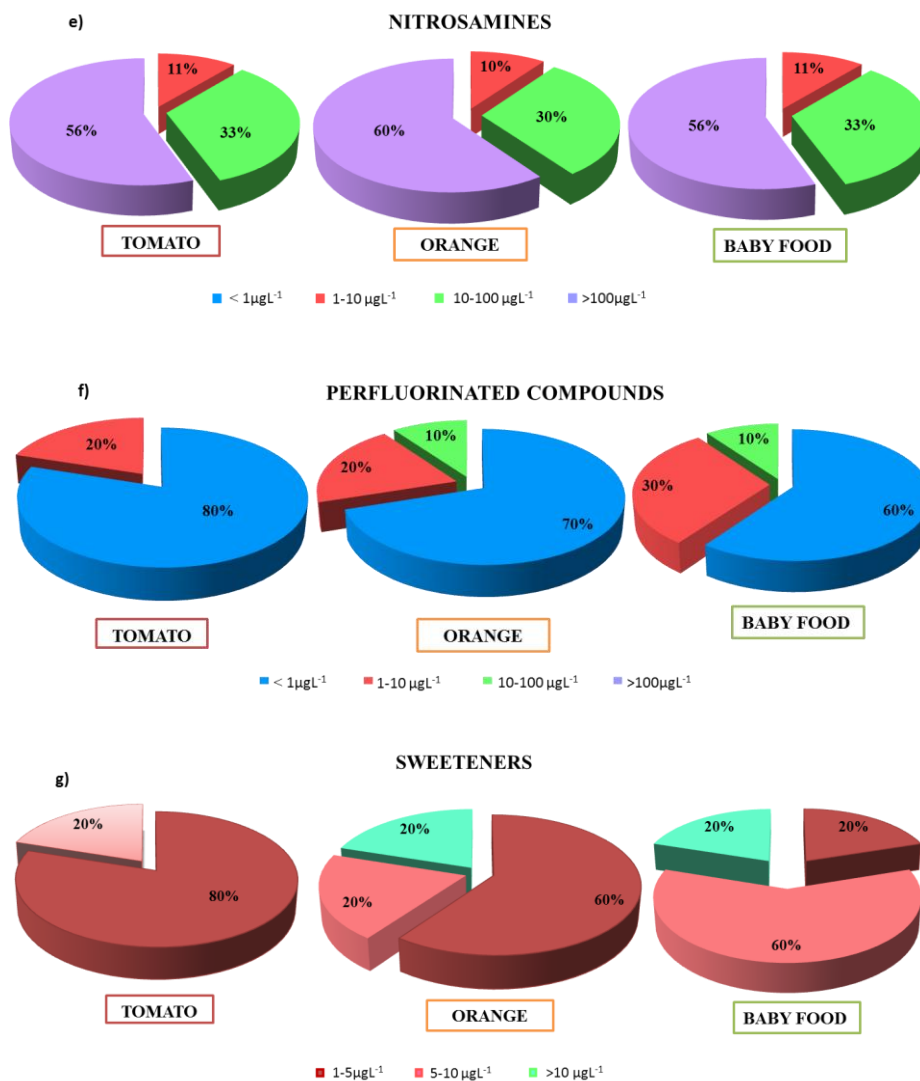


Figure S1 (cont). Percentage of a) pesticides; b) veterinary drugs; c) plasticizers; d) mycotoxins; e) nitrosamines; f) perfluorinated compounds; g) sweeteners, according to their limits of quantification (LOQs) in tomato, orange and baby food.

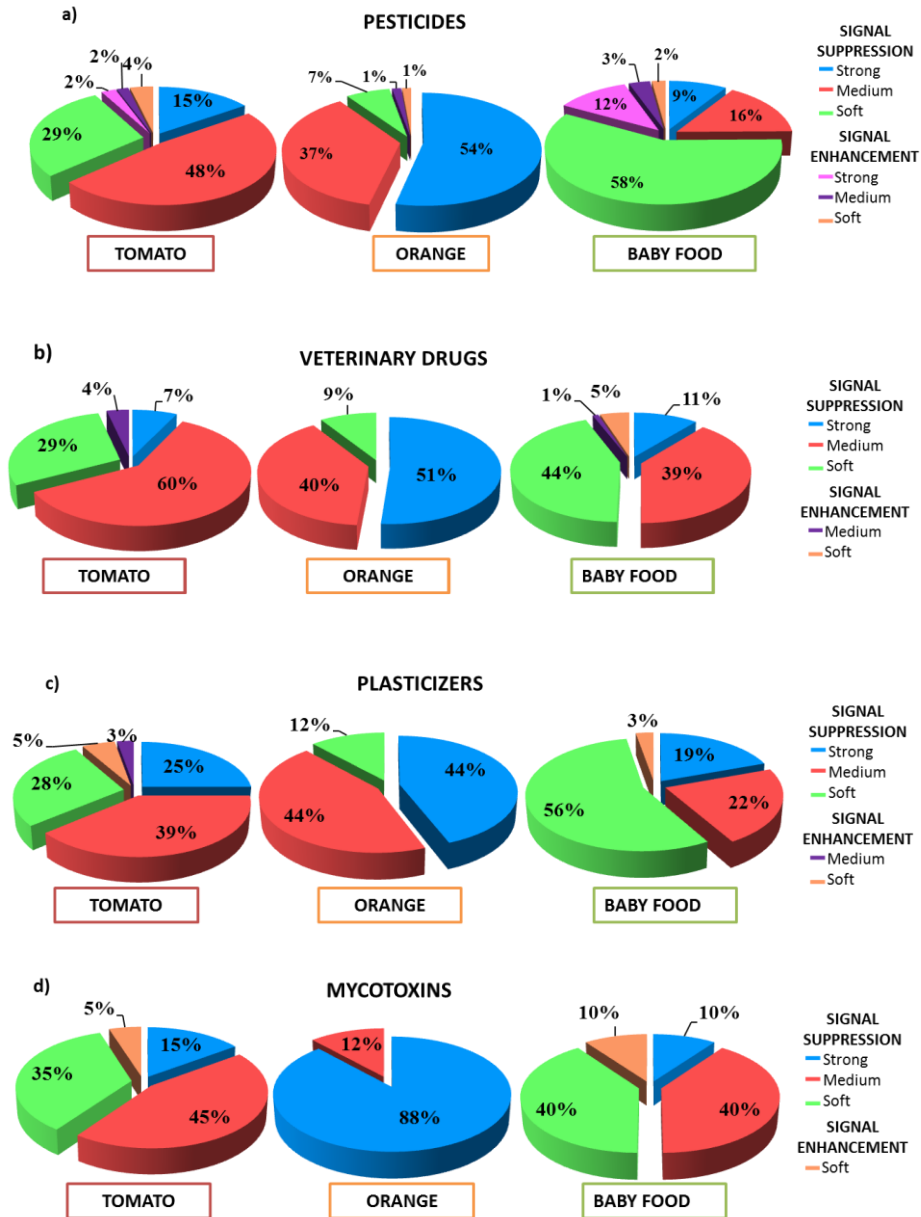


Figure S2. Percentages of a) pesticides; b) veterinary drugs; c) plasticizers; d) mycotoxins; e) nitrosamines; f) perfluorinated compounds; g) sweeteners, according to signal suppression or enhancement (soft, medium or strong) in tomato, orange and baby food extracts.

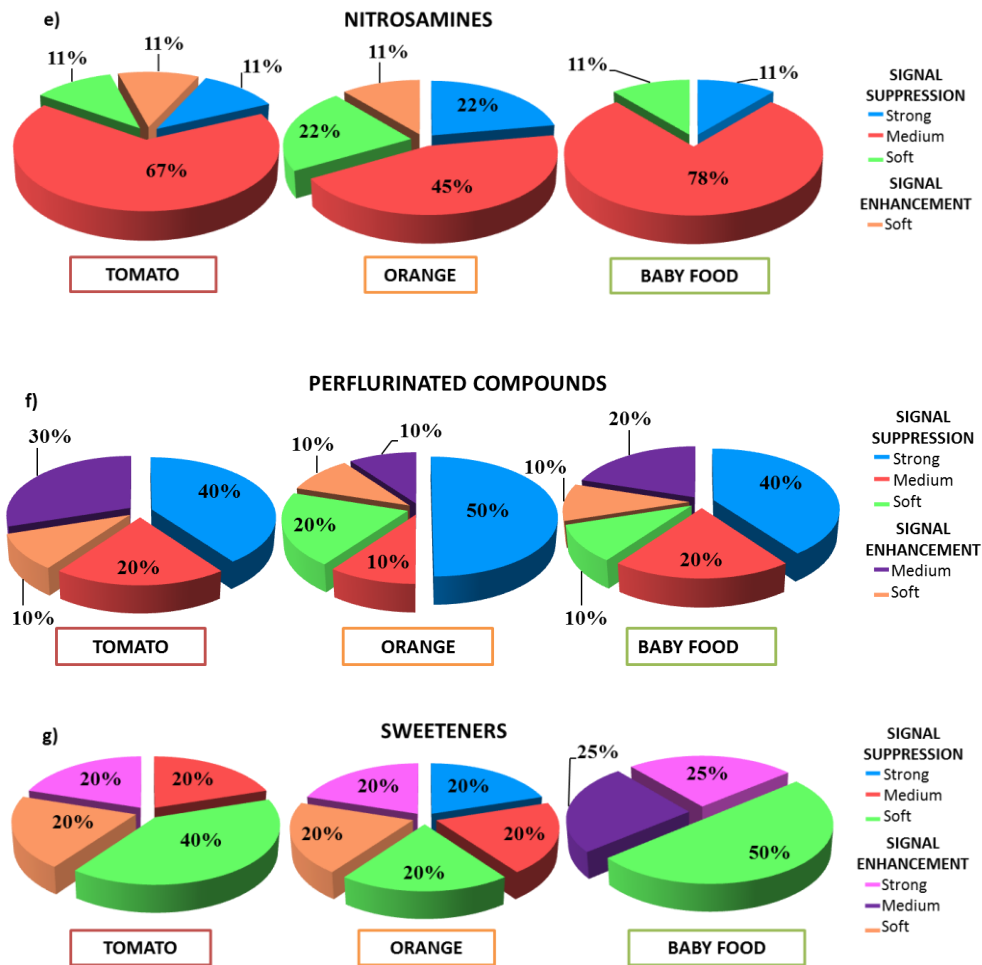


Figure S2 (cont). Percentages of a) pesticides; b) veterinary drugs; c) plasticizers; d) mycotoxins; e) nitrosamines; f) perfluorinated compounds; g) sweeteners, according to signal suppression or enhancement (soft, medium or strong) in tomato, orange and baby food extracts.

III.3.MÉTODO GENÉRICO DE TRATAMIENTO DE MUESTRA PARA LA DETERMINACIÓN SIMULTÁNEA DE PESTICIDAS Y MICOTOXINAS EN VINO MEDIANTE CROMATOGRAFÍA DE LÍQUIDOS-ESPECTROMETRÍA DE MASAS.

III.3. Método genérico de tratamiento de muestra para la determinación simultánea de pesticidas y micotoxinas en vino mediante cromatografía de líquidos-espectrometría de masas

III.3.1. Resumen

Dos clases importantes de contaminantes orgánicos que pueden encontrarse en muestras de vino son pesticidas y micotoxinas. Aunque existen estrictas normativas y controles exhaustivos de este tipo de compuestos en frutas, vegetales y aguas de consumo, se ha prestado poca atención a su contenido en productos derivados que se consumen habitualmente y que podrían contenerlos. En la UE sólo el contenido de una de las micotoxinas, en concreto la ochratoxina A, está regulado en vino. A pesar de la inexistencia de normativas que regulen su contenido, en la UE existe un amplio interés por la determinación de pesticidas y micotoxinas en vino debido a que es su principal productor y consumidor a nivel mundial. Por este motivo, técnicas analíticas como la cromatografía de líquidos y cromatografía de gases acopladas a espectrometría de masas han sido empleadas para la identificación de estos tóxicos en este tipo de muestras. Sin embargo, estas técnicas han sido mayoritariamente aplicadas para la determinación de un tipo u otro de contaminantes, pero no de forma simultánea. Hasta la fecha solo se conoce el desarrollo de 3 métodos que permitan su determinación simultánea y únicamente uno de ellos fue aplicado a vino.

En este capítulo se describe el desarrollo de un tratamiento de muestra genérico para la determinación simultánea de 60 pesticidas y 9 micotoxinas en vino tinto, basado en la aplicación de la cromatografía líquida-espectrometría de masas con analizador de tiempo de vuelo (LC-TOFMS). Los extractos de vino a los que se aplicó esta metodología fueron obtenidos mediante SPE empleando cartuchos de tipo polimérico. Para la selección del

cartucho apropiado se evaluó el efecto matriz para los compuestos del estudio empleando dos tipos de cartuchos diferentes (Oasis HLB® y Plexa®). En ambos casos se empleó como eluyente metanol y se trabajó con un factor de preconcentración 4:1. Una vez obtenidos los extractos, los compuestos de este estudio fueron identificados mediante LC-TOFMS, teniendo en cuenta tiempos de retención y valores de masa exacta. Una vez se comprobó que los cartuchos Oasis HLB® eran los que producían un menor efecto matriz para estos compuestos, se realizaron estudios de recuperación a dos niveles de concentración (2.5 y 25 $\mu\text{g L}^{-1}$), obteniéndose valores entre 70 y 120% para el 90% de los compuestos estudiados. Posteriormente, el método fue aplicado a 24 muestras de vino tinto procedentes de diferentes regiones de España. Los compuestos que se detectaron en la mayoría de las muestras fueron metalaxyl y Aflatoxina B₂.

III.3.2. Artículo

Abstract

In this work, a generic sample treatment method for simultaneous determination of multiclass pesticides and mycotoxins in wines is presented. The proposed method is based on solid-phase extraction (SPE) using polymeric-type SPE cartridges. To evaluate the proposed sample treatment, a liquid chromatography electrospray time-of-flight mass spectrometry method was used for testing 60 selected representative multiclass pesticides and 9 mycotoxins. Two different polymeric sorbents were evaluated, with hydrophilic-lipophilic-balanced (HLB) polymer cartridges being selected (OasisTM HLB) as the most suitable for the present study. The identification and confirmation of the compounds was based on retention time and accurate mass measurements of the protonated molecules ($[M+H]^+$). Limits of detection were below $1 \mu\text{g L}^{-1}$ for the 87% of the studied compounds. With the selected 4:1 preconcentration factor, 70% of the target compounds showed relatively low matrix effects, corresponding to signal suppressions lower than 30%. Recovery studies ($n = 10$) were carried out at two concentration levels, $2.5 \mu\text{g L}^{-1}$ and $25 \mu\text{g L}^{-1}$, obtaining mean recovery rates between 70 and 120% for the 90% of studied analytes. The relative standard deviation (RSD%) values of the entire procedure were below 15% in most cases (97% of the studied analytes). The proposed method was successfully applied to 24 red wine samples produced in different regions of Spain. The concentration levels of the target compounds found in the studied samples were in compliance with the current regulations. Aflatoxin B₂ and metalaxyl were the most detected compounds (75% and 50% of the studied samples, respectively).

Keywords: wine; pesticides; mycotoxins; food; sample treatment; liquid chromatography; mass spectrometry; electrospray; solid-phase extraction.

Introduction.

Europe is the main producer of wine in the world, with an estimated production in 2010 of 66.5% of the wine produced worldwide, being Italy, France and Spain the largest producing countries [1]. Europe is also leading the consumption of wine in the world, partly fostered for the health benefits associated to a moderate consumption of wine [2]. On the other hand, the increasing public concern about the potential health risks posed by the presence of toxic residues in the human diet has focused all sights on food quality and safety. The two important classes of toxic organics that could be present in wine are mycotoxins and pesticides. Mycotoxins are secondary metabolites produced by several hundreds of fungi that grow in food under particular circumstances [3]. Within this group of compounds, only the content of ochratoxin A in wine samples is regulated in the EU, establishing a maximum permitted limit of $2 \mu\text{g kg}^{-1}$ to those wines produced from 2005 harvest onwards [4]. In Spain, there is also an established generic maximum limit of $5 \mu\text{g kg}^{-1}$ for aflatoxin B₁ and a limit of $10 \mu\text{g kg}^{-1}$ for the sum of aflatoxins B₁, B₂, G₁ and G₂ in foodstuffs destined to human consumption [5].

Although there are extensive regulations for pesticide residues in fruits, vegetables, or drinking water, scarce attention is still devoted to derivate products -which may contain these commodities as an ingredient- such as wine. Despite the limited availability of specific regulation for pesticides in wine, several analytical methodologies have been reported, based on gas chromatography-mass spectrometry (GC-MS) and liquid chromatography-mass spectrometry (LC-MS). GC-MS (/MS) with quadrupole filters have been the most used [6-12], although time-of-flight mass spectrometers have been

also used in the last years [13, 14]. LC-MS(/MS) analyses of pesticides in wine have been usually performed by means of triple quadrupole analyzers operated in multiple reaction monitoring (MRM) mode [15-17], although the use of high resolution LC-MS instrumentation has been reported recently [17,18]. The development of analytical methods for testing mycotoxins in wine has been mainly focused in the determination of ochratoxin A (OTA). Liquid chromatography with fluorescence detection [20-22] and LC-MS/MS [23-25] have been the preferred techniques for the determination of OTA in wines. To date, only three multi-residue methods for the simultaneous determination of pesticides and mycotoxins in vegetable matrices have been described [26-28], although only one of has been validated in wine [28].

The sample preparation for multi-residue pesticide testing in wines has been recently reviewed by Pang et al. [29]. The need of generic, universal extraction methods covering a wide range of targeted organic contaminants of different physicochemical properties is totally confronted with dedicated cleanup step stages biased to a specific class of contaminants. Several methodologies have been proposed for pesticide extraction in wines. Amongst them: (a) liquid-liquid extraction without further purification steps [9,28] or combined with a clean-up step generally based on sorbent-based strategies such as solid-phase extraction (SPE) [28,30,31], (b) solid-phase extraction using many different type of cartridges [6,32], (c) solid-phase microextraction [10], (d) stir bar sorptive extraction [33], (e) sorptive extraction with disposable silicon discs [19], (f) matrix solid-phase dispersion [34], (g) membrane assisted solvent extraction [33] and (h) hollow-fiber liquid-phase microextraction [15,25]. In contrast, only three methods have been described for simultaneous extraction of pesticides and mycotoxins from vegetable matrices [26-28].

Solid-phase extraction (SPE) is a convenient sample preparation technique, which permits in a single step a preconcentration step, a separation from the bulk matrix, and extract cleanup [35]. It can be easily automated and the extracts obtained are clean enough for further LC-MS analyses. SPE has been used combined with either GC-MS or LC-MS for pesticide testing using C₁₈, polymer type and mixed-mode anion exchange SPE cartridges [6,7,17,18,32]. In SPE, specific analyte-sorbent interactions usually yield cleaner extracts, enhanced preconcentration factors and minor matrix effects. This performance is achieved at the expense of limiting multi-analyte capability, since the applicability of the method is biased towards a specific class of analytes/species. Polymer-based SPE sorbents are suitable for multi-residue analysis involving compounds of a wide range of physicochemical properties, and have been satisfactorily tested for pesticide residue analysis in wine [6,7,17]. Thanks to the use of highly selective and sensitive mass spectrometry instrumentation, the tendency in food safety testing, moves towards the development of methods with minor cleanup stages, covering as many compounds as possible in a single sample preparation stage and LC-MS run [26,27,35]. In this article, a generic sample treatment approach is proposed for the simultaneous testing of multiclass pesticides and mycotoxins in wines. The developed method uses a single SPE step with polymeric cartridges. Several representative multiclass pesticides and relevant mycotoxins were included in the study (60 representative multi-class pesticides and 9 mycotoxins). Two different SPE sorbents were assayed and the recovery rates and matrix effects carefully evaluated using liquid chromatography time-of-flight mass spectrometry (LC-TOFMS). To our knowledge, this is the first generic method for large-scale testing of multiclass pesticides and mycotoxins in beverages using SPE. The proposed method was applied to the analysis of 24 market-purchased red wine samples produced in different regions of Spain.

Experimental section

Chemicals and materials. Pesticide and mycotoxin analytical standards were purchased from Fluka, Pestanal® quality (Madrid, Spain) and Sigma-Aldrich (Madrid, Spain). Individual stock solutions of the studied compounds (ca. 500 µg mL⁻¹ each) were prepared in methanol or acetonitrile and stored at -20°C. HPLC-grade acetonitrile and methanol were obtained from Merck (Darmstadt, Germany). Formic acid was obtained from Fluka (Buchs, Switzerland). A Milli-Q-Plus ultra-pure water system from Millipore (Milford, MA, USA) was used throughout the study to obtain the HPLC-grade water used during the analyses. Oasis HLB™ SPE cartridges (200 mg, 6 mL) purchased from Waters (Milford, MA, USA) and Bond Elut™ Plexa SPE cartridges (200 mg, 6 mL) were obtained from Agilent Technologies (Madrid, Spain). A Supelco Visiprep™ (Bellefonte, PA, USA) SPE vacuum system was also used.

Sample treatment. The pesticides and mycotoxins were extracted using solid phase extraction with two polymer based SPE cartridges, namely Oasis HLB and Bond Elut Plexa. The cartridges were preconditioned with 4 mL of MeOH and 4 mL of ultrapure water at a flow rate of 2 mL min⁻¹. After the conditioning step, an aliquot of 4 mL of wine were passed through the cartridge at a flow rate of 1 mL min⁻¹. Then the cartridge was washed with 4 mL a mixture of MeOH/H₂O (5:95, v/v) and subsequently dried by vacuum during 1 min. The retained analytes were eluted with 2 x 4 mL of MeOH at 1 mL min⁻¹. This eluate was then evaporated until near dryness by a gentle nitrogen stream using a TurboVap LV from Zymark (Hopkinton, MA), with a water bath temperature of 37 °C and a N₂ pressure of 15 psi. The samples were then made up with 200 µL of MeOH and 800 µL of milli Q water (final preconcentration factor 4:1). Then this extract was filtered through a 0.45 µm PTFE filter (Millex FG, Millipore, Milford, MA, USA). For validation and

quantification purposes, matrix-matched standards were prepared by spiking the filtered (final) extracts with appropriate volume of working standard solutions of the studied analytes.

LC-Electrospray Time-of-Flight Mass Spectrometry. The separation of the species from the SPE extracts was carried out in a reversed phase C₁₈ analytical column of 50 mm x 4.6 mm and 1.8 μm particle size (Zorbax Rapid Resolution Eclipse XDB-C18) by means of an Agilent HPLC system (Agilent 1290 Infinity, Agilent Technologies, Santa Clara, CA, USA), consisting of vacuum degasser, auto-sampler and a binary pump. 20 μL of extract were injected in each study. Mobile phases A and B were water with 0.1% formic acid and acetonitrile respectively. The chromatographic method held the initial mobile phase composition (10% B) constant for 2 min. Then the content of B was increased up to 50% at 5 min, followed by a linear gradient to 100% B at 15 min and held constant for 3 min at 100% B. The flow-rate used was 0.5 mL min⁻¹.

The HPLC system was connected to a time-of-flight mass spectrometer Agilent TOF 6220 (Agilent Technologies, Santa Clara, CA, USA) equipped with an electrospray interface operating in positive ion mode, using the following operation parameters: capillary voltage: 4000 V; nebulizer pressure: 40 psig; drying gas: 9 L min⁻¹; gas temperature: 325 °C; fragmentor voltage (in-source CID fragmentation): 190 V. LC-MS accurate mass spectra were recorded across the range 50-1000 *m/z*. Accurate mass measurements of each peak from the total ion chromatograms were obtained by means of an automated calibrant delivery system using a dual-nebulizer electrospray source that introduces the flow from the outlet of the chromatograph together with a low flow of a calibrating solution (calibrant solution A, Agilent Technologies), which contains the internal reference masses (purine (C₅H₄N₄ at *m/z* 121.050873 and HP-921 [hexakis-(1H,1H,3H-tetrafluoropentoxy)-

phosphazene] ($C_{18}H_{18}O_6N_3P_3F_{24}$) at m/z 922.009798). Agilent MassHunter Data Acquisition software was used for method development and full-scan data acquisition. Agilent MassHunter Qualitative Analysis and Quantitative TOF Analysis software were used for data processing.

Results and discussion

Identification and quantification of multiclass pesticides and mycotoxins by LC-TOFMS. A total number of 69 analytes were selected in this study. Most of the pesticides included in this study were selected on the basis of their use in vine growing and published literature. From the 60 target pesticides, 26 were insecticides, 24 fungicides and 10 herbicides. Mycotoxins were selected on the basis of their previous finding in wine samples. Standard HPLC gradient conditions and electrospray ionization conditions were selected to achieve the best possible sensitivity and selectivity for the selected compounds. Default values were set for drying and nitrogen flow rates, vaporizer and drying temperatures considering the HPLC flow rate. Fragmentor voltage was studied in the range 160 – 250 V for in-source CID fragmentation, using a standard containing the mixture of compounds at a concentration level of $200 \mu\text{g L}^{-1}$. Finally fragmentor voltage was set at 190 V, as a compromise value between sensitivity for quantification and additional mass spectrum information for confirmation purposes.

The identification of the targeted species was performed by retention time matching (± 0.5 min of tolerance) combined with accurate mass measurements of the targeted protonated molecules and, when available, their main fragment ions (in-source CID fragmentation). The combination of these tools enables the unambiguous confirmation of the target compounds in the tested matrix, because of the typically high mass accuracy which permits accurate mass measurements of target ions within 2 ppm error in

most cases. Detailed results are showed in **Table 1**. Besides, some studied pesticides contain chlorine atoms (e.g. simazine, thiacloprid, penconazole), which offer an isotopic pattern that yields further information for the unambiguous identification of the target compounds. For quantitation purposes, extracted ion chromatograms (EICs) were used, setting a mass-window width of 20 ppm for the relative mass error tolerance. The protonated molecule ($[M+H]^+$) was used for quantitation purposes in all cases.

Table 1. Identification of the studied multiclass pesticides and mycotoxins tested by liquid chromatography electrospray time-of-flight mass spectrometry.

Compound	Elemental composition	RT (min)	Theoretical m/z	Experimental m/z	Error (ppm)
PESTICIDES					
Fungicides					
Azoxystrobin	C ₂₂ H ₁₇ N ₃ O ₅	8.50	404.1241	404.1241	0.00
Benalaxil	C ₂₀ H ₂₃ NO ₃	10.27	326.1751	326.1753	0.64
Bitertanol	C ₂₀ H ₂₃ N ₃ O ₂	9.10	338.1863	338.1865	0.59
Carbendazim	C ₉ H ₉ N ₃ O ₂	3.27	192.0768	192.0823	-1.56
Difenoconazole	C ₁₉ H ₁₇ Cl ₂ N ₃ O ₃	10.17	406.072	406.0710	-2.46
Dimethomorph (Z)	C ₂₁ H ₂₂ ClNO ₄	7.68	388.1310	388.1311	0.26
Dimethomorph (E)	C ₂₁ H ₂₂ ClNO ₄	7.45	388.1310	388.1311	0.26
Diniconazole	C ₁₅ H ₁₇ Cl ₂ N ₃ O	9.56	326.0822	326.0821	-0.31
Fenarimol	C ₁₇ H ₁₂ Cl ₂ N ₂ O	8.32	331.0399	331.0398	-0.30
Fenhexamid	C ₁₄ H ₁₇ Cl ₂ NO ₂	8.68	302.0709	302.0710	0.33
Flusilazole	C ₁₆ H ₁₅ F ₂ N ₃ Si	8.88	316.1076	316.1074	-0.63
Imazalil	C ₁₄ H ₁₄ Cl ₂ N ₂ O	5.86	297.0556	297.0550	-2.02
Iprodione	C ₁₃ H ₁₃ Cl ₂ N ₃ O ₃	11.03	330.0407	330.0402	-1.52
Isoprothiolane	C ₁₂ H ₁₈ O ₄ S ₂	9.49	291.072	291.0723	1.03
Kresoxim methyl	C ₁₈ H ₁₉ NO ₄	10.12	314.1387	314.1388	0.32
Metalaxyl	C ₁₅ H ₂₁ NO ₄	7.03	280.1543	280.1544	0.36
Myclobutanil	C ₁₅ H ₁₇ ClN ₄	8.44	289.1215	289.1210	-1.73
Procymidone	C ₁₃ H ₁₁ Cl ₂ NO ₂	9.56	284.0240	284.0242	0.70
Propiconazole	C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	9.64	342.0771	342.0775	1.17
Pyraclostrobin	C ₁₉ H ₁₈ N ₃ O ₄ Cl	10.82	388.1059	388.1059	0.00
Pyrimethanil	C ₁₂ H ₁₃ N ₃	6.95	200.1182	200.1181	-0.50

Tebuconazole	$C_{16}H_{22}ClN_3O$	8.82	308.1524	308.1525	0.32
Triadimefon	$C_{14}H_{16}ClN_3O_2$	8.70	294.1004	294.1002	-0.68
Triadimenol	$C_{14}H_{18}ClN_3O_2$	7.72	296.116	296.1167	2.36
Trifloxystrobin	$C_{20}H_{19}F_3N_2O_4$	11.49	409.137	409.1375	1.22
Herbicides					
Atrazine	$C_8H_{14}ClN_5$	7.03	216.1011	216.1010	-0.46
Buprofezine	$C_{16}H_{23}N_3OS$	10.36	306.1635	306.1639	1.31
Butachlor	$C_{17}H_{26}ClNO_2$	8.83	308.1417	308.1415	-0.65
Diuron	$C_5H_{11}Cl_2N_2O$	7.13	233.0243	233.0244	0.42
Fluometuron	$C_{10}H_{11}F_3N_2O$	6.85	233.0896	233.0899	1.29
Isoproturon	$C_{12}H_{18}N_2O$	7.03	207.1492	207.1494	0.97
Linuron	$C_9H_{10}Cl_2N_2O_2$	8.37	249.0192	249.0193	0.40
Metribuzin	$C_8H_{14}N_4OS$	6.52	215.0961	215.0962	0.46
Monuron	$C_9H_{11}ClN_2O$	6.17	199.0633	199.0637	2.01
Simazine	$C_7H_{12}ClN_5$	6.24	202.0854	202.0855	0.49
Insecticides					
Acetamiprid	$C_{10}H_{11}ClN_4$	5.45	223.0745	223.0742	-1.34
Carbofuran	$C_{12}H_{15}NO_3$	6.71	222.1124	222.1121	-1.35
Clothianidin	$C_6H_8ClN_5O_2S$	5.13	250.016	250.0159	-0.40
Dichlorvos	$C_4H_7Cl_2O_4P$	6.34	220.9532	220.9533	-0.45
Dimethoate	$C_5H_{12}NO_3PS_2$	5.40	230.0069	230.0068	-0.43
Etrimfos	$C_{10}H_{17}N_2O_4PS$	10.82	293.0719	293.0718	-0.34
Fenobucarb	$C_{12}H_{17}NO_2$	10.27	208.1332	208.1334	0.96
Fenthion	$C_{10}H_{15}O_3PS_2$	10.53	279.0273	279.0277	1.43
Imidacloprid	$C_9H_{10}ClN_5O_2$	5.23	256.0596	256.0596	0.00
Indoxacarb	$C_{22}H_{17}ClF_3N_3O_7$	11.29	528.078	528.0790	1.89
Malaoxon	$C_{10}H_{19}O_7PS$	6.47	315.0662	315.0661	-0.32
Malathion	$C_{10}H_{19}O_6PS_2$	8.32	331.0434	331.0434	0.00
Methiocarb	$C_{11}H_{15}NO_2S$	8.15	226.0896	226.0894	-0.88
Omethoate	$C_5H_{12}NO_4PS$	2.21	214.0298	214.0299	0.47
Paraoxon methyl	$C_8H_{10}NO_6P$	6.19	248.0319	248.0318	-0.40
Penconazole	$C_{13}H_{15}Cl_2N_3$	9.28	284.0716	284.0715	-0.35
Phosalone	$C_{12}H_{15}ClNO_4PS_2$	11.02	367.9941	367.9942	0.27
Phosphamidon	$C_{10}H_{19}ClNO_5P$	5.81	300.0762	300.0763	0.33
Pirimicarb	$C_{11}H_{18}N_4O_2$	4.59	239.1503	239.1505	0.84
Profenofos	$C_{11}H_{15}BrClO_3PS$	11.66	372.9424	372.9425	0.27
Quinalphos	$C_{12}H_{15}N_2O_3PS$	10.32	299.0614	299.0611	-1.00
Spinosyn A	$C_{41}H_{65}NO_{10}$	7.25	732.4681	732.4686	0.68
Spinosyn D	$C_{41}H_{65}NO_{10}$	7.74	746.4838	746.4840	0.27
Thiacloprid	$C_{10}H_9ClN_4S$	5.89	253.0309	253.0311	0.79

Thiamethoxam	$C_8H_{10}ClN_5O_3S$	4.77	292.0266	292.0264	-0.68
Triazophos	$C_{12}H_{16}N_3O_3PS$	9.41	314.0723	314.0726	0.96
Mycotoxins					
Aflatoxin B ₁	$C_{17}H_{12}O_6$	6.24	313.0707	313.0710	0.10
Aflatoxin B ₂	$C_{17}H_{14}O_6$	6.01	315.0863	315.0865	0.06
Aflatoxin G ₁	$C_{17}H_{12}O_7$	9.56	329.0656	329.0655	-0.03
Aflatoxin G ₂	$C_{17}H_{14}O_7$	5.82	331.0811	331.0812	0.30
Aflatoxin M ₁	$C_{17}H_{12}O_7$	6.03	329.0656	329.0656	0.00
Ergocornine	$C_{31}H_{39}N_5O_5$	5.41	562.3024	562.3021	-0.05
Fumonisin B ₁	$C_{34}H_{59}NO_{15}$	7.27	722.3958	722.3955	-0.04
Ochratoxin A	$C_{20}H_{18}ClNO_6$	8.02	404.0895	404.0893	-0.49

Optimization and performance of sample treatment. When dealing with multi-residue methods the use of SPE cartridges enabling simultaneously various types of interactions (hydrophilic and lipophilic) is usually more suitable than a specific SPE cartridge relying on a single mechanism [35,36]. In the case of pesticide testing, this is particularly important considering the wide array of species with different physicochemical properties. The target list of pesticides included in the method comprised species with different physicochemical properties and a wide variety of polarities. Therefore, polymer-based sorbents are the choice for this type of solid-phase extraction method [36]. In order to optimize the SPE procedure, two polymer-based SPE cartridges were evaluated. The selection of the cartridge was made on the basis of matrix effects (signal suppression), considered as a valid marker of cleanliness of SPE extracts. Matrix effects were studied by calculating slope ratios matrix/solvent. The use of Oasis HLB cartridges led to minor matrix effects (closer values to 1) for 75% of studied analytes. Moreover, correlation coefficients corresponding to matrix-matched calibration curves were closer to 1 using the extract obtained by Oasis HLB cartridges. Matrix effects obtained by the two tested SPE cartridges are compared for 30 selected

analytes in **Figure 1**. Finally, Oasis HLB cartridges were selected for further studies.

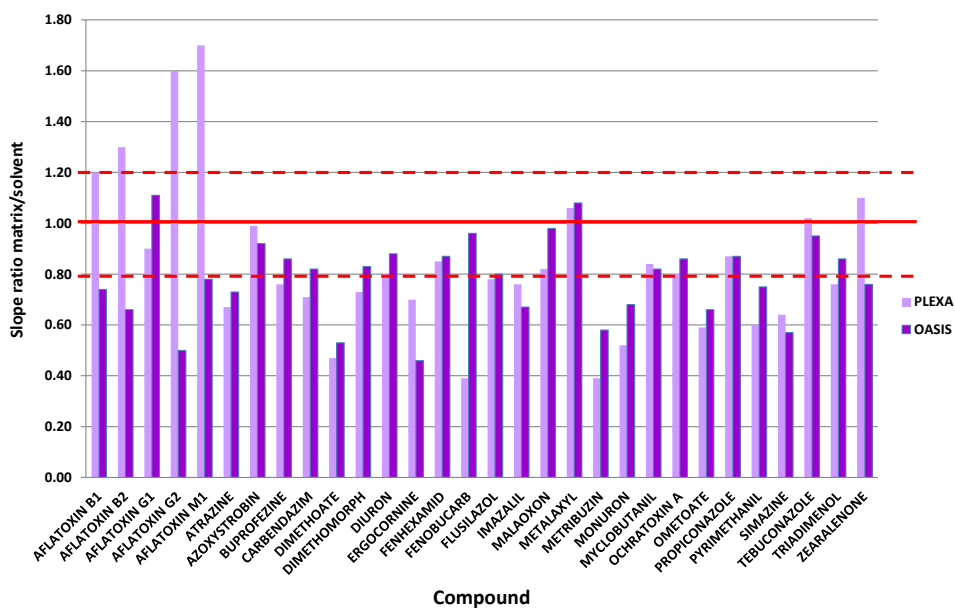


Figure 1. Results of the matrix effects obtained for 30 of the studied compounds using two types of SPE polymer-based cartridges evaluated. Dark bars correspond to Oasis HLB assay and bright bars correspond to Bond Elut Plexa SPE assay.

With regards to the sample volume loaded on the cartridges and the subsequent preconcentration factor implemented in the SPE procedure, we found that factors of 20:1 or higher involved complex extracts that yielded signal/sensitivity losses and soiled the MS inlet, making necessary a dedicated and daily cleaning and maintenance of the source. In addition, when using these relatively large preconcentration factors, matrix effects were remarkable (over 50 % suppression in some of the studied analytes). In contrast, the use of preconcentration factors of 10:1 (or lower) did not affect strongly the sensitivity and signal stability of the MS source, over large periods of operation. A preconcentration factor of 4:1 was found as appropriate, since it provides relatively clean extracts, compatible with LC-MS injection without any issue with instrument maintenance or quantitative

performance/matrix effects. Depending on the sensitivity of the instrument used for final determination this parameter can be adjusted to meet a required performance in terms of limits of detection.

The obtained extracts were analyzed with the developed LC-MS method, obtaining mean recoveries between 70 and 120% for the 90% of studied analytes at both concentration levels tested. The relative standard deviation (RSD%) values were below 15% in most cases (97% of the studied analytes), as shown in **Table 2**. These results evidences the suitability of the proposed method for multiclass testing of contaminants with different physicochemical properties such as those included in the present study. Since most of the compounds tested are representative of different classes, the method could cover a distinctly higher number of targeted species.

Table 2. Analytical parameters of the proposed method: linearity (R^2), limits of detection and quantification, recoveries and matrix effects.

Compound	LOD (μgL^{-1})	LOQ (μgL^{-1})	Average Recovery ^a (%)	RSD (%)	Regression coefficient (r^2)	Matrix effects
PESTICIDES						
Fungicides						
Azoxystrobin	0.04	0.13	91.97	1.68	0.9997	0.92
Benalaxil	0.43	1.42	93.15	3.49	0.9986	0.98
Bitertanol	1.14	3.79	78.31	14.24	0.9974	0.85
Carbendazim	0.43	1.45	90.76	2.76	0.9992	0.82
Difenoconazole	0.04	0.14	65.20	9.95	0.9972	0.72
Dimethomorph	0.13	0.43	89.91	2.95	0.9986	0.83
Diniconazole	0.18	0.60	87.52	2.64	0.9980	0.86
Fenarimol	0.13	0.45	88.44	2.91	0.9981	0.82
Fenhexamide	1.17	3.91	89.96	2.78	0.9995	0.87
Flusilazole	0.11	0.38	86.16	3.86	0.9921	0.80
Imazalil	0.09	0.30	93.40	1.55	0.9981	0.67
Iprodione	1.90	6.35	78.39	7.49	0.9970	0.72
Isoprothiolane	1.38	4.61	92.98	3.21	0.9987	0.80

Kresoxim methyl	2.60	8.68	89.48	4.08	0.9983	0.85
Metalaxyl	0.09	0.30	85.90	8.55	0.9994	1.08
Myclobutanil	0.08	0.25	90.72	1.69	0.9946	0.82
Procymidone	1.36	4.55	89.41	2.88	0.9984	0.62
Propiconazole	0.11	0.35	89.71	1.91	0.9983	0.87
Pyraclostrobin	0.12	0.41	78.91	12.64	0.9991	0.92
Pyrimethanil	0.05	0.16	86.66	1.31	0.9991	0.75
Tebuconazole	0.13	0.45	86.44	1.91	0.9990	0.95
Triadimefon	0.12	0.41	86.17	1.40	0.9981	0.90
Triadimenol	1.73	5.74	90.62	4.48	0.9988	0.86
Trifloxystrobin	0.18	0.59	73.68	9.71	0.9972	0.80
Herbicidas						
Atrazine	0.07	0.24	87.79	1.58	0.9977	0.73
Buprofezine	0.05	0.16	92.35	1.75	0.9978	0.86
Butachlor	0.11	0.38	99.25	24.08	0.9983	0.86
Diuron	1.98	6.60	90.46	2.45	0.9999	0.88
Fluometuron	0.30	1.01	86.71	3.38	0.9939	0.78
Isoproturon	0.23	0.76	95.58	1.79	0.9993	0.75
Linuron	0.68	2.25	88.32	2.13	0.9999	0.76
Metribuzin	0.26	0.85	90.67	4.42	0.9993	0.58
Monuron	0.27	0.90	90.09	1.77	0.9993	0.68
Simazine	0.25	0.84	83.14	1.59	0.9970	0.57
Insecticidas						
Acetamiprid	0.48	1.60	97.62	2.38	0.9961	0.45
Carbofuran	0.77	2.55	95.38	2.42	0.9996	0.70
Clothianidin	2.36	7.86	98.60	2.65	0.9998	0.40
Dichlorvos	1.07	3.57	57.17	4.33	0.9994	0.65
Dimethoate	1.95	6.52	83.19	18.87	0.9987	0.53
Etrimfos	0.04	0.14	87.1	1.37	0.9958	0.78
Fenobucarb	0.38	1.28	87.75	2.65	0.9994	0.96
Fenthion	0.96	3.21	43.38	6.40	0.9990	0.64
Imidacloprid	0.97	3.25	95.98	2.32	0.9957	0.36
Indoxacarb	0.39	1.32	59.50	11.50	0.9931	0.81
Malaoxon	0.15	0.50	93.49	2.69	0.9996	0.98
Malathion	0.49	1.64	96.75	2.93	0.9980	0.85
Methiocarb	2.36	7.86	85.64	2.33	0.9886	1.00
Omethoate	1.10	3.68	89.34	6.74	0.9956	0.66
Paraoxon	0.50	1.67	97.11	1.85	0.9990	0.55
Penconazole	0.09	0.29	80.81	8.99	0.9962	0.84

Phosalone	3.80	12.69	69.02	16.47	0.9950	1.13
Phosphamidon	0.09	0.29	96.32	1.91	0.9998	0.75
Pirimicarb	0.34	1.14	95.90	2.84	0.9984	0.38
Profenofos	0.41	1.38	65.01	6.30	0.9987	0.71
Quinalphos	0.32	1.07	71.74	4.43	0.9985	0.84
Spinosyn A	0.25	0.84	80.84	3.69	0.9952	0.70
Spinosyn D	0.40	1.34	70.27	6.79	0.9941	0.67
Thiacloprid	0.14	0.48	101.38	1.75	0.9977	0.57
Thiamethoxam	2.36	7.87	95.29	9.63	0.9978	0.18
Triazophos	0.11	0.36	91.09	3.03	0.9997	0.88
MYCOTOXINS						
Aflatoxin B ₁	0.51	1.71	67.10	1.43	0.9989	0.74
Aflatoxin B ₂	0.73	2.44	91.60	2.79	0.9994	0.66
Aflatoxin G ₁	0.74	2.49	87.09	2.66	0.9999	1.11
Aflatoxin G ₂	0.48	1.60	96.50	5.10	0.9967	0.50
Aflatoxin M ₁	0.09	0.30	75.11	2.48	0.9953	0.78
Ergocornine	0.10	0.35	89.12	5.82	0.9930	0.46
Fumonisin B ₁	0.80	2.68	91.26	2.48	0.9985	0.62
Ochratoxin A	0.11	0.36	117.41	4.00	0.9966	0.86
Zearalenone	1.87	6.25	88.09	3.37	0.9956	0.76

^a Average recovery obtained for fortified samples (n = 10) at two concentration levels: 2.5 µg L⁻¹ and 25 µg L⁻¹.

In order to evaluate the suitability of the SPE extracts for quantitative purposes, the effect of the matrix on the ionization suppression/enhancement of the analytes were compared to neat standards. The slopes obtained in the calibration with matrix-matched standards were compared with those obtained with solvent-based standards, calculating slope ratios matrix/solvent for each of the 69 studied analytes. The results obtained from the optimized method are detailed in **Table 2**. According to Ferrer-Amate *et al.* [27], matrix effects can be classified as: soft matrix effects (< 20 % signal suppression/enhancement), medium matrix effects (20-50 % signal suppression/enhancement) and strong matrix effects (50 % or higher).

As shown in **Table 2**, 51% of the compounds showed soft matrix effects, corresponding to a signal suppression or enhancement equal or lower than 20% (slope ratios in the range 0.8 – 1.2). These values are low enough to provide accurate quantitative data when matrix-matched standard calibration curves are used. Only 5 out of the 69 studied analytes showed strong matrix effects, corresponding to signal suppression higher than 50% (acetamiprid, clothianidin, ergocornine, imidacloprid and thiamethoxam). Compared to the previous method reported for multiclass testing of pesticides and mycotoxins based on partitioning with acetonitrile [28], the present SPE provides distinctly lower matrix effects (less than 10 % of analytes with major matrix effects compared to 40 % [28]) and involves clear advantages such as the preconcentration factor included and the benefits in terms of automation and speed of SPE compared to solvent partitioning.

Analytical performance. To evaluate the analytical features of the proposed method using the optimized SPE procedure and LC-TOFMS detection, calibration curves of the target 69 compounds were constructed (in the range 1-500 $\mu\text{g L}^{-1}$) using wine SPE extracts to prepare matrix-matched standards. Regression coefficients higher than 0.992 were obtained in all cases. The relative standard deviation (RSD %) ($n = 10$) values for run-to-run study were below 15% in most cases (97% of the studied analytes). The limits of quantification (LOQs) were estimated as the minimum concentration of analyte corresponding to a signal-to-noise ratio (S/N) = 10:1. This was experimentally calculated from the injection of matrix-matched standard solutions at low concentration levels, using the more abundant ion for each compound based on the signal from high-resolution raw (non-smoothed) extracted ion chromatograms with narrow mass windows (± 20 ppm relative mass error). Limits of detection ($S/N = 3$ criterion) were in the range 0.04 and 3.80 $\mu\text{g L}^{-1}$, and below 1 $\mu\text{g L}^{-1}$ for 87% of the compounds. The results

obtained are shown in **Table 2**. In most cases, LOQs were below $10 \mu\text{g L}^{-1}$, enabling the detection of all target compounds at low concentration levels. This is enough to meet European regulation for the content of pesticides in food [40,41], which establishes a default MRL of $10 \mu\text{g kg}^{-1}$. Further improvement could be accomplished using a preconcentration factor of 10:1. Regarding to mycotoxins, an LOD of $0.73 \mu\text{g L}^{-1}$ was obtained for aflatoxin B₁, below the established generic maximum limit of $5 \mu\text{g kg}^{-1}$ from Spanish regulation [5]. The same national regulation establishes a generic limit of $10 \mu\text{g kg}^{-1}$ for the sum of aflatoxins B₁, B₂, G₁ and G₂ in foodstuffs destined to human consumption, and the LODs for all of these compounds were below $10 \mu\text{g L}^{-1}$. Finally, the detection limit of ochratoxin A obtained by the proposed method is as low as $0.11 \mu\text{g L}^{-1}$, and the maximum permitted limit set by the EU for this compound is of $2 \mu\text{g kg}^{-1}$ to those wines produced from 2005 harvest onwards. As a conclusion, the results obtained with the proposed SPE method combined with LC-TOFMS can be considered satisfactory for the purpose studied. The use of LC-MS/MS in the MRM mode could further push down the concentration levels that could be detected with the proposed generic SPE method [42-44].

Determination of pesticides and mycotoxins in market purchased wine samples. The proposed method was applied to the analysis of 24 samples of red wine purchased in local markets. These samples corresponded to different brands from different harvesting regions of Spain. Only 10 out of the 69 studied compounds were detected in the studied samples, one mycotoxin and nine pesticides. The detected compounds, ordered by decreasing frequency of detection, were aflatoxin B₂ (detected in 21 of the studied samples), metalaxyl (11), azoxystrobin (8), pyrimethanil (7), tebuconazole (6), dimethomorph (5), carbendazim (4), penconazole (2), fenhexamid (1) and flusilazol (1). Detailed results of the compounds and

concentration levels detected in the analyzed wine samples can be found in

Table 3.

Table 3. Detailed results of the positive findings of the studied compounds in the analyzed red wine samples from Spain.

Sample	Azo (µg/L)	Car (µg/L)	Dim (µg/L)	Fen (µg/L)	Flu (µg/L)	Met (µg/L)	Pen (µg/L)	Pyr (µg/L)	Teb (µg/L)	Sum pest (µg/L)	AfB ₂ (µg/L)
1	ND	ND	ND	ND	ND	73.72	ND	ND	ND	73.72	8.49
2	2.81	100.69	1.67	ND	ND	57.45	ND	8.01	3.86	174.49	ND
3	7.65	ND	ND	ND	ND	191.10	ND	ND	2.64	201.39	6.06
4	ND	ND	ND	ND	ND	ND	ND	ND	ND	-	ND
5	ND	ND	ND	ND	ND	ND	ND	ND	ND	-	6.09
6	ND	26.96	ND	ND	ND	ND	ND	ND	ND	26.96	8.29
7	ND	ND	1.85	ND	ND	22.39	ND	3.71	ND	27.95	4.99
8	ND	ND	ND	ND	ND	ND	ND	3.68	11.26	14.94	5.19
9	ND	ND	ND	ND	ND	ND	ND	ND	ND	-	25.73
10	36.71	ND	ND	ND	ND	ND	ND	ND	10.98	47.69	2.73
11	ND	ND	ND	ND	ND	320.20	ND	ND	ND	320.20	8.18
12	3.62	62.99	4.12	ND	ND	ND	ND	4.45	ND	75.18	6.25
13	ND	ND	ND	ND	ND	ND	ND	ND	ND	-	8.64
14	ND	ND	ND	ND	ND	ND	ND	ND	ND	-	12.72
15	ND	ND	ND	ND	ND	8.71	ND	ND	ND	8.71	4.08
16	2.76	ND	4.09	ND	ND	33.71	ND	55.03	7.03	102.62	6.55
17	3.57	ND	ND	ND	ND	ND	2.26	ND	ND	5.83	5.02
18	ND	ND	ND	ND	ND	ND	ND	ND	ND	-	4.24
19	ND	44.73	8.54	ND	5.74	24.91	ND	ND	6.67	90.59	ND
20	28.28	ND	ND	10.52	ND	ND	1.89	ND	ND	40.69	10.62
21	8.24	ND	ND	ND	ND	ND	ND	4.89	ND	13.13	7.07
22	ND	ND	ND	ND	ND	26.02	ND	ND	ND	26.02	13.43
23	ND	ND	ND	ND	ND	ND	ND	ND	ND	-	10.10
24	ND	ND	ND	ND	ND	127.40	ND	1.66	ND	129.06	1.25

ND: non detected

Abbreviations: Azo: azoxystrobin; Car: carbendazim; Dim: dimetomorph; Fen: fenhexamid; Flu: flusilazole; Met: metalaxyl; Pen: penconazole; Pyr: pyrimethanil; Teb: tebuconazole; Sum pest: sum of pesticides; AfB₂: aflatoxin B₂.

Details of studied samples: 1. Arco Iris (Zamora, Spain, grape(g): Tempranillo, 2008); 2. Tres Reinos (La Rioja, Spain, g: non available (n/a), 2009); 3. Marqués de Dos

Palacios (Badajoz, Spain, g:n/a, 2010); 4.Viña Lameiriña (Orense, Spain, g: n/a, year n/a); 5. Cosechero Cantineo (non available location, g: n/a, 2011); 6. Tío de la Bota (non available location, g:n/a, 2011);7. Elegido (non available location, g:n/a, 2011); 8. Don Ramón Fuente Jalón (Zaragoza, Spain, g: Tempranillo and Garnacha, 2008); 9. Señorío de los Llanos (Valdepeñas, Spain, g:Tempranillo, year n/a); 10. Ribera de los Molinos (Toledo, Spain, g: Tempranillo, Garnacha, Merlot and Cabernet Sauvignon, 2010); 11. Señorío del Alange (Badajoz, Spain, g: Tempranillo, year n/a); 12. Castillo San Asensio (Logroño, Spain; g: n/a, year n/a); 13. Dominio de la Fuente (Cuenca, Spain, g: Tempranillo, 2009); 14. Carrefour (1) (non available location, g: n/a, 2011); 15. Castillo San Simon (Jumilla, g: Tempranillo and Monastrell, 2003); 16. Mayor de Castilla Ribera de Duero (Burgos, g: n/a, 2010); 17. Cortujo el Anchurón (Granada, Spain, g: Tempranillo and Merlot, 2006); 18. Guadalvín (Málaga, Spain; g: Syrah, year n/a); 19. Torre Tallada (Valencia, Spain; g: Tempranillo and Monastrell, year n/a); 20. Santa Elisa (Toledo, Spain, g:Tempranillo and Syrah, 2009); 21. Camino de la Dehesa Ribera de Duero (Soria, Spain, g: n/a, 2009); 22. Cumbre de Gredos (Pozuelo de Alarcón, Spain; g: n/a, 2011); 23. Peñasol (Valdepeñas, Spain; g: n/a, 2011); 24.Carrefour (2) (non available location, g:n/a, 2011).

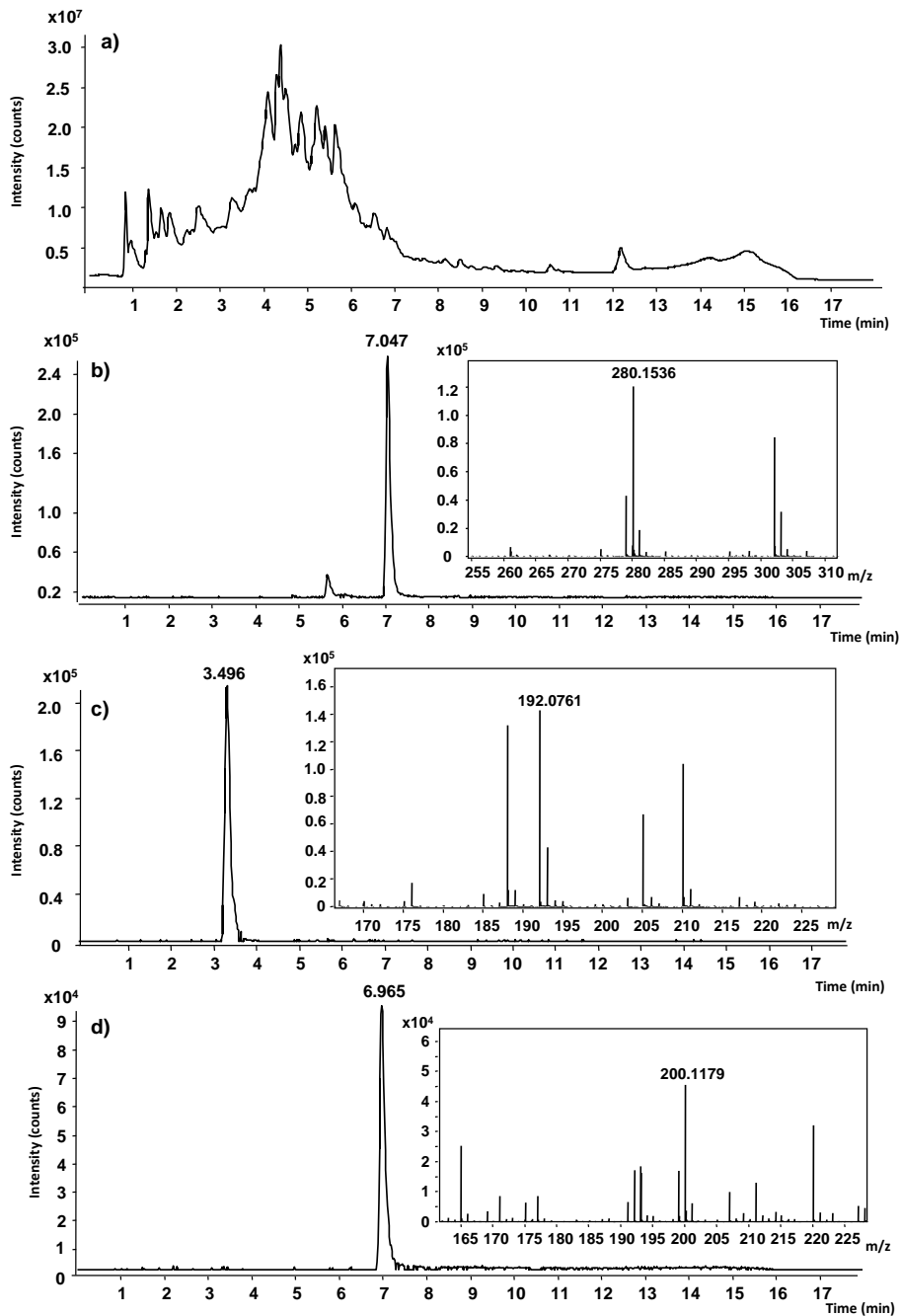


Figure 2. a) Total ion chromatogram (TIC) from the LC-TOFMS analysis of a red wine sample (M2). Positive findings of b) metalaxyl ($57.45 \mu\text{g L}^{-1}$), c) carbendazim ($100.69 \mu\text{g L}^{-1}$) and d) Pyrimethanil ($8.01 \mu\text{g L}^{-1}$) in the studied wine sample.

Aflatoxin B₂ was detected in the 87.5% of the studied samples, but the content of aflatoxins in wine or grapes is not regulated in the EU by a maximum permitted limit, as the content of ochratoxin A [4,40]. Under Spanish law, nevertheless, there is an established generic maximum limit of 5 µg kg⁻¹ for aflatoxin B₁ and a limit of 10 µg kg⁻¹ for the sum of aflatoxins B₁, B₂, G₁ and G₂ in foodstuffs destined to human consumption [5]. Taking into account a maximum production of 70 L of wine from 100 kg of grapes, the maximum permitted limit for the above mentioned sum of aflatoxins would be 14.3 µg L⁻¹ in a wine sample, and the content of aflatoxin B₂ exceeded this value in one of the studied samples (M9). Regarding to pesticide findings, all detected compounds were fungicides used during grapes cultivation. Metalaxyl was the fungicide most frequently detected in the analyzed wine samples, at concentration levels within the range 8.7 – 320.2 µg L⁻¹. As an example, **Figure 2** shows the confirmation of the presence of metalaxyl, carbendazim and pyrimethanil in a wine sample (M2). There is not an EU harmonized maximum residue level (MRL) established for metalaxyl in wines. Only Switzerland and Italy have set MRLs for some pesticides in wines. On the basis of the 1 mg kg⁻¹ MRL established in the EU for metalaxyl in grapes [41], and taking into account the transformation factor of 70 L of wine from 100 kg of grapes, all of the studied samples fulfilled the regulation requirements. Similarly, concentration levels of all detected pesticides in the studied wine samples were below the MRLs established in the EU in grapes destined to wine production. The sum of the concentrations of pesticide residues exceeded 100 µg L⁻¹ on some of the studied red wine samples though.

Conclusions

In this work, a generic sample treatment method for large-scale simultaneous determination of multiclass pesticides and mycotoxins in wines

has been proposed, based on solid-phase extraction (SPE) using polymeric-type SPE cartridges. A liquid chromatography electrospray time-of-flight mass spectrometry method was used to evaluate the sample treatment method with the 60 selected representative multiclass pesticides and 9 mycotoxins. The results in terms of sensitivity, cleanliness of extracts and matrix effects compares well against previous works described for simultaneous testing of pesticides and mycotoxins. High recovery rates were obtained for different classes of pesticides and mycotoxins showing the versatility and broad applicability of the proposed approach. To our knowledge this is the first SPE method described for pesticide and mycotoxins in wine. The method was successfully applied to the analysis of 24 market-purchased red wine samples from Spain. Aflatoxin B₂ and metalaxyl were the most detected compounds, in the 75% and 50% of the studied samples, respectively.

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*III.4. DETERMINACIÓN DE 355 PESTICIDAS
MULTICLASE EN MERMELADAS MEDIANTE
CROMATOGRAFÍA DE LÍQUIDOS DE ALTA
RESOLUCIÓN/ESPECTROMETRÍA DE MASAS DE
TIEMPO DE VUELO (UHPLC-TOFMS).*

III.4. Determinación de 355 pesticidas multiclase en mermeladas mediante cromatografía de líquidos de alta resolución/espectrometría de masas de tiempo de vuelo (UHPLC-TOFMS)

III.4.1. Resumen

Para mejorar el rendimiento de las cosechas en cultivos de frutas y verduras se emplea una gran cantidad y variedad de pesticidas. Debido a que su uso es cada vez más frecuente, existen diferentes normativas que regulan su empleo, con el objetivo de no poner en riesgo la salud del consumidor. Estas normativas son aplicables a muestras de fruta, verdura, aguas de consumo humano y potitos. Sin embargo, en la legislación vigente no se presta atención al contenido de estos contaminantes en productos derivados, como es el caso de las mermeladas obtenidas a base de fruta. En el ámbito de la química analítica se conoce esta falta de legislación, pero no por ello se deja de prestar atención a este tipo de productos. Se conocen hasta la fecha un amplio número de métodos que emplean LC-MS/MS con triple cuadrupolo como analizador en modo SRM para la determinación de pesticidas en este tipo de muestras. Una alternativa al empleo de esta técnica es el uso de LC-HRMS con Orbitrap o Q-TOF. Esta última técnica proporciona alta especificidad debido al alto poder de resolución y exactitud de masas, permitiendo el análisis de un amplio número de compuestos en un único análisis.

En este capítulo se detalla el desarrollo de un método multiresiduo para la determinación de 355 pesticidas en mermeladas obtenidas a base de fruta usando para el tratamiento de las muestras un método genérico (QuEChERS) y para el análisis de los extractos previamente obtenidos, UHPLC-TOFMS. Después de desarrollar el método analítico, se creó una base de datos que contenía valores de masa exacta y tiempo de retención de cada uno de los

pesticidas incluidos en este estudio, para lo cual fue necesario el empleo de patrones analíticos. La información necesaria fue recopilada en un archivo csv, compatible con el software empleado posteriormente para el análisis de estos pesticidas en las muestras seleccionadas. Una vez fue creada la base de datos, el método fue validado en mermelada en términos de límites de detección y cuantificación, efecto matriz y linealidad. Finalmente, el método fue aplicado a 54 muestras de mermeladas obtenidas a base de fruta. Los resultados obtenidos mostraron que en todas las muestras el contenido de los pesticidas detectados era inferiores a los límites máximos de residuos (LMRs) establecidos excepto en una de ellas. Esto puede indicar que no constituye un gran riesgo el consumo de productos derivados, pero sí que pone de manifiesto la necesidad de emplear LMRs que regulen el contenido de pesticidas en ellos, para así garantizar que su consumo es seguro.

III.4.2. Artículo

Abstract

While comprehensive regulations enforce the presence of pesticide residues in fruits, vegetables, baby food or drinking water, yet limited attention is devoted to derivate products, which may contain these commodities as an ingredient, such as the case of fruit-based jams, scarcely studied so far. In this study, the presence and concentration levels of over 350 multiclass pesticides was examined in a total of 54 market samples collected in Spain from different companies. For this purpose, a multi-residue screening method covering 355 species was developed using ultra-high performance liquid chromatography-time-of-flight mass spectrometry (UHPLC-TOFMS). The method was based on an experimental library with retention time/accurate mass data for the 355 selected analytes. Prior to analysis, a simple sample extraction step based on liquid partitioning with acetonitrile and a cleanup step with dispersive solid-phase extraction (QuEChERS) was implemented. The identification and confirmation of the compounds was based on retention time and the accurate mass measurements of the protonated molecules ($[M+H]^+$). Screening method limits of quantitation were below $10 \mu\text{g Kg}^{-1}$ for 90% of the studied compounds. The proposed method was successfully applied to 54 market-purchased jams samples. The concentration levels found were in compliance with the current regulations with the exception of a sample (M23), which contained monocrotophos. 41 % of the samples were found free of pesticides; 26 % of the samples contained only one pesticide while 33 % contained at least two or more pesticides. The concentration range of the pesticides detected was $0.3\text{-}506 \mu\text{g kg}^{-1}$. The relatively low concentration levels detected suggest that part of the pesticide residues in the actual fruits used to prepare the derivative product have been partially abated during processing stages.

Introduction

Over 1000 active substances against pests are used worldwide in current agricultural practice due to its undisputable benefits for crop protection [1]. Their application results in improved crop yields and enables international trade and consumption of fresh fruits and vegetables. However, some pesticides may eventually cause a range of adverse effects on human health. Thus, different organizations have established regulatory controls intended to limit exposure of the general population to pesticide residues [2] by setting maximum residue levels (MRLs) for selected pesticide/commodity combinations usually in the range 0.01-10 mg kg⁻¹ [3-6]. These low MRLs and the great number of potential residues have prompted the development and improvement of multi-residue methods (MRMs), which should be comprehensive in order to enable official laboratories to exert an effective control [7,8].

Up-to-date, liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) using triple quadrupole instrumentation operated in the selected reaction monitoring (SRM) mode is the mainstream technique in pesticide testing [9-18]. This approach is based on multiple MS/MS experiments, where both precursor or transition and retention time are defined using standards *a priori*. The MRM methods developed so far cover typically between 50 and 200 compounds.

As an alternative, liquid chromatography-high resolution mass spectrometry (LC-HRMS) using either orbital ion trap or (quadrupole) time-of-flight (Q-TOF) instruments has recently become an extensively used in selected food and environmental testing laboratories [19-23]. LC-HRMS provides high specificity due to both high mass accuracy and mass resolution. It also enables the screening of several hundreds of compounds with high

sensitivity within the same run without limiting the number of simultaneously observed target compounds. Both the accurate mass of each scan and the higher mass resolving power provide a greater degree of reduction in chemical noise, thereby enhancing selectivity. Liquid chromatography time-of-flight mass spectrometry (LC-TOFMS) has been proven to be a sensitive and selective method for the determination and confirmation of pesticide residues in vegetables and fruits, obtaining limits of detection (LODs) in compliance with established MRLs [11,23-27]. Finally, both non-target and unknown analysis are feasible by means of accurate mass measurements without the need to use standards *a priori*.

While comprehensive regulations enforce the presence of pesticide residues in fruits, vegetables, baby food or drinking water, limited attention is devoted to derivate products, which may contain these commodities as an ingredient, such as the case of fruit-based jams, scarcely studied so far [28-31]. In this study, the presence and concentration levels of over 350 multiclass pesticides was examined in a total of 54 market samples collected in Spain from different companies. For this purpose, a multi-residue screening method covering 355 species was developed using ultra-high performance liquid chromatography-time-of-flight mass spectrometry (UHPLC-TOFMS). The method was based on an experimental library with retention time/accurate mass data for the 355 selected analytes. Prior to analysis, a simple sample extraction step based on liquid partitioning with acetonitrile and a cleanup step with dispersive solid-phase extraction (QuEChERS) was implemented.

Experimental section.

Chemical and reagents. The selected pesticides targeted in this work are shown in **Table 1**. A significant number (122) of the pesticides listed in the

Annex I of Commission Implementing Regulation 788/2012 were included in the targeted list [32]. Pesticide analytical standards were purchased from Fluka, Pestanal® quality (Madrid, Spain) and Sigma–Aldrich (Madrid, Spain), magnesium sulphate anhydrous (MgSO_4) and sodium acetate (AcNa) from Sigma–Aldrich (Madrid, Spain); and primary-secondary amine (PSA) from Bond-Elut® (Varian Inc., Palo Alto, CA, USA). Individual stock solutions of the studied compounds (*ca.* $500 \mu\text{g mL}^{-1}$ each) were prepared in methanol or acetonitrile and stored at -20°C . HPLC-grade acetonitrile and methanol were obtained from Merck (Darmstadt, Germany). Formic acid was obtained from Fluka (Buchs, Switzerland). A Milli-Q-Plus ultra-pure water system from Millipore (Milford, MA, USA) was used throughout the study to obtain the HPLC-grade water used during the analyses.

Jam samples. Fifty-four market-purchased fruit-based jam samples were studied including both own-brand products and international companies (15 international brands and 39 own-brand products from the Spanish market).

Table 1. Identification of the studied 355 multiclass pesticides tested by UHPLC-TOFMS.

Compound	Rt (min)	Elemental composition m	Theoretical m/z	Ion detected	Experimental m/z	LOQ (μgkg^{-1})
1-Naphtalene-acetamide	4.34	C ₁₂ H ₁₁ ON	185.0841	[M+H] ⁺	186.0913	4.2
2-Hydroxybiphenyl	5.60	C ₁₂ H ₁₀ O	170.0732	[M+H] ⁺	171.0804	208
3,3-dichloro-benzidine	5.67	C ₁₂ H ₁₀ Cl ₂ N ₂	252.0221	[M+H] ⁺	253.0294	2.0
3,5-Dichloroaniline	5.50	C ₆ H ₅ Cl ₂ N	160.9872	[M+H] ⁺	161.9872	1.6
Abamectin	7.59	C ₄₈ H ₇₂ O ₁₄	872.4922	[M+Na] ⁺	895.4814	1.8
Acephate	0.82	C ₄ H ₁₀ NO ₃ PS	183.0119	[M+Na] ⁺	206.0011	128
Acetamiprid	4.03	C ₁₀ H ₁₁ ClN ₄	222.0672	[M+H] ⁺	223.0745	11.7
Acibenzolar S-methyl	5.72	C ₈ H ₆ N ₂ O ₂ S	209.9922	[M+H] ⁺	210.9994	66.7
Aclonifen	6.36	C ₁₂ H ₉ ClN ₂ O ₃	264.0302	[M+H] ⁺	265.0374	18.6
Alachlor	6.20	C ₁₄ H ₂₀ ClNO ₂	269.1183	[M+H] ⁺	270.1255	103
Albendazole	4.52	C ₁₂ H ₁₅ N ₃ O ₂ S	265.0885	[M+H] ⁺	266.0958	3.0
Aldicarb	4.30	C ₇ H ₁₄ N ₂ O ₂ S	190.0776	[M+Na] ⁺	213.0668	1.5
Aldicarb sulfone	2.80	C ₇ H ₁₄ N ₂ O ₄ S	222.0674	[M+Na] ⁺	245.0566	22.9
Aldicarb sulfoxide	1.62	C ₇ H ₁₄ N ₂ O ₃ S	206.0725	[M+Na] ⁺	229.0617	48.7
Allethrin	7.13	C ₁₉ H ₂₆ O ₃	302.1882	[M+H] ⁺	303.1955	5.0
Ametryn	4.48	C ₉ H ₁₇ N ₅ S	227.1205	[M+H] ⁺	228.1278	1.9
Aminocarb	1.01	C ₁₁ H ₁₆ N ₂ O ₂	208.1212	[M+H] ⁺	209.1285	9.0
Amitrol	0.31	C ₂ H ₄ N ₄	84.0436	[M+H] ⁺	85.0509	13.8
Anilazine	5.87	C ₉ H ₅ Cl ₃ N ₄	273.9580	[M+H] ⁺	274.9653	8.5
Anilofos	6.52	C ₁₃ H ₁₉ ClNO ₃ PS ₂	367.0232	[M+H] ⁺	368.0305	8.5
Atrazine	5.01	C ₈ H ₁₄ ClN ₅	215.0938	[M+H] ⁺	216.1011	1.5
Atrazine desethyl	3.80	C ₆ H ₁₀ ClN ₅	187.0625	[M+H] ⁺	188.0697	4.6
Atrazine desisopropyl	3.08	C ₅ H ₈ ClN ₅	173.0468	[M+H] ⁺	174.0541	1.7
Azaconazole	5.04	C ₁₂ H ₁₁ Cl ₂ N ₃ O ₂	299.0228	[M+H] ⁺	300.0301	0.8
Azinphos-ethyl	6.24	C ₁₂ H ₁₆ N ₃ O ₃ PS ₂	345.0371	[M+Na] ⁺	368.0263	1.8
Azinphos-methyl	5.71	C ₁₀ H ₁₂ N ₃ O ₃ PS ₂	317.0058	[M+Na] ⁺	339.9950	10.4
Azoxystrobin	5.85	C ₂₂ H ₁₇ N ₃ O ₅	403.1168	[M+H] ⁺	404.1241	0.8
Barban	6.08	C ₁₁ H ₉ Cl ₂ NO ₂	257.0010	[M+H] ⁺	258.0083	22.0
Benalaxyl	6.40	C ₂₀ H ₂₃ NO ₃	325.1678	[M+H] ⁺	326.1751	2.5
Bendiocarb	4.87	C ₁₁ H ₁₃ NO ₄	223.0845	[M+Na] ⁺	246.0737	1.6
Bensulfuron methyl	5.41	C ₁₆ H ₁₈ N ₄ O ₇ S	410.0896	[M+H] ⁺	411.0969	4.7
Bensulide	6.49	C ₁₄ H ₂₄ NO ₄ PS ₃	397.0605	[M+Na] ⁺	420.0497	1.3
Bifenazate	5.98	C ₁₇ H ₂₀ N ₂ O ₃	300.1474	[M+H] ⁺	301.1547	217
Bitertanol	6.06	C ₂₀ H ₂₃ N ₃ O ₂	337.1790	[M+H] ⁺	338.1863	7.5
Boscalid	5.90	C ₁₈ H ₁₂ Cl ₂ N ₂ O	342.0327	[M+H] ⁺	343.0399	3.5

Brodifacoum	7.57	C ₃₁ H ₂₃ BrO ₃	522.0831	[M+H] ⁺	523.0903	24.9
Bromacil	4.49	C ₉ H ₁₃ BrN ₂ O ₂	260.0160	[M+H] ⁺	261.0233	53.2
Bromadiolone iso1	6.74	C ₃₀ H ₂₃ BrO ₄	526.0780	[M+Na] ⁺	549.0672	9.2
Bromadiolone iso2	6.82	C ₃₀ H ₂₃ BrO ₄	526.0780	[M+Na] ⁺	549.0672	26.2
Bromophos methyl	7.14	C ₈ H ₈ BrCl ₂ O ₃ PS	363.8492	[M+H] ⁺	364.8565	42.8
Bromoxynil	5.11	C ₇ H ₃ Br ₂ ON	274.8581	[M+H] ⁺	275.8654	69.9
Bromuconazol iso1	5.84	C ₁₃ H ₁₂ BrCl ₂ N ₃ O	374.9541	[M+H] ⁺	375.9614	2.3
Bromuconazol iso2	5.66	C ₁₃ H ₁₂ BrCl ₂ N ₃ O	374.9541	[M+H] ⁺	375.9614	2.4
Bupirimate	5.50	C ₁₃ H ₂₄ N ₄ O ₃ S	316.1569	[M+H] ⁺	317.1642	0.4
Buprofezin	6.41	C ₁₆ H ₂₃ N ₃ OS	305.1562	[M+H] ⁺	306.1635	7.3
Butachlor	7.21	C ₁₇ H ₂₆ ClNO ₂	311.1652	[M+H] ⁺	312.1725	64.5
Butocarboxim	4.17	C ₇ H ₁₄ N ₂ O ₂ S	190.0776	[M+Na] ⁺	213.0668	6.2
Butoxycarboxim	2.54	C ₇ H ₁₄ N ₂ O ₄ S	222.0674	[M+Na] ⁺	245.0564	119
Buturon	5.42	C ₁₂ H ₁₃ ClN ₂ O	236.0716	[M+H] ⁺	237.0789	1.5
Cadusafos	6.48	C ₁₀ H ₂₃ O ₂ PS ₂	270.0877	[M+H] ⁺	271.0950	1.4
Carbaryl	5.02	C ₁₂ H ₁₁ NO ₂	201.0790	[M+Na] ⁺	224.0682	24.5
Carbendazim	2.36	C ₉ H ₉ N ₃ O ₂	191.0695	[M+H] ⁺	192.0768	1.4
Carbofuran	4.87	C ₁₂ H ₁₅ NO ₃	221.1052	[M+H] ⁺	222.1125	10.2
Carbofuran 3-hydroxy	3.75	C ₁₂ H ₁₅ NO ₄	237.1001	[M+H] ⁺	238.1074	2.5
Carboxine	5.11	C ₁₂ H ₁₃ NO ₂ S	235.0667	[M+H] ⁺	236.0740	3.6
Carfentazone ethyl	6.40	C ₁₅ H ₁₄ Cl ₂ F ₃ N ₃ O ₃	411.0364	[M+Na] ⁺	434.0257	10.4
Chlofentezin	6.63	C ₁₄ H ₈ Cl ₂ N ₄	302.0126	[M+H] ⁺	303.0199	45.0
Chlorbromuron	5.79	C ₉ H ₁₀ BrClN ₂ O ₂	291.9614	[M+H] ⁺	292.9687	14.9
Chlordimeform	3.37	C ₁₀ H ₁₃ ClN ₂	196.0767	[M+H] ⁺	197.0840	3.1
Chlorfenvinfos	6.31	C ₁₂ H ₁₄ Cl ₃ O ₄ P	357.9695	[M+Na] ⁺	380.9587	0.8
Chlorfluazuron	7.37	C ₂₀ H ₉ Cl ₃ F ₅ N ₃ O ₃	538.9630	[M+H] ⁺	539.9702	8.1
Chloridazon	3.78	C ₁₀ H ₈ ClN ₃ O	221.0356	[M+H] ⁺	222.0429	1.1
Chlorotoluron	4.96	C ₁₀ H ₁₃ ClN ₂ O	212.0716	[M+H] ⁺	213.0789	2.1
Chloroxuron	5.73	C ₁₅ H ₁₅ ClN ₂ O ₂	290.0822	[M+H] ⁺	291.0895	2.8
Chlorpropham	6.00	C ₁₀ H ₁₂ ClNO ₂	213.0557	C ₇ H ₆ ClNO ₂ ⁺	172.0160	13.0
Chlorpyrifos	7.28	C ₉ H ₁₁ Cl ₃ NO ₃ PS	348.9263	[M+H] ⁺	349.9336	49.5
Chlorpyrifos methyl	6.74	C ₇ H ₇ Cl ₃ NO ₃ PS	321.9023	[M+H] ⁺	321.9023	9.3
Chlorsulfuron	4.98	C ₁₂ H ₁₂ ClN ₅ O ₄ S	357.0299	[M+H] ⁺	358.0371	2.2
Chlothianidin	3.74	C ₆ H ₈ ClN ₅ O ₂ S	249.0087	[M+H] ⁺	250.0160	5.3
Cinosulfuron	4.81	C ₁₅ H ₁₉ N ₅ O ₇ S	413.1005	[M+H] ⁺	414.1078	10.5
Clomazone	5.42	C ₁₂ H ₁₄ ClNO ₂	239.0713	[M+H] ⁺	240.0786	5.9
Coumaphos	6.59	C ₁₄ H ₁₆ ClO ₅ PS	362.0145	[M+H] ⁺	363.0217	2.7
Cyanazine	4.65	C ₉ H ₁₃ ClN ₆	240.0890	[M+H] ⁺	241.0963	5.0
Cyazofamid	6.35	C ₁₃ H ₁₃ ClN ₄ O ₂ S	324.0448	[M+H] ⁺	325.0521	9.9

Cycloate	6.71	C ₁₁ H ₂₁ NOS	215.1344	[M+H] ⁺	216.1417	2.4
Cycloheximid	4.23	C ₁₅ H ₂₃ NO ₄	281.1627	[M+H] ⁺	282.1700	15.7
Cycloxdim	6.89	C ₁₇ H ₂₇ NO ₃ S	325.1712	[M+H] ⁺	326.1784	6.5
Cyphenothrin	7.80	C ₂₄ H ₂₅ NO ₃	375.1834	[M+Na] ⁺	398.1727	16.3
Cyprodinil	5.39	C ₁₄ H ₁₅ N ₃	225.1266	[M+H] ⁺	226.1339	1.3
Cyproconazol	5.56	C ₁₅ H ₁₈ ClN ₃ O	291.1138	[M+H] ⁺	292.1211	1.1
Cyromacin	0.51	C ₆ H ₁₀ N ₆	166.0967	[M+H] ⁺	167.1040	2.2
DEET	5.07	C ₁₂ H ₁₇ NO	191.1310	[M+H] ⁺	192.1383	1.7
Demeton-S-methyl	4.61	C ₆ H ₁₅ O ₃ PS ₂	230.0200	[M+Na] ⁺	253.0092	2.5
Desethyl terbutylazine	4.64	C ₇ H ₁₂ ClN ₅	201.0781	[M+H] ⁺	202.0854	6.0
Desmedipham	5.65	C ₁₆ H ₁₆ N ₂ O ₄	300.1110	[M+H] ⁺	301.1183	72.5
Desmetryn	4.07	C ₈ H ₁₅ N ₅ S	213.1048	[M+H] ⁺	214.1121	2.0
Diafenthiuron	7.54	C ₂₃ H ₃₂ N ₂ OS	384.2235	[M+H] ⁺	385.2308	13.3
Dichlofenthion	7.24	C ₁₀ H ₁₃ Cl ₂ O ₃ PS	313.9700	[M+H] ⁺	314.9773	69.2
Dichlofluanid	6.33	C ₉ H ₁₁ Cl ₂ FN ₂ O ₂ S ₂	331.9623	[M+Na] ⁺	354.9515	12.5
Dichloran	5.47	C ₆ H ₄ Cl ₂ N ₂ O ₂	205.9650	[M+H] ⁺	206.9723	59.2
Dichlorvos	4.62	C ₄ H ₇ Cl ₂ O ₄ P	219.9459	[M+H] ⁺	220.9532	3.1
Dicrotophos	3.40	C ₈ H ₁₆ NO ₅ P	237.0766	[M+H] ⁺	238.0839	11.7
Diethofencarb	5.69	C ₁₄ H ₂₁ NO ₄	267.1471	[M+H] ⁺	268.1543	51.0
Difenacoum isomer1	7.32	C ₃₁ H ₂₄ O ₃	444.1725	[M+H] ⁺	445.1798	12.9
Difenacoum isomer2	7.21	C ₃₁ H ₂₄ O ₄	445.1725	[M+H] ⁺	446.1798	12.7
Difenoconazole	6.37	C ₁₉ H ₁₇ Cl ₂ N ₃ O ₃	405.0647	[M+H] ⁺	406.0720	0.5
Difenoaxuron	5.21	C ₁₆ H ₁₈ N ₂ O ₃	286.1317	[M+H] ⁺	287.1390	1.2
Diflubenzuron	6.06	C ₁₄ H ₉ ClF ₂ N ₂ O ₂	310.0321	[M+Na] ⁺	333.0213	15.1
Diflufenican	6.81	C ₁₉ H ₁₁ F ₅ N ₂ O ₂	394.0741	[M+H] ⁺	395.0813	6.6
Dimethametryn	5.27	C ₁₁ H ₂₁ N ₅ S	255.1518	[M+H] ⁺	256.1590	0.8
Dimethenamid	5.73	C ₁₂ H ₁₈ ClNO ₂ S	275.0747	[M+H] ⁺	276.0820	1.8
Dimethoate	3.92	C ₅ H ₁₂ NO ₃ PS ₂	228.9996	[M+Na] ⁺	251.9888	12.8
Dimethomorph iso.1	5.43	C ₂₁ H ₂₂ ClNO ₄	387.1237	[M+H] ⁺	388.1310	1.5
Dimethomorph iso.2	5.52	C ₂₁ H ₂₂ ClNO ₄	387.1237	[M+H] ⁺	388.1310	1.5
Diniconazol	6.15	C ₁₅ H ₁₇ Cl ₂ N ₃ O	325.0749	[M+H] ⁺	326.0821	0.8
Diphenylamine	6.16	C ₁₂ H ₁₁ N	169.0891	[M+H] ⁺	170.0964	1.3
Disulfoton	4.32	C ₈ H ₁₉ O ₂ PS ₃	274.0285	[M+H] ⁺	275.0358	40.5
Diuron	5.14	C ₉ H ₁₀ Cl ₂ N ₂ O	232.0170	[M+H] ⁺	233.0243	5.0
DMST solution	5.07	C ₉ H ₁₄ N ₂ O ₂ S	214.0776	[M+H] ⁺	215.0849	107
Edifenphos	6.27	C ₁₄ H ₁₅ O ₂ PS ₂	310.0251	[M+H] ⁺	311.0324	1.7
Emamectin benzoate	5.72	C ₄₉ H ₇₅ NO ₁₃	885.5238	[M+H] ⁺	886.5311	0.4
EPN	6.81	C ₁₄ H ₁₄ NO ₄ PS	323.0381	[M+Na] ⁺	324.0454	13.3
Epoxiconazole	5.78	C ₁₇ H ₁₃ ClFN ₃ O	329.0731	[M+H] ⁺	330.0804	0.8

Eprinomectin	7.13	C ₅₀ H ₇₅ NO ₁₄	913.5188	[M+Na] ⁺	936.5080	2.1
EPTC	6.31	C ₉ H ₁₉ NOS	189.1187	[M+H] ⁺	190.1260	6.2
Etaconazol	5.73	C ₁₄ H ₁₅ Cl ₂ N ₃ O ₂	327.0541	[M+H] ⁺	328.0614	0.6
Ethiofencarb	5.12	C ₁₁ H ₁₅ NO ₂ S	225.0823	[M+Na] ⁺	248.0716	0.3
Ethion	7.38	C ₉ H ₂₂ O ₄ P ₂ S ₄	383.9876	[M+Na] ⁺	406.9768	6.7
Ethiprole	5.63	C ₁₃ H ₉ Cl ₂ F ₃ N ₄ OS	395.9826	[M+H] ⁺	396.9899	2.9
Ethofumesate	6.02	C ₁₃ H ₁₈ O ₅ S	286.0875	[M+H] ⁺	287.0948	182
Ethoxyquin	4.82	C ₁₄ H ₁₉ NO	217.1467	[M+H] ⁺	218.1539	1.8
Etofenprox	7.96	C ₂₅ H ₂₈ O ₃	376.2038	[M+Na] ⁺	399.1931	20.0
Etoprofos	5.87	C ₈ H ₁₉ O ₂ PS ₂	242.0564	[M+H] ⁺	243.0637	2.1
Etoazole	7.34	C ₂₁ H ₂₃ F ₂ NO ₂	359.1697	[M+H] ⁺	360.1770	0.0
Etrimphos	6.55	C ₁₀ H ₁₇ N ₂ O ₄ PS	392.0647	[M+H] ⁺	293.0719	0.8
Famphur	5.68	C ₁₀ H ₁₆ NO ₅ PS ₂	325.0208	[M+H] ⁺	326.0280	1.4
Fenamidone	5.73	C ₁₇ H ₁₇ N ₃ OS	311.1092	[M+H] ⁺	312.1165	0.3
Fenamiphos	5.76	C ₁₃ H ₂₂ NO ₃ PS	303.1058	[M+H] ⁺	304.1131	3.3
Fenamiphos sulfone	4.73	C ₁₃ H ₂₂ NO ₅ PS	335.0956	[M+H] ⁺	336.1029	1.7
Fenamiphos sulfoxide	4.31	C ₁₃ H ₂₂ NO ₄ PS	319.1007	[M+H] ⁺	320.1080	0.3
Fenarimol	5.71	C ₁₇ H ₁₂ Cl ₂ N ₂ O	330.0327	[M+H] ⁺	331.0399	1.8
Fenchlorphos	7.09	C ₈ H ₈ Cl ₃ O ₃ PS	319.8997	[M+H] ⁺	320.9070	37.2
Fenhexamid	5.89	C ₁₄ H ₁₇ Cl ₂ NO ₂	301.0636	[M+H] ⁺	302.0709	3.4
Fenhexamid 4-o-glucoside	4.76	C ₂₀ H ₂₇ NO ₇ Cl ₂	463.1165	[M+H] ⁺	464.1237	7.8
Fenitrothion	6.18	C ₉ H ₁₂ NO ₅ PS	277.0174	[M+H] ⁺	278.0247	2.6
Fenobucarb	6.40	C ₁₂ H ₁₇ NO ₂	207.1259	[M+H] ⁺	208.1332	12.9
Fenoxaprop-P-ethyl	6.83	C ₁₈ H ₁₆ ClNO ₅	361.0717	[M+H] ⁺	362.0790	0.3
Fenoxycarb	6.15	C ₁₇ H ₁₉ NO ₄	301.1314	[M+H] ⁺	302.1387	90.9
Fenpiclonil	5.54	C ₁₁ H ₆ Cl ₂ N ₂	235.9908	[M+H] ⁺	236.9981	2.0
Fenpropathrin	7.59	C ₂₂ H ₂₃ NO ₃	349.1678	[M+Na] ⁺	372.1570	29.6
Fenpropidine	4.96	C ₁₉ H ₃₁ N	273.2456	[M+H] ⁺	274.2529	0.2
Fenpropimorphe	5.00	C ₂₀ H ₃₃ NO	303.2562	[M+H] ⁺	304.2635	0.3
Fenthion	6.51	C ₁₀ H ₁₅ O ₃ PS ₂	278.0200	[M+H] ⁺	279.0273	10.8
Fenuron	3.70	C ₉ H ₁₂ N ₂ O	164.0950	[M+H] ⁺	165.1022	1.6
Fenvalerate	7.74	C ₂₅ H ₂₂ ClNO ₃	419.1288	[M+Na] ⁺	442.1180	51.4
Fipronil	6.33	C ₁₂ H ₄ Cl ₂ F ₆ N ₄ OS	435.9387	[M+H] ⁺	436.9460	1.9
Fluazifop-buthyl	7.19	C ₁₉ H ₂₀ F ₃ NO ₄	383.1344	[M+H] ⁺	384.1417	1.1
Flucythrinate	7.44	C ₂₆ H ₂₃ F ₂ NO ₄	541.1595	[M+Na] ⁺	474.1487	20.8
Fludioxonil	5.73	C ₁₂ H ₆ F ₂ N ₂ O ₂	248.0397	[M+Na] ⁺	271.0290	74.6
Flufenacet	6.19	C ₁₄ H ₁₃ F ₄ N ₃ O ₂ S	363.0665	[M+H] ⁺	364.0737	2.7
Flufenoxuron	7.23	C ₂₁ H ₁₁ ClF ₆ N ₂ O ₃	488.0362	[M+H] ⁺	489.0435	18.3
Fluochloralin	6.96	C ₁₂ H ₁₃ ClF ₃ N ₃ O ₄	355.0547	[M+H] ⁺	356.0619	9.9

Fluomethuron	5.00	$C_{10}H_{11}F_3N_2O$	232.0823	$[M+H]^+$	233.0896	2.6
Fluquinconazole	5.94	$C_{16}H_8Cl_2FN_5O$	375.0090	$[M+H]^+$	376.0163	8.9
Fluroxypyr	4.61	$C_7H_5Cl_2FN_2O_3$	253.9661	$[M+H]^+$	254.9734	59.0
Flusilazole	5.97	$C_{16}H_{15}F_2N_3Si$	315.1003	$[M+H]^+$	316.1076	0.3
Flutolanil	6.14	$C_{17}H_{16}F_3NO_2$	323.1133	$[M+H]^+$	324.1206	0.7
Flutriafol	5.02	$C_{16}H_{13}F_2N_3O$	301.1027	$[M+H]^+$	302.1099	2.0
Forchlorfenuron	4.98	$C_{12}H_{10}ClN_3O$	247.0512	$[M+H]^+$	248.0585	1.0
Fosthiazate	4.97	$C_9H_{18}NO_3PS_2$	283.0466	$[M+Na]^+$	306.0358	1.2
Fuberidazol	3.22	$C_{11}H_8N_2O$	184.0637	$[M+H]^+$	185.0709	0.2
Furalaxyl	5.59	$C_{17}H_{19}NO_4$	301.1314	$[M+H]^+$	302.1387	0.7
Furmecyclox	6.21	$C_{14}H_{21}NO_3$	251.1521	$[M+H]^+$	252.1594	2.1
Griseofulvin	5.15	$C_{17}H_{17}ClO_6$	352.0714	$[M+H]^+$	353.0786	1.4
Haloxyfop	6.08	$C_{15}H_{11}ClF_3NO_4$	361.0329	$[M+H]^+$	362.0401	1.5
Hexaflumuron	6.68	$C_{16}H_8Cl_2F_6N_2O_3$	459.9816	$[M+H]^+$	460.9889	19.9
Hexazinone	4.38	$C_{12}H_{20}N_4O_2$	252.1586	$[M+H]^+$	253.1659	1.1
Hexythiazox	7.30	$C_{17}H_{21}ClN_2O_2S$	352.1012	$[M+H]^+$	353.1085	8.4
Hydramethylnon	6.03	$C_{25}H_{24}F_6N_4$	494.1905	$[M+H]^+$	495.1978	0.3
Imazalil	4.59	$C_{14}H_{14}Cl_2N_2O$	296.0483	$[M+H]^+$	297.0556	0.1
Imazamethabenz-methyl	4.19	$C_{16}H_{20}N_2O_3$	288.1474	$[M+H]^+$	289.1547	2.2
Imazamox	3.86	$C_{15}H_{19}N_3O_4$	305.1376	$[M+H]^+$	306.1448	1.1
Imazapyr	3.47	$C_{13}H_{15}N_3O_3$	261.1113	$[M+H]^+$	262.1186	2.6
Imazaquin	4.63	$C_{17}H_{17}N_3O_3$	311.1270	$[M+H]^+$	312.1343	1.6
Imidacloprid	3.87	$C_9H_{10}ClN_5O_2$	255.0523	$[M+H]^+$	256.0596	26.1
Indoxacarb	6.83	$C_{22}H_{16}ClF_3N_3O_7$	527.0707	$[M+Na]^+$	550.0599	1.7
Ioxynil	5.46	$C_7H_3I_2NO$	370.8304	$[M+H]^+$	371.8377	24.9
Iprodione	6.66	$C_{13}H_{13}N_3Cl_2O_3$	329.0334	$[M+H]^+$	330.0407	76.3
Iprovalicarb	5.67	$C_{18}H_{28}N_2O_3$	320.2100	$[M+H]^+$	321.2173	0.4
Isazophos	6.27	$C_9H_{17}ClN_3O_3PS$	313.0417	$[M+H]^+$	314.0490	1.4
Isocarbophos	5.61	$C_{11}H_{16}NO_4PS$	289.0538	$[M+Na]^+$	312.0430	0.9
Isofenphos	6.88	$C_{15}H_{24}NO_4PS$	345.1164	$[M+Na]^+$	368.1056	1.1
Isoprocab	5.25	$C_{11}H_{15}NO_2$	193.1103	$[M+H]^+$	194.1176	66.4
Isoproturon	5.10	$C_{12}H_{18}N_2O$	206.1419	$[M+H]^+$	207.1492	1.0
Isoxaben	6.01	$C_{18}H_{24}N_2O_4$	332.1736	$[M+H]^+$	333.1809	1.2
Isoxaflutole	4.76	$C_{15}H_{12}F_3NO_4S$	359.0439	$[M+H]^+$	360.0512	22.9
Karbutilate	4.71	$C_{14}H_{21}N_3O_3$	279.1583	$[M+H]^+$	280.1656	6.9
Kresoxim methyl	6.41	$C_{18}H_{19}NO_4$	313.1314	$[M+Na]^+$	336.1206	1.8
Lenacil	4.70	$C_{13}H_{18}N_2O_2$	234.1368	$[M+H]^+$	235.1441	8.3
Linuron	5.69	$C_9H_{10}Cl_2N_2O_2$	248.0119	$[M+H]^+$	249.0192	2.7
Lufenuron	7.06	$C_{17}H_8Cl_2F_8N_2O_3$	509.9784	$[M+H]^+$	510.9857	36.5

Malaoxon	4.82	C ₁₀ H ₁₉ O ₇ PS	314.0589	[M+Na] ⁺	337.0481	1.0
Malathion	6.14	C ₁₀ H ₁₉ O ₆ PS ₂	330.0361	[M+H] ⁺	331.0433	17.4
Mebendazole	4.55	C ₁₆ H ₁₃ N ₃ O ₃	295.0957	[M+H] ⁺	296.1030	0.9
Mefenacet	5.86	C ₁₆ H ₁₄ N ₂ O ₂ S	298.0776	[M+H] ⁺	299.0849	1.1
Mepanipirim	5.91	C ₁₄ H ₁₃ N ₃	223.1109	[M+H] ⁺	224.1182	0.2
Mephosfolam	4.42	C ₈ H ₁₆ NO ₃ PS ₂	269.0309	[M+H] ⁺	270.0382	0.4
Mepronil	6.03	C ₁₇ H ₁₉ NO ₂	269.1416	[M+H] ⁺	270.1489	1.1
Mercaptodimethur (Methiocarb)	5.61	C ₁₁ H ₁₅ NO ₂ S	225.0823	[M+H] ⁺	226.0896	303
Mesotrion	4.84	C ₁₄ H ₁₃ NO ₇ S	339.0413	[M+H] ⁺	340.0485	2.1
Metaflumizone	6.99	C ₂₄ H ₁₆ F ₆ N ₄ O ₂	506.1177	[M+H] ⁺	507.1250	0.9
Metalaxyl	5.12	C ₁₅ H ₂₁ NO ₄	279.1471	[M+H] ⁺	280.1543	2.5
Metamitron	3.68	C ₁₀ H ₁₀ N ₄ O	202.0855	[M+H] ⁺	203.0927	1.2
Metazachlor	5.30	C ₁₄ H ₁₆ ClN ₃ O	277.0982	[M+Na] ⁺	300.0874	5.1
Methabenzthiazuron	4.86	C ₁₀ H ₁₁ N ₃ OS	221.0623	[M+H] ⁺	222.0696	6.0
Methamidophos	0.59	C ₂ H ₆ NO ₂ PS	141.0013	[M+H] ⁺	142.0086	16.4
Methidathion	5.70	C ₆ H ₁₀ N ₂ O ₄ PS ₃	301.9619	[M+Na] ⁺	324.9511	2.3
Methiocarb sulfoxide	3.70	C ₁₁ H ₁₅ NO ₃ S	241.0773	[M+H] ⁺	242.0845	6.8
Methomyl	2.92	C ₅ H ₁₀ N ₂ O ₂ S	162.0463	[M+Na] ⁺	185.0355	14.3
Methoxyfenozide	6.03	C ₂₂ H ₂₈ N ₂ O ₃	368.2100	[M+H] ⁺	369.2173	1.1
Metobromuron	5.28	C ₉ H ₁₁ BrN ₂ O ₂	258.0004	[M+H] ⁺	259.0077	6.4
Metolachlor	6.14	C ₁₅ H ₂₂ ClNO ₂	283.1339	[M+H] ⁺	284.1412	1.8
Metoxuron	4.39	C ₁₀ H ₁₃ ClN ₂ O ₂	228.0666	[M+H] ⁺	229.0738	1.5
Metribuzin	4.68	C ₈ H ₁₄ N ₄ OS	214.0888	[M+H] ⁺	215.0961	1.2
Metsulfuron methyl	4.84	C ₁₄ H ₁₅ N ₅ O ₆ S	381.0743	[M+H] ⁺	382.0816	0.9
Mevinphos	4.10	C ₇ H ₁₃ O ₆ P	224.0450	[M+H] ⁺	225.0523	32.1
Miconazole nitrate	5.32	C ₁₈ H ₁₄ Cl ₄ N ₂ O	413.9860	[M+H] ⁺	414.9933	0.3
Molinate	5.82	C ₉ H ₁₇ NOS	187.1031	[M+H] ⁺	188.1104	17.4
Monocrotophos	3.24	C ₇ H ₁₄ NO ₅ P	223.0610	[M+H] ⁺	224.0682	7.3
Monolinuron	5.12	C ₉ H ₁₁ ClN ₂ O ₂	214.0509	[M+H] ⁺	215.0582	16.9
Monuron	4.54	C ₉ H ₁₁ ClON ₂	198.0560	[M+H] ⁺	199.0633	1.3
Myclobutanil	5.80	C ₁₅ H ₁₇ ClN ₄	288.1142	[M+H] ⁺	289.1215	3.2
N,N-Diethyl-2-naphtholoxypromamide	5.95	C ₁₇ H ₂₁ O ₂ N	271.1572	[M+H] ⁺	272.1645	2.0
Naptalam	4.81	C ₁₈ H ₁₃ NO ₃	291.0895	[M+H] ⁺	292.0968	53.8
Neburon	6.24	C ₁₂ H ₁₆ Cl ₂ N ₂ O	274.0640	[M+H] ⁺	275.0715	1.8
Nitenpyram	3.03	C ₁₁ H ₁₅ ClN ₄ O ₂	270.0884	[M+H] ⁺	271.0956	4.7
N-Methylcarbamate	4.88	C ₁₂ H ₁₅ NO ₃	221.1052	[M+H] ⁺	222.1125	7.4
Norflurazone	5.24	C ₁₂ H ₉ ClF ₃ N ₃ O	303.0386	[M+H] ⁺	304.0459	1.5
Novaluron	6.81	C ₁₇ H ₉ ClF ₈ N ₂ O ₄	492.0123	[M+H] ⁺	493.0196	2.9

Nuarimol	5.32	$C_{17}H_{12}ClFN_2O$	314.0622	$[M+H]^+$	315.0695	2.1
Ofurace	5.12	$C_{14}H_{16}ClNO_3$	281.0819	$[M+H]^+$	282.0891	1.6
Omethoate	1.09	$C_5H_{12}NO_4PS$	213.0225	$[M+H]^+$	214.0298	476
Orbencarb	6.56	$C_{12}H_{16}ClNOS$	257.0641	$[M+H]^+$	258.0714	1.2
Oryzalin	6.15	$C_{12}H_{18}N_4O_6S$	346.0947	$[M+H]^+$	347.1020	9.2
Oxadiazon (oxidiazinon)	7.24	$C_{15}H_{18}Cl_2N_2O_3$	344.0694	$[M+H]^+$	345.0757	79.6
Oxadixyl	4.60	$C_{14}H_{18}N_2O_4$	278.1267	$[M+H]^+$	279.1339	25.0
Oxamyl	2.85	$C_7H_{13}N_3O_3S$	219.0678	$[M+Na]^+$	242.0570	5.3
Oxfendazole	4.03	$C_{15}H_{13}N_3O_3S$	315.0678	$[M+H]^+$	316.0751	1.9
Oxyfluorfen	7.14	$C_{15}H_{11}ClF_3NO_4$	361.0329	$[M+H]^+$	362.0401	14.3
Paclobutrazol	5.49	$C_{15}H_{20}ClN_3O$	293.1295	$[M+H]^+$	294.1368	0.8
Parathion	6.51	$C_{10}H_{14}NO_5PS$	291.0330	$[M+H]^+$	292.0403	13.7
Parathion-methyl	5.96	$C_8H_{10}NO_5PS$	263.0017	$[M+H]^+$	264.0090	15.1
Penconazole	6.04	$C_{13}H_{15}Cl_2N_3$	283.0643	$[M+H]^+$	284.0716	0.5
Pencycuron	6.68	$C_{19}H_{21}ClN_2O$	328.1342	$[M+H]^+$	329.1415	0.8
Pendimethalin	7.27	$C_{13}H_{19}N_3O_4$	281.1376	$[M+H]^+$	282.1448	93.8
Phenmedipham	5.66	$C_{16}H_{16}N_2O_4$	300.1110	$[M+Na]^+$	323.1002	0.8
Phenothrin	8.00	$C_{23}H_{26}O_3$	350.1882	$[M+H]^+$	351.1955	8.3
Phentoate	6.55	$C_{12}H_{17}O_4PS_2$	320.0306	$[M+H]^+$	321.0379	122
Phorate	6.67	$C_7H_{17}O_2PS_3$	260.1280	$[M+Na]^+$	283.0020	14.2
Phosalone	6.76	$C_{12}H_{15}ClNO_4PS_2$	366.9869	$[M+H]^+$	367.9941	14.8
Phosphamidon	4.41	$C_{10}H_{19}ClNO_5P$	299.0689	$[M+H]^+$	300.0762	3.1
Phoxim	6.71	$C_{12}H_{15}N_2O_3PS$	298.0541	$[M+H]^+$	299.0614	72.5
Picloram	3.28	$C_6H_3Cl_3N_2O_2$	239.9260	$[M+H]^+$	240.9333	11.7
Picolinafen	6.97	$C_{19}H_{12}F_4N_2O_2$	376.0835	$[M+H]^+$	377.0908	2.9
Piperonyl butoxide	7.02	$C_{19}H_{30}O_5$	338.2093	$[M+Na]^+$	361.1985	0.1
Piperophos	6.75	$C_{14}H_{28}NO_3PS_2$	353.1248	$[M+H]^+$	354.1321	0.4
Pirimicarb	3.58	$C_{11}H_{18}N_4O_2$	238.1430	$[M+H]^+$	239.1503	1.1
Pirimiphos methyl	6.59	$C_{11}H_{20}N_3O_3PS$	305.0963	$[M+H]^+$	306.1036	0.5
Pretilachlor	6.84	$C_{17}H_{26}ClNO_2$	311.1652	$[M+H]^+$	312.1725	2.3
Prochloraz	5.55	$C_{15}H_{16}Cl_3N_3O_2$	375.0308	$[M+H]^+$	376.0381	2.8
Procymidone	6.16	$C_{13}H_{11}Cl_2NO_2$	283.0167	$[M+H]^+$	284.0240	12.6
Promecarb	5.74	$C_{12}H_{17}NO_2$	207.1259	$[M+Na]^+$	230.1151	1.9
Prometon	4.15	$C_{10}H_{19}N_5O$	225.1590	$[M+H]^+$	226.1662	3.2
Prometryn	4.90	$C_{10}H_{19}N_5S$	241.1361	$[M+H]^+$	242.1434	0.7
Propachlor	5.31	$C_{11}H_{14}ClNO$	211.0764	$[M+H]^+$	212.0837	1.7
Propamocarb	1.19	$C_9H_{20}N_2O_2$	188.1525	$[M+H]^+$	189.1598	4.1
Propanil	5.50	$C_9H_9Cl_2NO$	217.0061	$[M+H]^+$	218.0134	2.0
Propaquizafop	6.94	$C_{22}H_{22}ClN_3O_5$	443.1248	$[M+H]^+$	444.1321	1.6

Propargite	7.46	C ₁₉ H ₂₆ O ₄ S	350.1552	[M+Na] ⁺	373.1444	3.2
Propazine	5.45	C ₉ H ₁₆ ClN ₅	229.1094	[M+H] ⁺	230.1167	0.6
Propetamphos	6.16	C ₁₀ H ₂₀ NO ₄ PS	281.0851	[M+H] ⁺	282.0923	4.4
Propiconazole	6.17	C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	341.0698	[M+H] ⁺	342.0771	2.3
Propisochlor	6.44	C ₁₅ H ₂₂ ClNO ₂	283.1339	[M+Na] ⁺	306.1231	1.7
Propoxur	4.81	C ₁₁ H ₁₅ NO ₃	209.1052	[M+Na] ⁺	232.0944	3.4
Propyzamid	5.93	C ₁₂ H ₁₁ Cl ₂ NO	255.0218	[M+H] ⁺	256.0290	2.9
Proquinazid	7.52	C ₁₄ H ₁₇ IN ₂ O ₂	372.0335	[M+H] ⁺	373.0407	0.6
Prosulfocarb	6.94	C ₁₄ H ₂₁ NOS	251.1344	[M+H] ⁺	252.1417	3.3
Prosulfuron	5.67	C ₁₅ H ₁₆ F ₃ N ₅ O ₄ S	419.0875	[M+H] ⁺	420.0948	1.8
Pymetrozin	0.65	C ₁₀ H ₁₁ N ₅ O	217.0964	[M+H] ⁺	218.1036	3.5
Pyracarbolid	4.89	C ₁₃ H ₁₅ NO ₂	217.1103	[M+H] ⁺	218.1176	1.2
Pyraclostrobin	6.60	C ₁₉ H ₁₈ ClN ₃ O ₄	387.0986	[M+H] ⁺	388.1059	1.9
Pyranocoumarin	6.47	C ₂₀ H ₁₈ O ₄	322.1205	[M+H] ⁺	323.1278	15.8
Pyrazon	3.84	C ₁₀ H ₈ ClN ₃ O	221.0356	[M+H] ⁺	222.0429	1.6
Pyridaben	7.68	C ₁₉ H ₂₅ ClN ₂ OS	364.1376	[M+H] ⁺	365.1449	8.8
Pyridaphenthion	5.93	C ₁₄ H ₁₇ N ₂ O ₄ PS	340.0647	[M+H] ⁺	341.0719	1.7
Pyrifenox isomer 1	4.57	C ₁₄ H ₁₂ Cl ₂ N ₂ O	294.0327	[M+H] ⁺	295.0399	1.1
Pyrifenox isomer 2	4.65	C ₁₄ H ₁₂ Cl ₂ N ₂ O	294.0327	[M+H] ⁺	295.0399	0.5
Pyrimethanil	4.71	C ₁₂ H ₁₃ N ₃	199.1109	[M+H] ⁺	200.1182	0.8
Pyriproxifen	7.18	C ₂₀ H ₁₉ NO ₃	321.1365	[M+H] ⁺	322.1438	0.5
Pyroquilon	4.29	C ₁₁ H ₁₁ NO	173.0841	[M+H] ⁺	174.0913	0.5
Quinalphos	6.41	C ₁₂ H ₁₅ N ₂ O ₃ PS	298.0541	[M+H] ⁺	299.0614	4.2
Quinmerac	3.72	C ₁₁ H ₈ ClNO ₂	221.0244	[M+H] ⁺	222.0316	8.8
Quinoclamine	4.61	C ₁₀ H ₆ ClNO ₂	207.0087	[M+H] ⁺	208.0160	10.0
Quinoxifen	6.87	C ₁₅ H ₈ Cl ₂ FNO	306.9967	[M+H] ⁺	308.0040	2.0
Quizalofop-p-ethyl	6.92	C ₁₉ H ₁₇ ClN ₂ O ₄	372.0877	[M+H] ⁺	373.0950	3.8
Rotenone	6.20	C ₂₃ H ₂₂ O ₆	394.1416	[M+H] ⁺	395.1489	4.2
Secbumeton	4.07	C ₁₀ H ₁₉ N ₅ O	225.1590	[M+H] ⁺	226.1662	0.2
Sethoxydim	7.13	C ₁₇ H ₂₉ NO ₃ S	327.1868	[M+H] ⁺	328.1941	0.6
Siduron isomer 1	5.50	C ₁₄ H ₂₀ N ₂ O	232.1576	[M+H] ⁺	233.1648	0.1
Siduron isomer 2	5.56	C ₁₄ H ₂₀ N ₂ O	232.1576	[M+H] ⁺	233.1648	0.5
Simazine	4.48	C ₇ H ₁₂ ClN ₅	201.0781	[M+H] ⁺	202.0854	61.9
Spinosyn A	5.43	C ₄₁ H ₆₅ NO ₁₀	731.4608	[M+H] ⁺	732.4681	0.1
Spinosyn D	5.62	C ₄₂ H ₆₇ NO ₁₀	745.4765	[M+H] ⁺	746.4838	0.2
Spiromesifen	7.68	C ₂₃ H ₃₀ O ₄	370.2144	[M+Na] ⁺	393.2036	1.4
Spirotetramat	5.60	C ₂₁ H ₂₇ NO ₅	373.1889	[M+H] ⁺	374.1962	0.9
Sulcotrione	4.90	C ₁₄ H ₁₃ ClO ₅ S	328.0172	[M+H] ⁺	329.0245	1.6
Sulfometuron methyl	4.91	C ₁₅ H ₁₆ N ₄ O ₅ S	364.0841	[M+H] ⁺	365.0914	19.2

Sulfotep	6.66	$C_8H_{20}O_5P_2S_2$	322.0227	$[M+H]^+$	323.0300	3.5
Sulprofos	7.30	$C_{12}H_{19}O_2PS_3$	322.0285	$[M+H]^+$	323.0358	2.4
Tau-fluvalinate	7.85	$C_{26}H_{22}ClF_3N_2O_3$	502.1271	$[M+H]^+$	503.1344	15.3
TCPP	5.70	$C_9H_{18}Cl_3O_4P$	326.0008	$[M+Na]^+$	348.9900	7.0
Tebuconazole	5.93	$C_{16}H_{22}ClN_3O$	307.1451	$[M+H]^+$	308.1524	3.8
Tebufenpyrad	6.92	$C_{18}H_{24}ClN_3O$	333.1608	$[M+H]^+$	334.1681	2.9
Tebutam	6.05	$C_{15}H_{23}NO$	233.1780	$[M+H]^+$	234.1852	1.1
Tebuthiuron	4.32	$C_9H_{16}N_4OS$	228.1045	$[M+H]^+$	229.1118	1.1
Teflubenzuron	6.73	$C_{14}H_6Cl_2F_4N_2O_2$	379.9742	$[M+H]^+$	380.9815	28.2
Tembotrione	5.75	$C_{17}H_{16}ClF_3O_6S$	440.0308	$[M+H]^+$	441.0381	9.5
Temephos	7.19	$C_{16}H_{20}O_6P_2S_3$	465.9897	$[M+H]^+$	466.9970	15.0
Tepraloxymid	5.85	$C_{17}H_{24}ClNO_4$	341.1394	$[M+H]^+$	342.1467	6.7
Terbacil	4.50	$C_9H_{13}ClN_2O_2$	216.0666	$[M+Na]^+$	239.0558	58.0
Terbufos	7.16	$C_9H_{21}O_2PS_3$	288.0441	$[M+Na]^+$	311.0333	5.1
Terbumeton	4.19	$C_{10}H_{19}N_5O$	225.1590	$[M+H]^+$	226.1662	0.2
Terbutylazine	5.59	$C_9H_{16}ClN_5$	229.1094	$[M+H]^+$	230.1167	0.6
Terbutryn	4.96	$C_{10}H_{19}N_5S$	241.1361	$[M+H]^+$	242.1434	1.2
Tetrachovinphos	6.12	$C_{10}H_9Cl_4O_4P$	363.8993	$[M+H]^+$	364.9065	2.8
Thiabendazole	3.06	$C_{10}H_7N_3S$	201.0361	$[M+H]^+$	202.0433	0.5
Thiacloprid	4.36	$C_{10}H_9ClN_4S$	252.0236	$[M+H]^+$	253.0309	2.0
Thiamethoxam	3.48	$C_8H_{10}ClN_5O_3S$	291.0193	$[M+H]^+$	292.0266	44.3
Thidiazuron	4.54	$C_9H_8N_4OS$	220.0419	$[M+H]^+$	221.0492	0.8
Thiocyclam	0.84	$C_5H_{11}NS_3$	181.0054	$[M+H]^+$	182.0126	33.6
Thiodicarb	4.81	$C_{10}H_{18}N_4O_4S_3$	354.0490	$[M+Na]^+$	377.0382	2.6
Thiofanox	5.00	$C_9H_{18}N_2O_2S$	218.1089	$[M+Na]^+$	241.0981	3.6
Thiophanate methyl	4.79	$C_{12}H_{14}N_4O_4S_2$	342.0456	$[M+H]^+$	343.0529	4.7
Tolclofos methyl	6.66	$C_9H_{11}Cl_2O_3PS$	299.9544	$[M+H]^+$	300.9616	2.4
Tolyfluanid	6.61	$C_{10}H_{13}Cl_2FN_2O_2S$ 2	345.9780	$[M+Na]^+$	368.9672	2.5
Tralkoxidym	7.27	$C_{20}H_{27}NO_3$	329.1991	$[M+H]^+$	330.2064	0.6
Transfluthrin	7.39	$C_{15}H_{12}Cl_2F_4O_2$	370.0150	$[M+H]^+$	371.0223	36.4
Triadimefon	5.86	$C_{14}H_{16}ClN_3O_2$	293.0931	$[M+H]^+$	294.1004	1.8
Triadimenol	5.50	$C_{14}H_{18}ClN_3O_2$	295.1088	$[M+H]^+$	296.1160	21.3
Triallat	7.38	$C_{10}H_{16}Cl_3NOS$	303.0018	$[M+H]^+$	304.0091	9.1
Triasulfuron	4.95	$C_{14}H_{16}ClN_5O_5S$	401.0561	$[M+H]^+$	402.0633	1.0
Triazophos	6.15	$C_{12}H_{16}N_3O_3PS$	313.0650	$[M+H]^+$	314.0723	0.8
Triazoxid	4.20	$C_{10}H_6ClN_5O$	247.0261	$[M+H]^+$	248.0334	0.5
Trichlorfon	3.58	$C_4H_8Cl_3O_4P$	255.9226	$[M+H]^+$	256.9299	12.2
Triclocarban	6.67	$C_{13}H_9Cl_3ON_2$	313.9780	$[M+H]^+$	314.9853	2.7
Tridemorph	5.53	$C_{19}H_{39}NO$	297.3032	$[M+H]^+$	298.3105	0.7

Trifloxystrobin	6.87	$C_{20}H_{19}F_3N_2O_4$	408.1297	$[M+H]^+$	409.1370	3.2
Triflumizole	6.06	$C_{15}H_{15}ClF_3N_3O$	345.0856	$[M+H]^+$	346.0929	12.7
Triflumuron	6.44	$C_{15}H_{10}ClF_3N_2O_3$	358.0332	$[M+H]^+$	359.0405	12.8
Trinexapac-ethyl	5.35	$C_{13}H_{16}O_5$	252.0998	$[M+H]^+$	253.1071	8.2
Triticonazole	5.52	$C_{17}H_{20}ClN_3O$	317.1295	$[M+H]^+$	318.1368	1.6
XMC	5.69	$C_{10}H_{13}NO_2$	179.0946	$[M+H]^+$	180.1019	32.7
Zoxamide	6.51	$C_{14}H_{16}Cl_3NO_2$	335.0247	$[M+H]^+$	336.0319	0.9
α -Cypermethrin	7.65	$C_{22}H_{19}Cl_2NO_3$	415.0742	$[M+Na]^+$	438.0634	51.5

Sample Treatment. The employed procedure (so-called “QuEChERS”) described elsewhere [33] comprised the following steps: a representative 10 g portion of previously homogenized sample was weighed in a 200 mL PTFE centrifuge tube. Then 10 mL of acetonitrile were added, and the tube was vigorously shaken for 1 min. After this time, 1 g of sodium acetate and 4 g of MgSO_4 were added, and the shaking process was repeated for 1 minute. The extract was then centrifuged (3700 rpm) for 3 min. An amount of 5 mL of the supernatant (acetonitrile phase) was then taken with a pipet and transferred to a 15 mL graduated centrifuge tube containing 250 mg of primary-secondary amine (PSA) and 750 mg of MgSO_4 that was then energetically shaken for 20 seconds. The extract was then centrifuged again (3700 rpm) for 3 minutes. Thus, an extract containing the equivalent of 1 g of sample per mL in nearly 100% acetonitrile was obtained. An amount of 1 mL of this extract was then evaporated to near dryness under a gentle nitrogen stream using a Turbo Vap LV from Zymark (Hopkinton, MA), with a water bath temperature of 37 °C and a N_2 pressure of 15 psi and reconstituted to 1 mL of 20% MeOH. Prior to UPLC-TOFMS analysis, the extract was filtered through a 0.45 μm PTFE filter (Millex FG, Millipore, Milford, MA).

UHPLC-TOFMS analysis. An Agilent 1290 Infinity UHPLC system consisting of a vacuum degasser, an autosampler and a binary pump (Agilent Technologies, Santa Clara, CA) equipped with an analytical column C18 50 mm \times 2.1 mm, 1.8 μm particle size (ZORBAX Eclipse Plus C18) was used. For each determination, 20 μL of the sample extract was injected. Mobile phases A and B were mill-Q water with 0.1% (v/v) formic acid, and acetonitrile with 0.1% (v/v) formic acid respectively. The chromatographic method held the initial mobile phase composition (10% B) constant for 2 min, followed by a linear gradient to 100% B up to 8 min, and kept for 2 min at 100% B. After each run 8 min of post-run equilibration was performed with the initial

mobile phase composition. The flow rate was 0.5 mL min⁻¹. The UHPLC system was connected to an Agilent 6220 TOF time-of flight mass spectrometer equipped with an electrospray interface operated in the positive ionization mode, using the following operation parameters: capillary voltage, 3500 V; nebulizer pressure, 40 psi; drying gas flow rate, 9 L min⁻¹; gas temperature, 325 °C; skimmer voltage, 65 V; octopole rf, 250 V; fragmentor voltage: 190 V. High-resolution TOFMS accurate mass spectra were recorded across the range m/z 50–1000. Accurate mass measurements were obtained using an automated accurate-mass calibrant delivery system to provide continuous mass correction. The instrument performed the internal mass calibration automatically, using a dual-nebulizer electrospray source with an automated calibrant delivery system, which introduces the flow from the outlet of the chromatograph together with a low flow (approximately 10 µL min⁻¹) of a calibrating solution containing the internal reference masses purine (C₅H₅N₄/[M+H]⁺/at m/z 121.050 873) and HP-0921 ([hexakis-(1H,1H,3H-tetrafluoropentoxo)-phosphazene] (C₁₈H₁₉O₆N₃P₃F₂₄)/[M+H]⁺/ at m/z 922.009 798). The full-scan data recorded was processed with Agilent MassHunter Software (version B.04.00).

Screening method: development of accurate-mass database of pesticides.

The screening method was based on “Find by Formula” application of the software used. Standard solutions of the targeted pesticides were organized in different mixtures containing *ca.* 30-40 compounds each at a concentration of *ca.* 500 µg L⁻¹. These solutions were analyzed by UHPLC-TOFMS to collect the retention time data and relevant mass spectra information. For the automatic screening method, an excel spreadsheet was constructed containing the elemental composition and exact mass data for each pesticide as well as their retention times. This file was put into *csv (comma separated values)* file format for use by the Agilent TOF automated

data analysis (“*Find by Formula*”) software. The data included are summarized in **Table 1**, where the retention time, molecular formula and accurate masses of the selected ions are shown for each the 355 compounds tested.

“Find by formula” software application tool searches the selected targeted list of retention time/accurate mass (elemental composition) pairs in the LC-MS raw datafile. The two main parameters previously optimized affecting search criteria were: accurate mass tolerance (± 10 mDa mass window was selected for screening purposes) and retention time tolerance window (fixed at ± 0.25 min). Retention times RSD were typically well below this tolerance (*eg.* < 0.1 - 0.2 %). To each individual positive finding, the retention time and experimental accurate mass bias is provided along with the isotope pattern matching score, which is based on the comparison of the experimental data with the theoretical values of the assigned elemental composition of the tentative positive. This score coefficient -scaled up to 100- considers: the relative abundance of the different isotope signals of the detected species, the space (*m/z* gap) between these signals and the relative mass error.

Results and discussion

Screening method for the determination of 355 multiclass pesticides by UHPLC–TOFMS. A total number of 355 pesticides were targeted in this study. Standard UHPLC-ESIMS mobile phases, elution gradient and electrospray ionization conditions were selected to achieve appropriate sensitivity and selectivity for the majority of the selected compounds. Default values were set for nitrogen flow rates, and drying temperatures considering the HPLC flow rate. Fragmentor voltage was studied in the range 160–250 V for in-source CID fragmentation. It was set at 190 V, as a compromise value between sensitivity for quantitation and additional fragmentation

information for confirmation purposes [27]. All the targeted compounds were detected in the positive ionization mode, and the protonated molecule ($[M+H]^+$) was used for identification purposes in most cases (299 compounds). Sodium adducts ($[M+Na]^+$) were used for the rest of compounds (55) because the relative intensity of the sodium adduct ions was distinctly higher than the corresponding protonated molecule. Only in one case (chlorpropam), a fragment was used instead. It is worth to mention the distribution of the pesticides throughout the chromatogram. As shown in **Figure 1**, where the m/z value and retention time of each detected compound are represented, the distribution of the species is not even. Actually, most of the compounds elute between 4 and 7.5 minutes. Only moderately polar species exhibited retention times below 4 minutes. The coeluting species do not represent any problem in terms of selectivity as all the species are distinctly separated either by retention time and/or by accurate mass. The presence of such large number of co-eluting species would be eventually an issue in the case of using LC-MS/MS instrumentation (multiple reaction monitoring mode), as many MS/MS transitions would be necessarily traced within the same time segment, thus reducing the acquisition time for each individual transition and the sensitivity as well. In contrast, the use of full-scan acquisition mode greatly simplifies method development.

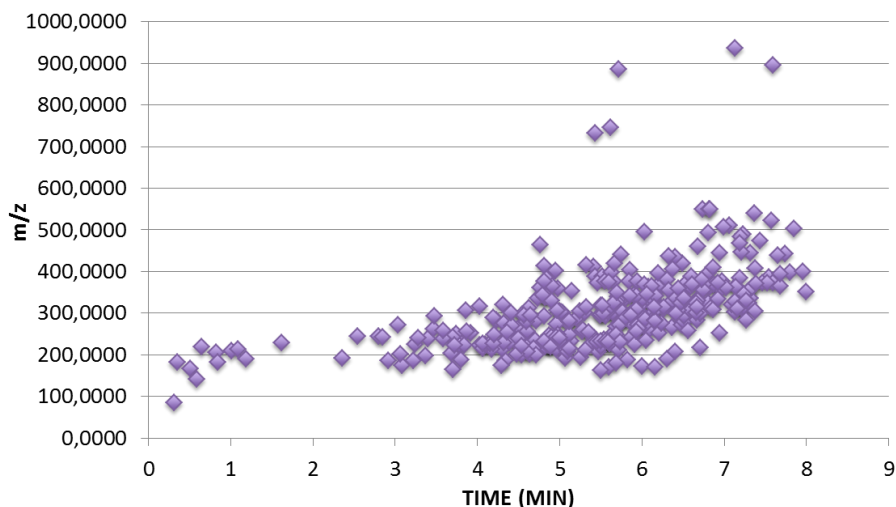


Figure 1. 2D-Plot distribution of the 355 studied compounds according to their m/z values and retention time.

The identification of the targeted species was performed in an automated fashion, by retention time matching (± 0.25 min of tolerance) combined with accurate mass measurements of the targeted ions (mainly protonated molecules). For positive findings additional measurements of fragment ions (in-source CID fragmentation) were also conducted. Furthermore, as some studied pesticides contain chlorine (or bromine) atoms, the isotopic pattern which yields further information for the unambiguous identification of the target compounds can be used by means of a software feature which provides a score coefficient.

For quantitation purposes, extracted ion chromatograms (EICs) were used, setting a mass-window width of ± 20 ppm. The protonated molecule ($[M+H]^+$) was used for quantitation purposes in all cases. As an example, **Figure 2** shows the total ion chromatogram obtained from a jam matrix-matched standard spiked at $10 \mu\text{g kg}^{-1}$, with the EICs of terbutryn, pyrimethanil and thiabendazole.

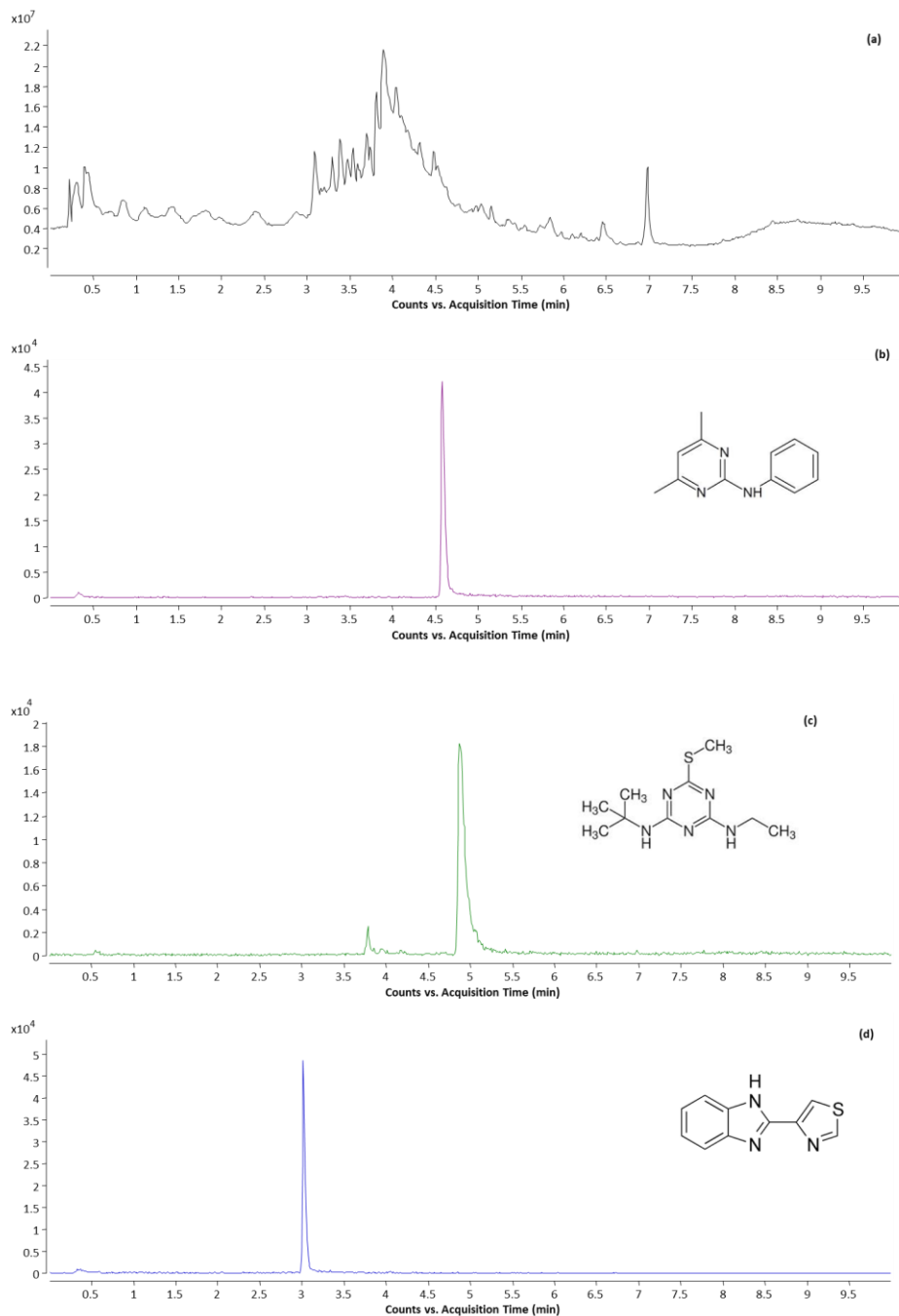


Figure 2. UHPLC-TOFMS analysis of pesticides in jam: (a) Total ion chromatogram of a jam extract spiked with pesticides at $10 \mu\text{g kg}^{-1}$; Extracted ion chromatograms of: (b) terbutryny, (c) pyrimethanil; (d) thiabendazole.

Analytical performance. The linearity of the method was studied by preparing calibration curves using matrix-matched standards in matrix spiked at five concentration levels from 1 to 1000 $\mu\text{g kg}^{-1}$. The results are shown in **Table S1** (Supplementary Information) with correlation coefficients higher than 0.999 in the majority of cases. The screening method limits of quantitation (LOQs) were calculated as the minimum concentration of analyte whose extracted ion chromatogram (with a narrow mass window extraction of ± 20 ppm without smooth filters) showed a signal-to-noise ratio at (S/N) 10:1 respectively. This was experimentally calculated from the injection of matrix-matched standard solutions at low concentration levels, using the more abundant ion for each compound based on the signal from high-resolution raw (non-smoothed) extracted ion chromatograms. LOQs were below 10 $\mu\text{g kg}^{-1}$ for over 70% of the pesticides tested, while LODs were below 10 $\mu\text{g kg}^{-1}$ for 90 % of the species and below 1 $\mu\text{g kg}^{-1}$ for over 50%. Results obtained (**Table 1**) are summarized in **Figure 3**.

With the aim to provide more accurate quantitative results, matrix-matched calibration was addressed using a pool of different fruit-based jams. Matrix effects (ME) were also estimated in order to assess the impact of the matrix on the ionization suppression/enhancement on the analytes (compared to neat standards). For this purpose, the slopes obtained in the calibration with jam extracts were compared with those obtained with solvent-based standards, calculating slope ratios matrix/solvent (ME) for each of the targeted compounds. ME significantly > 1 means signal enhancement while ME significantly < 1 means signal suppression (the more common phenomenon).

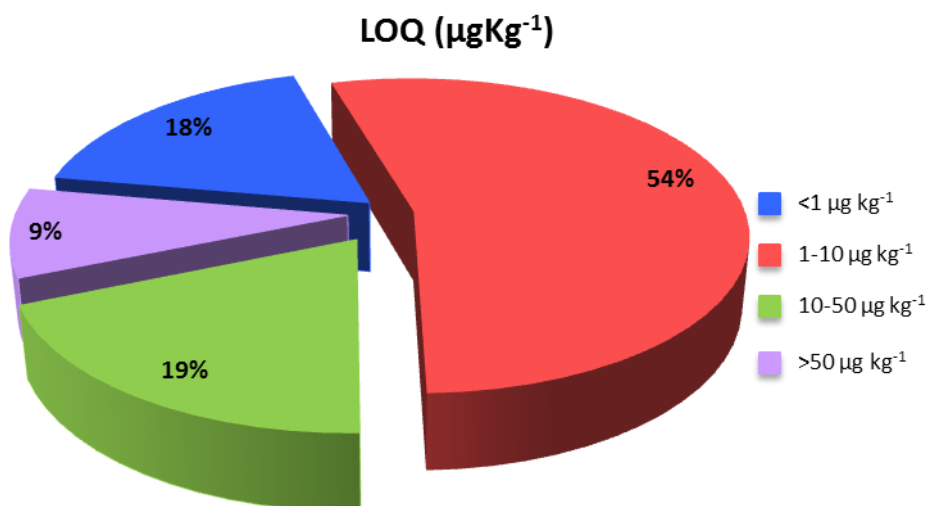


Figure 3. Diagram with the distribution of compounds classified according to their limits of quantification.

The experiment was accomplished with analytes separated in different mixtures to avoid coelutions and prevent analyte/analyte interactions that may affect the matrix effects overall results. A summary of the results is also included in **Figure 4a**, divided in three groups: minor matrix effects (<25% suppression/enhancement), moderate matrix effects (25-50% suppression/enhancement) and strong matrix effects (>50% suppression/enhancement): 25% of the analytes (ca. 90 compounds) showed minor matrix effects, below the 25% of signal suppression/enhancement, while 51% (ca. 185 compounds) displayed moderate matrix effects (25-50% of suppression). On the other hand, 23% of the compounds studied (ca. 80 compounds) showed strong matrix effects, with signal suppression or enhancement higher than 50%. The detailed results are described in **Table S1** (Supplementary Information). The 2D-plot, which represents the matrix effect coefficients of the compounds throughout the chromatographic run

(Figure 4b), shows an even distribution of the matrix effects with signal suppression in most cases.

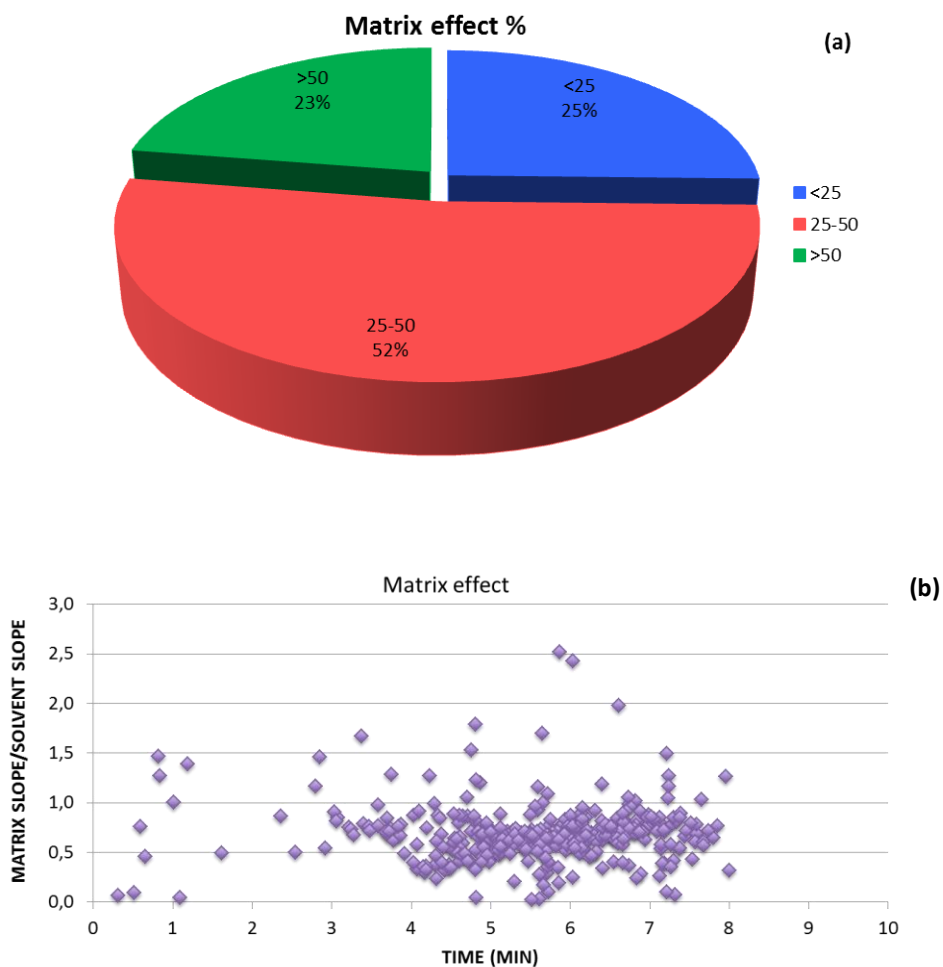


Figure 4a. Diagram with the distribution of compounds classified according to minor (<25%), moderate (25-50%) and strong matrix effects (>50%); b) 2D-Plot representing the occurrence of matrix effects throughout the chromatographic run.

Determination of pesticides in market purchased jams samples. The proposed method was applied to 54 market-purchased fruit-based jams of different flavours, including both own-brand products (39) and international companies (15 samples from international brands) obtained from the local market. Identification was performed with accurate mass measurements of the selected ion and retention time matching. Additional confirmation was provided with an additional fragment ion or with the ^{37}Cl isotope signal. Accurate mass measurements were within 5 ppm (relative mass error) in most cases. **Table 2** shows the details of the samples analysed, pesticides detected and concentration levels in each sample. As can be seen, these values may be considered relatively low in the range from 0.3 to 506 $\mu\text{g kg}^{-1}$. In most samples, the detected concentrations were below 50 $\mu\text{g kg}^{-1}$. Only in one case (sample M23), a concentration higher than the maximum residue limit for pesticides was reported (monocrotophos: 112 $\mu\text{g kg}^{-1}$) while the MRL of monocrotophos in peach is 10 $\mu\text{g kg}^{-1}$. **Figure 5** represents the summary of the results obtained in terms of number of pesticides detected per sample. 41% of the samples were found free of the pesticide tested; 26% of the samples contained only one pesticide while 33% contained at least two or more pesticides. Examples of the detection of pesticides in different samples are outlined in **Figure 6**, showing the detection of carbofuran 3-hydroxy (25.9 $\mu\text{g kg}^{-1}$), fenhexamid (51.1 $\mu\text{g kg}^{-1}$) and spinosad (118 $\mu\text{g kg}^{-1}$) in different samples.

Table 2. Determination of multi-class pesticides in 54 market fruit-based jams by UHPLC-TOFMS.

SAMPLE	COMPOUND(S)	THEORETICAL M/Z	EXPERIMENTAL M/Z	ERROR (PPM)	CONCENTRATION (μGKG^{-1})	SAMPLE TYPE
M1	Not Detected	-	-	-	-	Plum (Light)
M2	Difenoconazole	406.0720	406.0714	-1.5	3.7	Apricot (Light)
	Difenoconazole (^{37}Cl)	408.0717	408.0695	-5.4		
M3	Not Detected	-	-	-	-	Seville Orange
M4	Not Detected	-	-	-	-	Peach (Light)
M5	Azoxystrobin	404.1241	404.1245	1.0	8.7	Strawberry (Light)
	Azoxystrobin F ₁	372.0979	372.0965	-3.8		
	Myclobutanil	289.1215	289.1217	0.7	Detected (<LOQ)	
	Myclobutanil (^{37}Cl)	291.1185	291.1161	-8.2		
M6	Carbofuran 3-hydroxy	238.1074	238.1068	-2.5	25.9	Tomato
	Carbofuran 3-hydroxy F ₁	163.0754	163.0748	-3.6		
M7	Not Detected	-	-	-	-	Blueberry
M8	Pyrimethanil	200.1182	200.1181	-0.5	4.3	Blackberry
M9	Not Detected	-	-	-	-	Apple
M10	Fenhexamid	302.0709	302.0715	2.0	51.1	Berries (mix)
	Fenhexamid F ₁	97.1011	97.1011	0		
	Pirimicarb	239.1503	239.1508	2.1	5.0	
	Pyrimethanil	200.1182	200.1180	-1.0	39.2	
	Pyrimethanil F ₁	183.0917	183.0929	6.6		
M11	Azoxystrobin	404.1241	404.1240	-0.2	13.5	Tomato
	Azoxystrobin F ₁	372.0979	372.0980	0.3		
	Iprovalicarb F ₅	119.0855	119.0855	0	Detected (<LOQ)	
	Iprovalicarb F ₇	91.0542	91.0548	6.6		
M12	Myclobutanil	289.1215	289.1215	0	2.8	Strawberry
	Myclobutanil F ₂	70.0399	70.0408	12.9		
	Spinosyn A	732.4681	732.4681	0	Detected (<LOQ)	
M13	Not Detected	-	-	-	-	Plum
M14	Difenoconazole	406.0720	406.0718	-0.5	5.0	Apricot
	Difenoconazole (^{37}Cl)	408.0690	408.0704	3.4		
M15	Not Detected	-	-	-	-	Peach
M16	Not Detected	-	-	-	-	Orange

M17	Not Detected	-	-	-	-	Peach
M18	Fenarimol	331.0399	331.0396	-0.9	5.2	Strawberry
	Fenarimol (³⁷ Cl)	333.0369	333.0351	-5.4		
	Fenhexamid	302.0709	302.0711	0.7	61.6	
	Fenhexamid F ₁	97.1011	97.1012	1.0		
	Fenhexamid 4-o-glucoside	464.1237	464.1248	2.4	17.3	
	Fenhexamid 4-o-glucoside (Na aduct)	486.1057	486.1067	2.1		
	Myclobutanil	289.1215	289.1227	4.2	5.2	
	Myclobutanil F ₂	70.0399	70.0409	14.3		
	Spinosyn A	731.4608	732.4685	0.5	5.7	
M19	Not Detected	-	-	-	-	Peach
M20	Carbendazim	192.0768	192.0768	0	6.2	Plum
	Carbendazim F ₁	160.0505	160.0502	-1.9		
M21	1-naphtalene-acetamide F ₁	141.0699	141.0687	-8.5	54.8	Apricot
M22	Fenarimol	331.0399	331.0403	1.2	6.0	Strawberry (Diet)
	Fenarimol (³⁷ Cl)	333.0369	333.0347	-6.6		
	Fenhexamid	302.0709	302.0710	0.3	506	
	Fenhexamid F ₁	97.1011	97.1012	1.0		
	Fenhexamid 4-o-glucoside	464.1237	464.1235	-0.4	34.7	
	Fenhexamid 4-o-glucoside (Na aduct)	486.1057	486.1060	0.6		
	Myclobutanil	289.1215	289.1216	0.3	24.6	
	Myclobutanil F ₂	70.0399	70.4000	1.4		
	Penconazole	284.0716	284.0709	-2.5	1.8	
	Penconazole (³⁷ Cl)	286.0686	286.0677	-3.1		
		Pyrimethanil	200.1182	200.1177	-2.5	
	Pyrimethanil F ₁	183.0917	183.0910	-3.8		
M23	Monocrotophos	224.0682	224.0690	3.6	112	Peach (Diet)
	Monocrotophos F ₁	193.0260	193.0253	-3.7		
M24	Not Detected	-	-	-	-	Blueberry
M25	Azoxystrobin	404.1241	404.1242	0.2	34.2	Raspberry
	Azoxystrobin F ₁	372.0979	372.0985	1.6		
	Pyrimethanil	200.1182	200.1182	0	18.2	
	Pyrimethanil F ₁	183.0917	183.0928	6.0		
M26	Azoxystrobin	404.1241	404.1230	-2.7	11.0	Strawberry
	Azoxystrobin F ₁	372.0979	372.0987	2.1		
M27	Carbendazim	192.0768	192.0762	-3.1	52.1	Strawberry (Diet)
	Carbendazim F ₁	160.0505	160.0500	-3.1		
		Myclobutanil	289.1215	289.1222	2.4	

	Myclobutanil (³⁷ Cl)	291.1185	291.1219	11.6	(<LOQ)	
	Thiophanate methyl	343.0529	343.0526	-0.9	169	
	Thiophanate methyl F ₁	311.0267	311.0278	3.5		
M28	Not Detected	-	-	-	-	Peach
M29	Not Detected	-	-	-	-	Peach (Diet)
M30	Fenhexamid	302.0718	302.0711	0.7	97.3	Strawberry
	Fenhexamid F ₁	97.1011	97.1008	-3.1		
	Fenhexamid 4-o-glucoside	464.1237	464.1223	-3.0	12.6	
	Fenhexamid 4-o-glucoside F ₁	302.0709	302.0710	0.3		
	Myclobutanil	289.1215	289.1217	0.7	5.3	
	Myclobutanil F ₂	70.0399	70.0395	-5.7		
	Spinosyn A	732.4681	732.4680	-0.1	0.51	
M31	Myclobutanil	289.1215	289.1215	0	6.2	Strawberry (Diet)
	Myclobutanil F ₂	70.0399	70.0403	5.7		
	Penconazole	284.0716	284.0718	0.7	1.5	
	Penconazole F ₂	158.9763	158.9761	-1.3		
	Pyrimethanil	200.1182	200.1182	0	7.0	Strawberry (Diet)
	Pyrimethanil	183.0917	183.0903	-7.6		
	Spinosyn A F ₁	732.4681	732.4678	-0.4	0.34	
	Tolyfluanid (Na aduct)	368.9672	368.9677	1.4	187	
	Tolyfluanid F ₁	237.9654	237.9652	-0.8		
M32	Not Detected	-	-	-	-	Peach
M33	Tebuconazole	308.1524	308.1526	0.6	11.1	Peach (Diet)
	Tebuconazole F ₂	70.0400	70.0413	18.6		
M34	Tebuconazole	308.1524	308.1523	-0.3	5.1	Apricot
	Tebuconazole (³⁷ Cl)	310.1494	310.1511	5.5		
M35	Not Detected	-	-	-	-	Plum
M36	Not Detected	-	-	-	-	Plum (Diet)
M37	Myclobutanil	289.1215	289.1221	2.1	Detected	Strawberry
	Myclobutanil (³⁷ Cl)	291.1185	291.1201	5.4	(<LOQ)	
	Metalaxyl F ₂	220.1332	220.1314	-8.2	14.2	
	Metalaxyl F ₃	192.1383	192.1375	-4.2		
M38	Not Detected	-	-	-	-	Peach
M39	Not Detected	-	-	-	-	Plum
M40	Not Detected	-	-	-	-	Plum (Diet)
M41	Fenhexamid	302.0709	302.0710	0.3	109	Strawberry
	Fenhexamid F ₁	97.1011	97.1008	-3.1		

	Fenhexamid 4-o-glucoside	464.1237	464.1246	1.9	26.2	
	Fenhexamid 4-o-glucoside (Na adduct)	486.1057	486.1063	1.2		
	Myclobutanil	289.1215	289.1213	-0.7	10.6	
	Myclobutanil F ₂	70.0399	70.0406	10.0		
	Penconazole	284.0716	284.0718	0.7	2.4	
	Penconazole (³⁷ Cl)	286.0686	286.0709	8.0		
M42	Not Detected	-	-	-	-	Peach
M43	Not Detected	-	-	-	-	Plum
M44	Azoxystrobin	404.1241	404.1243	0.5	151	Strawberry
	Azoxystrobin F ₁	372.0979	372.0980	0.3		
	Fenhexamid	302.0724	302.0720	3.6	33.22	
	Fenhexamid F ₁	97.1011	97.0998	-13.4		
	Myclobutanil	289.1215	289.1213	-0.7	34.29	
	Myclobutanil F ₂	70.0399	70.0407	11.4		
	Penconazole	284.0716	284.0714	-0.7	11.49	
	Penconazole F ₂	158.9763	158.9762	-0.6		
	Pirimicarb	239.1503	239.1501	-0.8	2.2	
	Spinosyn A	732.4681	732.4678	-0.4	0.60	
	Triadimenol	296.1160	296.1187	9.1	54.4	
Triadimenol F ₂	99.0804	99.0804	-2.0			
M45	Amitrol	85.0509	85.0498	-12.9	215	Apricot
	Difenoconazole	406.0720	406.0704	-3.9	5.15	
	Difenoconazole (³⁷ Cl)	408.0690	408.0698	2.0		
M46	Imazapyr	262.1186	262.1186	0	6.8	Plum
	Imazapyr F ₁	234.1237	234.1242	2.1		
M47	Metalaxyl	280.1543	280.1550	2.5	28.5	Strawberry
	Metalaxyl F ₃	192.1383	192.1383	0		
	Pyrimethanil	200.1182	200.1182	0	9.3	
	Pyrimethanil F ₁	183.0917	183.0926	4.9		
	Thiabendazole	202.0433	202.0429	-2.0	3.3	
Thiabendazole F ₁	175.0324	175.0320	-2.3			
M48	Not Detected	-	-	-	-	Peach
M49	Imazalil	297.0556	297.0550	-2.0	27.4	Orange
	Imazalil F ₁	158.9763	158.9753	-6.3		
M50	Fenhexamid	302.0709	302.0717	2.7	210	Strawberry (Diet)
	Fenhexamid F ₁	97.1011	97.1001	-10.3		
	Fenhexamid 4-o-glucoside	464.1237	464.1253	3.5	15.8	
	Fenhexamid 4-o-glucoside F ₁	302.0709	302.0700	-3.0		

	Flusilazole	316.1076	316.1081	1.6	0.91	
	Flusilazole F ₁	247.0749	247.0753	1.6		
	Metalaxyl	280.1543	280.1543	0	65.8	
	Metalaxyl F ₂	220.1332	220.1335	1.4		
	Pyraclostrobin	388.1059	388.1058	-0.3	12.3	
	Pyraclostrobin F ₁	163.0633	163.0630	-1.8		
M51	Azoxystrobin	404.1241	404.1225	-3.9	53.4	Strawberry
	Azoxystrobin F ₁	372.0979	372.0964	-4.0		
	Cyproconazol	292.1211	292.1210	-0.3	5.6	
	Cyproconazol (³⁷ Cl)	294.1181	294.1164	-5.8		
	Penconazole	284.0716	284.0710	-2.1	45.8	
	Penconazole F ₂	158.9763	158.9764	0.6		
	Spinosyn A	732.4681	732.4685	0.5	118	
	Spinosyn A F ₁	544.3633	544.3642	1.7		
	Spinosyn D	746.4838	746.4844	0.8		
	Spinosyn D F ₁	558.3789	558.3825	6.4		
	Tebufenpyrad	334.1681	334.1684	0.9	11.0	
	Tebufenpyrad F ₁	145.0527	145.0520	-4.8		
	Triadimenol	296.1160	296.1162	0.7	325	
	Triadimenol F ₂	99.0804	99.0802	-2.0		
M52	Cyprodinil	226.1339	226.1334	-2.2	19.5	Peach
	Cyprodinil F ₁	133.0760	133.0761	0.8		
M53	Pyrimethanil	200.1182	200.1185	1.5	2.3	Plum
	Pyrimethanil F ₂	107.0604	107.0598	-5.6		
	Tebuconazole	308.1524	308.1525	0.3	7.3	
	Tebuconazole F ₁	70.0400	70.0396	-5.7		
M54	Diphenylamine	170.0964	170.0964	0	10.2	Orange

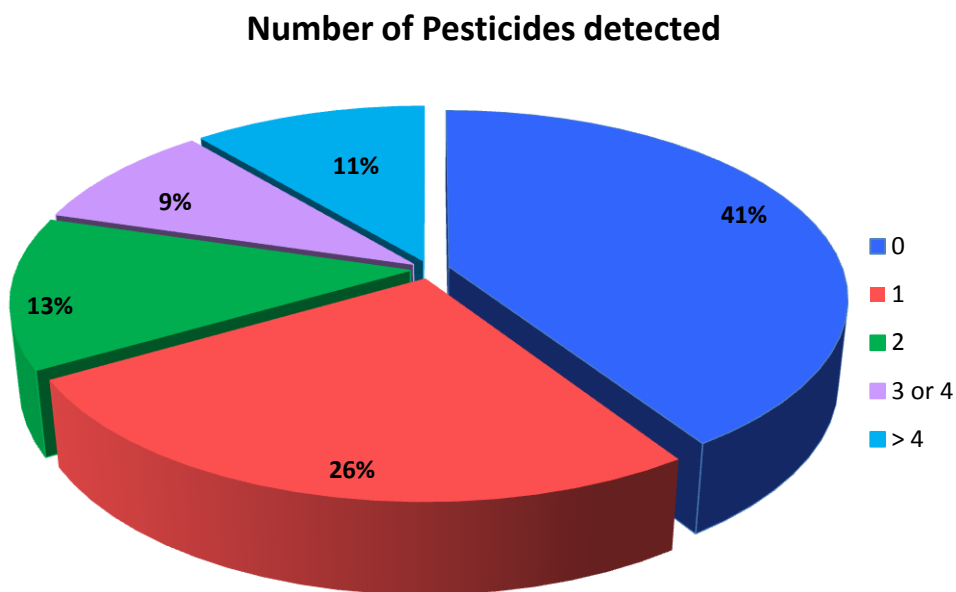


Figure 5. Cake diagram with the percentages classifying the analyzed samples according to the number of pesticides detected.

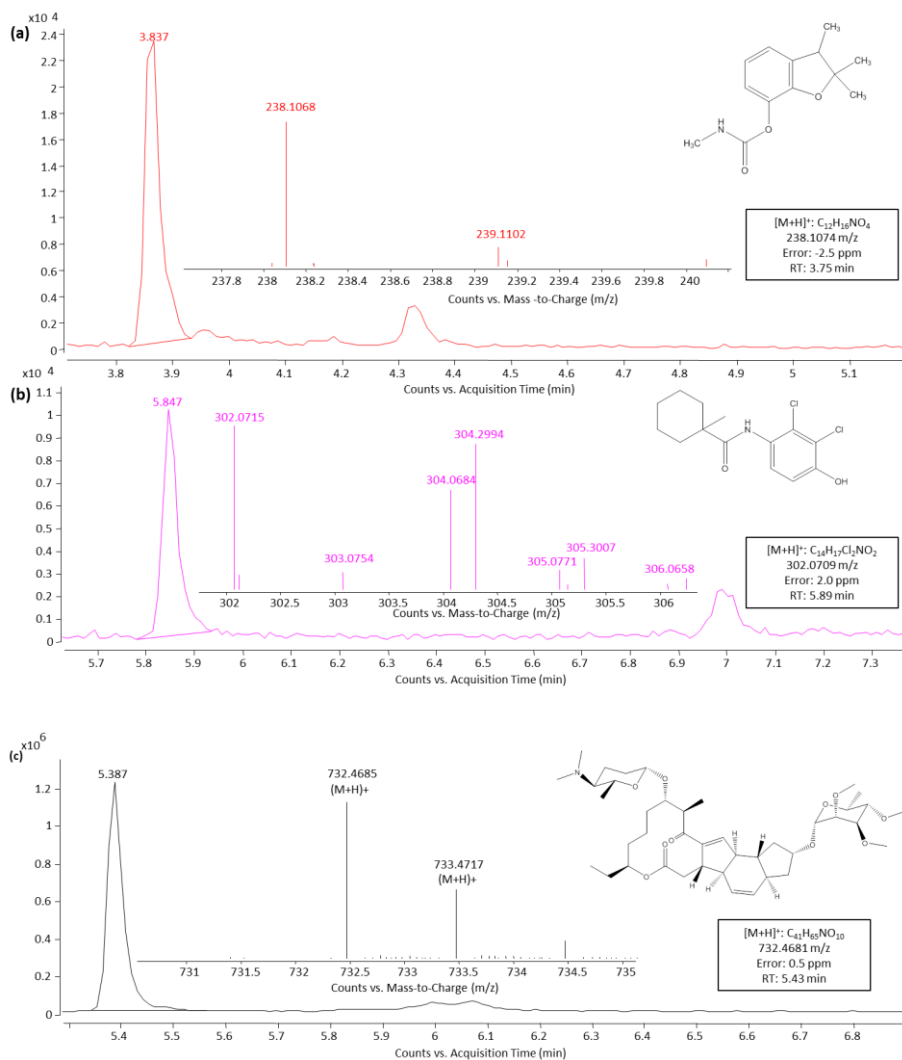


Figure 6. Examples of the application of proposed UHPLC-TOFMS screening method for the analysis of 355 pesticide residues in market samples: (a) Extracted ion chromatogram and accurate mass spectra (inset) of carbofuran-3-hydroxy, detected in sample M6 ($25.9 \mu\text{g kg}^{-1}$); (b) Extracted ion chromatogram and accurate mass spectra (inset) of fenhexamid, detected in sample M10 ($51.1 \mu\text{g kg}^{-1}$); (c) Extracted ion chromatogram and accurate mass spectra (inset) of spinosad (Spinosyn A), detected in sample M51 ($118 \mu\text{g kg}^{-1}$).

Conclusions

Unlike fruit and vegetables which are extensively studied and carefully controlled, derivative products such as beverages or other fruit-based commodities have not been tested in such extent. In this study, a reconnaissance study on the presence and occurrence of over 350 multiclass pesticides in jams was undertaken by means of a screening method based on UHPLC-TOFMS and accurate mass measurements. The proposed method was successfully applied to 54 jams samples (15 international brands and 39 own-brand products from the Spanish market). The results obtained revealed the presence of pesticides at relatively low concentration levels being in most cases in the low $\mu\text{g kg}^{-1}$ range. Only in one sample, the concentration exceeded the MRL set for the corresponding commodity. These results suggest that part of the pesticide residues in the actual fruits used to prepare the derivative product eventually have been partially abated during processing stages.

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III.4.3. Anexo.

Tabla S1. Linearity and matrix effect studies.

Compound	Matrix regression equation	Linearity (matrix) r^2	Matrix effect	Solvent calibration slope
1-Naphtalene-acetamide	$y = 274.99x - 1134.1$	0.9991	0.87	316.05
2-Hydroxybiphenyl	$y = 3.572x + 1333$	1.0000	0.93	3.852
3,3-Dichlorobenzidine	$y = 2489x - 18028$	0.9992	0.63	3965.5
3,5-Dichloroaniline	$y = 2002.9x + 1493.1$	0.9999	0.68	2956.5
Abamectin	$y = 1168.8x - 7000.1$	0.9998	0.69	1701.7
Acephate	$y = 289.11x + 30740$	0.9963	1.47	196.93
Acetamidrid	$y = 506.36x - 3442$	0.9999	0.87	581.24
Acibenzolar S-methyl	$y = 29.013x + 3297.3$	0.9999	1.09	26.73
Aclonifen	$y = 26.257x + 1076.4$	0.9995	0.70	37.525
Alachlor	$y = 37.477x + 520.92$	1.0000	0.85	44.008
Albendazole	$y = 6042.6x - 46147$	0.9995	0.52	11633
Aldicarb	$y = 833.71x - 8416.8$	0.9993	0.38	2217.3
Aldicarb sulfone	$y = 873.16x - 948$	0.9999	1.16	751.01
Aldicarb sulfoxide	$y = 145.72x + 55.974$	0.9997	0.49	296.32
Allethrin	$y = 402.16x + 6667.3$	1.0000	0.80	500.78
Ametryn	$y = 7021x - 49556$	0.9998	0.37	18736
Aminocarb	$y = 2713x - 24273$	0.9993	1.01	2694
Amitrol	$y = 103.98x - 4210$	0.9999	0.06	1630.7
Anilazine	$y = 17.877x + 198.17$	0.9992	2.52	7.098
Anilofos	$y = 340.12x + 1045.2$	0.9994	0.68	502.08
Atrazine	$y = 4080.8x - 32683$	0.9995	0.47	8606.3
Atrazine desethyl	$y = 3309.1x - 24344$	0.9996	0.65	5093.7
Atrazine desisopropyl	$y = 7926.1x - 59239$	0.9997	0.85	9319.3
Azaconazole	$y = 6927.4x + 26299$	1.0000	0.48	14313
Azinphos-ethyl	$y = 211.46x - 344.03$	0.9998	0.45	467.46
Azinphos-methyl	$y = 41.504x + 1953.3$	0.9993	0.29	142.76
Azoxystrobin	$y = 731.99x + 7883.6$	0.9995	0.74	993.28
Barban	$y = 9.3462x + 287.12$	0.9907	0.62	15.153
Benalaxyl	$y = 966.25x - 1877.9$	0.9994	0.74	1314.2
Bendiocarb	$y = 145.55x + 5516.5$	0.9965	1.20	121.19
Bensulfuron methyl	$y = 889.23x + 53324$	0.9993	0.55	1605.1
Bensulide	$y = 879.47x + 515.56$	0.9995	0.76	1158.7
Bifenazate	$y = 325.66x - 77241$	1.0000	0.68	476.63
Bitertanol	$y = 307.69x + 352.74$	0.9992	0.67	459.37

Boscalid	$y = 1062.9x - 6583.6$	1.0000	0.78	1368.8
Brodifacoum	$y = 29.367x + 1902.7$	0.9999	0.60	48.606
Bromacil	$y = 4.046x + 1718.5$	0.9923	0.55	7.4115
Bromadiolone isomer 1	$y = 32.959x + 2329.2$	0.9957	0.99	33.427
Bromadiolone isomer 2	$y = 29.734x + 1377.7$	0.9935	1.02	29.191
Bromophos methyl	$y = 2.64x - 249$	0.9999	0.54	4.9067
Bromoxynil	$y = 5.4233x + 180.33$	0.9999	0.47	11.506
Bromuconazol isomer 1	$y = 424.04x - 1570.3$	0.9997	0.71	597.08
Bromuconazol isomer 2	$y = 451.57x - 1246.9$	0.9996	0.64	703.16
Bupirimate	$y = 13150x - 68385$	0.9994	0.65	20184.00
Buprofezin	$y = 9531.2x - 25035$	1.0000	0.62	15382.00
Butachlor	$y = 228.15x - 42535$	0.9999	1.50	152.52
Butocarboxim	$y = 571.17x - 1642.3$	0.9997	0.30	1920.4
Butoxycarboxim	$y = 957.72x + 3232.3$	0.9993	0.50	1920.4
Buturon	$y = 6147.2x + 5594.1$	1.0000	0.54	11476
Cadusafos	$y = 4086.5x - 2901.5$	0.9999	0.70	5807.3
Carbaryl	$y = 58.553x + 3341.4$	1.0000	0.72	81.687
Carbendazim	$y = 4234.4x - 1705.4$	0.9996	0.86	4899.8
Carbofuran	$y = 230.97x + 271.3$	1.0000	0.70	329.39
Carbofuran 3-hydroxy	$y = 1185.5x + 13162$	0.9999	1.28	922.74
Carboxine	$y = 1216.5x + 15272$	0.9977	0.62	1963
Carfentazone ethyl	$y = 59.79x - 23.863$	0.9998	1.19	50.237
Chlofentezin	$y = 17.987x - 88.333$	0.9999	0.71	25.343
Chlorbromuron	$y = 64.54x + 2957.2$	0.9998	0.62	104.2
Chlordimeform	$y = 3283.2x + 125.88$	0.9999	1.67	1963
Chlorfenvinfos	$y = 299.99x + 12719$	0.9995	0.48	620.36
Chlorfluazuron	$y = 47.347x + 1939.1$	0.9999	0.54	87.391
Chloridazon	$y = 3283.5x - 25607$	1.0000	0.62	5323.3
Chlorotoluron	$y = 1140.3x - 4715$	0.9999	0.55	2065.4
Chloroxuron	$y = 1386.4x - 3022.6$	0.9995	0.66	2106.5
Chlorpropham	$y = 63.435x + 1946.8$	0.9999	0.56	112.37
Chlorpyrifos	$y = 7.1146x + 242.49$	0.9996	0.78	9.1381
Chlorpyrifos methyl	$y = 7.6464x + 108.55$	0.9993	0.37	20.713
Chlorsulfuron	$y = 149.33x - 124.16$	0.9992	0.60	249.82
Chlothianidin	$y = 46.626x + 133.7$	0.9999	0.74	63.366
Cinosulfuron	$y = 1337.9x + 6660.7$	0.9997	0.82	1632.4
Clomazone	$y = 962.88x + 6822.9$	0.9976	0.66	1468.9
Coumaphos	$y = 502.24x + 1194.6$	0.9999	0.85	594.34
Cyanazine	$y = 4301x - 22761$	0.9993	0.59	7280

Cyazofamid	$y = 276.1x - 745.19$	0.9999	0.73	380.76
Cycloate	$y = 824.23x + 7871.7$	0.9992	0.66	1251.5
Cycloheximid	$y = 201.22x + 1852.7$	1.0000	1.27	158.42
Cycloxidim	$y = 966.81x - 4842.1$	0.9999	0.28	3392.4
Cyphenothrin	$y = 60.1x - 2103.2$	0.9975	0.65	92.635
Cyprodinil	$y = 20992x + 64498$	0.9999	0.70	30166
Cyproconazol	$y = 4430.5x - 15157$	0.9998	0.68	6555.3
Cyromacin	$y = 408.24x - 8568.4$	0.9993	0.10	4285.30
DEET	$y = 6820.7x - 34721$	0.9996	0.59	11508
Demeton-S-methyl	$y = 300.64x - 1825.4$	0.9993	0.41	740.03
Desethyl terbuthylazine	$y = 517.44x - 3977$	0.9999	0.47	1091.8
Desmedipham	$y = 146x + 13291$	0.9995	1.70	85.959
Desmetryn	$y = 10781x - 8824.2$	0.9999	0.33	32543
Diafenthuron	$y = 1396.3x - 80221$	1.0000	0.43	3265.9
Dichlofenthion	$y = 4.0167x - 87.333$	0.9999	1.27	3.1553
Dichlofluanid	$y = 47.353x + 322.33$	1.0000	0.61	78
Dichloran	$y = 2.9775x + 224.07$	0.9986	0.41	7.26
Dichlorvos	$y = 285.78x - 4241$	0.9994	0.66	434.67
Dicrotophos	$y = 1009.2x + 9111.9$	1.0000	0.79	1277.6
Diethofencarb	$y = 18.226x + 1236.5$	0.9991	0.68	26.729
Difenacoum isomer 1	$y = 37.57x + 14503$	0.9996	0.08	497.61
Difenacoum isomer 2	$y = 42.824x + 14241$	0.9999	0.10	437.73
Difenoconazole	$y = 2788.4x - 6519.9$	0.9997	0.66	4228
Difenoxuron	$y = 2257.3x - 6352.9$	0.9998	0.71	3169.8
Diflubenzuron	$y = 21.734x + 1063.3$	0.9999	0.73	29.637
Diflufenican	$y = 390.15x + 5452.5$	0.9999	0.69	562.08
Dimethametryn	$y = 25444x - 52135$	0.9986	0.56	45083
Dimethenamid	$y = 3975.4x + 16618$	0.9997	0.76	5232.2
Dimethoate	$y = 115.84x - 331.23$	0.9994	0.49	238.46
Dimethomorph isomer 1	$y = 288.67x - 258.04$	0.9992	0.70	411.17
Dimethomorph isomer 2	$y = 234.07x + 67.753$	1.0000	0.73	321.91
Diniconazol	$y = 5659.2x + 38569$	0.9998	0.52	10916
Diphenylamine	$y = 2614.8x - 3456.8$	0.9998	0.59	4399.5
Disulfoton	$y = 4.9454x + 504.11$	0.9999	0.23	21.297
Diuron	$y = 333.98x + 381.96$	0.9995	0.60	552.21
DMST solution	$y = 22.262x + 2167.1$	0.9923	0.70	31.588
Edifenphos	$y = 657.26x - 83.528$	0.9991	0.70	939.53
Emamectin benzoate	$y = 7721.6x + 145702$	0.9996	0.35	21988
EPN	$y = 53.143x + 5171.6$	0.9989	0.69	77.308

Epoxiconazole	$y = 19604x - 7859.3$	0.9999	0.69	28288
Eprinomectin	$y = 619.77x - 2549.3$	0.9993	0.85	730.77
EPTC	$y = 1797.7x - 27402$	0.9990	0.92	1949.2
Etaconazol	$y = 9065.3x + 93760$	0.9999	0.40	22532
Ethiofencarb	$y = 409.39x + 919.06$	0.9990	0.50	824.40
Ethion	$y = 80.438x + 1381.1$	0.9992	0.54	147.94
Ethiprole	$y = 260.28x - 73.824$	0.9997	0.73	355.4
Ethofumesate	$y = 8.5667x + 878.67$	0.9999	0.63	13.687
Ethoxyquin	$y = 1054.7x - 7159.3$	1.0000	0.05	23308
Etofenprox	$y = 78.02x - 200$	0.9999	1.26	61.862
Etoprofos	$y = 757.01x - 11155$	0.9995	0.62	1216.5
Etoazole	$y = 110795x + 337235$	0.9999	0.81	137554
Etrimphos	$y = 8862x + 26421$	1.0000	0.40	22049
Famphur	$y = 1803x + 9268.6$	0.9996	0.54	3362.8
Fenamidone	$y = 28796x + 50124$	1.0000	0.67	42757
Fenamiphos	$y = 1321.3x - 2549.9$	0.9998	0.65	2017.90
Fenamiphos sulfone	$y = 6692.9x + 8861.8$	1.0000	0.42	16043
Fenamiphos sulfoxide	$y = 6678x + 150936$	1.0000	0.46	14463
Fenarimol	$y = 1023.3x - 318.08$	0.9992	0.68	1513.6
Fenchlorphos	$y = 3.5639x - 20.721$	0.9997	0.71	5.0077
Fenhexamid	$y = 362.73x + 3112.4$	0.9999	0.66	549.63
Fenhexamid 4-o-glucoside	$y = 1527.8x - 11616$	0.9998	0.71	2156.8
Fenitrothion	$y = 49.949x + 20.134$	0.9995	0.59	84.89
Fenobucarb	$y = 368.09x + 622$	0.9999	0.81	451.8
Fenoxaprop P ethyl	$y = 11684x + 33357$	1.0000	0.81	14373
Fenoxycarb	$y = 138.09x + 2492.5$	0.9999	0.74	187.26
Fenpiclonil	$y = 651.15x + 2885.6$	1.0000	0.56	1170.3
Fenpropathrin	$y = 55.144x - 1026.2$	0.9985	0.78	70.581
Fenpropidine	$y = 16899x - 82357$	1.0000	0.74	22858
Fenpropimorphe	$y = 11029x + 65266$	0.9991	0.64	17364
Fenthion	$y = 122x + 1874.5$	0.9990	0.67	183.28
Fenuron	$y = 1513.4x - 5912$	1.0000	0.68	2226.7
Fenvalerate	$y = 9.5019x - 610.85$	0.9998	0.72	13.20
Fipronil	$y = 240.87x + 3898.5$	1.0000	0.51	474.23
Fluazifop-buthyl	$y = 2685.3x - 46367$	0.9993	0.71	3776.6
Flucythrinate	$y = 40.461x - 517.56$	1.0000	0.66	61.211
Fludioxonil	$y = 3.0175x + 4777.5$	0.9999	0.10	30.16
Flufenacet	$y = 1545.2x + 4677.7$	0.9999	0.71	2174
Flufenoxuron	$y = 38.892x - 885.67$	1.0000	1.04	37.22

Fluochloralin	$y = 128.4x + 673.48$	0.9997	0.76	169.3
Fluomethuron	$y = 1486.2x - 2993.4$	0.9998	0.63	2364.5
Fluquinconazole	$y = 69.475x + 12.689$	1.0000	0.83	83.898
Fluroxypyr	$y = 8.1792x - 67.462$	0.9998	0.55	14.862
Flusilazole	$y = 16792x - 7709.9$	0.9991	0.76	22083
Flutolanil	$y = 10223x + 13879$	0.9997	0.83	12245
Flutriafol	$y = 3414.2x - 16223$	0.9999	0.67	5125.00
Forchlorfenuron	$y = 5858.7x + 60339$	0.9999	0.40	14502
Fosthiazate	$y = 5942.5x + 17764$	0.9991	0.74	7977.7
Fuberidazol	$y = 9150x + 10452$	0.9998	0.75	12140
Furalaxyl	$y = 15325x + 61002$	1.0000	0.71	21553
Furmecyclox	$y = 2065.1x + 13498$	0.9990	0.72	2856.1
Griseofulvin	$y = 4931.4x - 16375$	0.9999	0.64	7758.5
Haloxypop	$y = 3650.2x + 9746.1$	0.9996	0.75	4844.9
Hexaflumuron	$y = 21.036x - 371.5$	0.9999	0.82	25.659
Hexazinone	$y = 17263x - 66146$	0.9994	0.68	25269
Hexythiazox	$y = 57.611x + 504.92$	1.0000	0.85	67.605
Hydramethylnon	$y = 37086x - 92528$	0.9993	2.43	15293
Imazalil	$y = 4744.9x - 29964$	0.9996	0.50	9575.8
Imazamethabenz-methyl	$y = 6578.6x - 35547$	0.9992	0.36	18249
Imazamox	$y = 24213x - 79615$	0.9996	0.67	36342
Imazapyr	$y = 3039.1x - 10793$	1.0000	0.76	3997.2
Imazaquin	$y = 3144.1x - 7731.9$	0.9999	0.47	6644.1
Imidacloprid	$y = 85.93x + 5416$	0.9998	0.78	110.01
Indoxacarb	$y = 483.14x - 2182.7$	0.9995	0.77	626.1
Ioxynil	$y = 10.659x - 60.462$	0.9969	0.58	18.458
Iprodione	$y = 6.78x + 856$	1.0000	0.39	17.25
Iprovalicarb	$y = 6446.4x + 63347$	0.9999	0.47	13778
Isazophos	$y = 7298.4x + 68879$	1.0000	0.47	15690
Isocarbophos	$y = 824.06x + 2015.5$	0.9996	0.60	1371.40
Isofenphos	$y = 7473.6x + 1704$	0.9999	0.91	8187.9
Isoprocab	$y = 31.245x + 2700.5$	0.9998	0.49	63.878
Isoproturon	$y = 2676.2x - 2731.4$	0.9997	0.52	5157.8
Isoxaben	$y = 13686x - 25327$	0.9998	0.87	15713
Isoxaflutole	$y = 601.23x + 22160$	0.9976	1.53	393.14
Karbutilate	$y = 2289x - 2974.2$	1.0000	0.87	2642
Kresoxim methyl	$y = 399.81x + 28958$	0.9988	0.34	1190
Lenacil	$y = 211.28x - 1058.2$	1.0000	1.05	200.76
Linuron	$y = 157.42x + 154.69$	0.9993	0.61	257.2

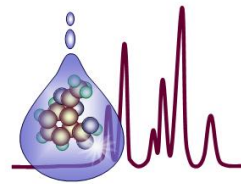
Lufenuron	$y = 11.361x - 216.72$	1.0000	0.84	13.528
Malaoxon	$y = 3638.1x - 2963.6$	0.9999	1.23	2957.80
Malathion	$y = 15.696x - 95.5$	0.9991	0.90	17.52
Mebendazole	$y = 5289.2x - 60919$	0.9994	0.64	8216.6
Mefenacet	$y = 1803x + 391223$	0.9901	0.20	9231.9
Mepanipyrim	$y = 62094x + 275995$	0.9987	0.62	100908
Mephosfolam	$y = 6288.8x + 137181$	0.9991	0.32	19769
Mepronil	$y = 5018.1x + 223559$	0.9986	0.25	20012
Mercaptodimethur (Methiocarb)	$y = 7.57x + 453$	0.9999	0.03	255.17
Mesotrion	$y = 913.38x - 4590.2$	0.9999	0.71	1279.8
Metaflumizone	$y = 3296.4x - 14250$	1.0000	0.88	3747.3
Metalaxyl	$y = 881.24x - 3317.3$	0.9999	0.75	1179.3
Metamitron	$y = 4466.9x - 49466$	0.9995	0.70	6364.6
Metazachlor	$y = 420.32x + 10046$	0.9998	0.20	2065.2
Methabenzthiazuron	$y = 893.47x - 6789.3$	0.9998	0.51	1761
Methamidophos	$y = 142.43x + 1664.2$	0.9991	0.76	187.66
Methidathion	$y = 240.12x + 140.33$	0.9994	0.52	464.49
Methiocarb sulfoxide	$y = 336.35x + 524.69$	1.0000	0.84	399.51
Methomyl	$y = 700.84x + 42132$	1.0000	0.54	1297.1
Methoxyfenozide	$y = 2461x + 916.82$	1.0000	0.77	3205.8
Metobromuron	$y = 103.3x + 503.85$	0.9990	0.72	144.04
Metolachlor	$y = 521.06x + 337.15$	0.9995	0.64	818.64
Metoxuron	$y = 5106.3x + 59297$	0.9998	0.40	12894
Metribuzin	$y = 4923.4x - 35260$	0.9999	0.49	10082
Metsulfuron methyl	$y = 4787.2x - 29709$	0.9997	0.65	7338.8
Mevinphos	$y = 123.91x - 5605.7$	0.9972	0.92	135.36
Miconazole nitrate	$y = 7572.1x - 4854$	0.9999	0.67	11377
Molinate	$y = 283.15x - 1690.4$	1.0000	0.56	505.89
Monocrotophos	$y = 149.15x - 143.04$	0.9997	0.73	203.80
Monolinuron	$y = 190.16x - 1339.7$	0.9996	0.55	343.19
Monuron	$y = 610.76x + 84.68$	1.0000	0.60	1023.3
Myclobutanil	$y = 2618.7x + 12309$	0.9998	0.66	3987.4
N,N-Diethyl-2-naphthoxypropamide	$y = 1304.6x + 15768$	0.9997	0.52	2529.8
Naptalam	$y = 32.866x + 326.14$	0.9999	0.52	62.741
Neburon	$y = 952.59x - 716.98$	0.9991	0.65	1465.90
Nitenpyram	$y = 942.51x - 2250.6$	0.9999	0.90	1042.1
N-Methylcarbamathe	$y = 353.17x - 271.39$	0.9999	0.67	524.64
Norflurazone	$y = 828.18x + 151.86$	0.9997	0.62	1332
Novaluron	$y = 239.92x + 1385.4$	0.9996	0.74	323.53

Nuarimol	$y = 3987.3x + 1884.1$	0.9999	0.74	5380.1
Ofurace	$y = 684.92x + 3013.3$	0.9994	0.88	775.84
Omethoate	$y = 14.296x + 14830$	0.9999	0.05	313.87
Orbencarb	$y = 2256.9x + 5833.5$	1.0000	0.65	3479.3
Oryzalin	$y = 56.944x + 94.129$	0.9977	0.79	71.868
Oxadiazon (oxidiazinon)	$y = 66.42x - 1254$	0.9999	1.16	57.027
Oxadixyl	$y = 105.05x - 1640.5$	0.9990	0.80	131.92
Oxamyl	$y = 792.94x + 257.39$	0.9989	1.46	544.17
Oxfendazole	$y = 2318.5x - 39838$	0.9994	0.39	5889.6
Oxyfluorfen	$y = 15.334x + 286.04$	0.9993	0.58	26.661
Paclobutrazol	$y = 31777x + 125099$	0.9990	0.65	48937
Parathion	$y = 11.989x + 309.13$	1.0000	0.73	16.352
Parathion-methyl	$y = 31.129x + 590.08$	0.9991	0.57	54.45
Penconazol	$y = 3829.5x + 9264$	0.9995	0.59	6468.3
Pencycuron	$y = 18293x + 10282$	0.9993	0.82	22344
Pendimethalin	$y = 5.7533x + 419.33$	0.9999	0.58	9.99
Phenmedipham	$y = 2946.8x + 22457$	1.0000	1.00	2946.8
Phenothrin	$y = 246.6x + 616.71$	0.9999	0.32	771.72
Phentoate	$y = 4.36x + 1116$	0.9999	0.63	6.92
Phorate	$y = 21.693x + 426.5$	0.9918	0.80	27.064
Phosalone	$y = 3.8733x + 240.33$	0.9999	0.96	4.0181
Phosphamidon	$y = 5048.3x + 18164$	0.9963	0.55	9169.7
Phoxim	$y = 77.156x + 20738$	0.9999	0.91	84.447
Picloram	$y = 187.63x - 2670.1$	0.9998	0.68	276.63
Picolinafen	$y = 458.35x - 1315.3$	0.9992	0.85	540.21
Piperonyl butoxide	$y = 29845x + 136508$	0.9999	0.86	34748
Piperophos	$y = 27495x + 121459$	1.0000	0.74	37290
Pirimicarb	$y = 8518.9x - 35481$	0.9997	0.76	11166
Pirimiphos methyl	$y = 22369x - 66513$	1.0000	0.64	35055.00
Pretilachlor	$y = 3808.4x + 180996$	0.9927	0.24	15636
Prochloraz	$y = 8973.1x - 36270$	0.9998	0.65	389.14
Procymidone	$y = 23.859x + 206.9$	0.9999	0.84	28.538
Promecarb	$y = 414.87x + 609.57$	0.9999	0.64	649.24
Prometon	$y = 8973.1x - 36270$	0.9997	0.35	25369
Prometryn	$y = 10960x - 2876.2$	0.9999	0.45	24175
Propachlor	$y = 6234.3x + 21037$	0.9993	0.69	9095.1
Propamocarb	$y = 6536.9x - 60548$	0.9999	1.39	4708.70
Propanil	$y = 336.13x - 1006.5$	0.9993	0.70	482.5
Propaquizafop	$y = 1197.2x + 5468.5$	0.9992	0.74	1626.4

Propargite	$y = 332.22x - 1512.9$	0.9991	0.72	463.49
Propazine	$y = 5803.2x - 2404.6$	0.9995	0.53	10943
Propetamphos	$y = 740.7x + 663.89$	1.0000	0.95	779.67
Propiconazole	$y = 5116x + 114265$	0.9902	0.54	9547.6
Propisochlor	$y = 1478.6x + 25336$	0.9999	0.67	2221.4
Propoxur	$y = 353.1x + 16657$	0.9983	0.32	1094
Propyzamid	$y = 136.5x + 99.403$	0.9997	0.70	195.67
Proquinazid	$y = 2342.6x + 2090.2$	0.9993	0.79	2957.8
Prosulfocarb	$y = 482.23x - 1946.8$	1.0000	0.63	767.21
Prosulfuron	$y = 1377.9x + 9305.2$	0.9999	0.17	8196.9
Pymetrozin	$y = 5279.1x + 49190$	0.9999	0.46	11492
Pyracarbolid	$y = 7365.7x + 71256$	1.0000	0.40	18362
Pyraclostrobin	$y = 644.16x + 16623$	0.9948	0.59	1096.1
Pyranocoumarin	$y = 1203.5x - 10561$	0.9999	0.76	1579.3
Pyrazon	$y = 939.06x - 13733$	0.9993	0.76	1237.3
Pyridaben	$y = 138.53x + 1630.3$	0.9992	0.61	227.68
Pyridaphenthion	$y = 940.39x + 480.37$	0.9991	0.68	1382
Pyrifenox isomer 1	$y = 4341.8x - 20259$	0.9999	0.63	6880.7
Pyrifenox isomer 2	$y = 12898x - 899.48$	0.9998	0.87	14901
Pyrimethanil	$y = 8278.1x - 10453$	0.9998	0.41	20097
Pyriproxifen	$y = 7321.6x - 34124$	0.9991	0.73	10066
Pyroquilon	$y = 5820.5x + 25629$	0.9995	0.99	5879.3
Quinalphos	$y = 1139.6x - 4753.9$	0.9993	0.75	1526.5
Quinmerac	$y = 259.17x - 386.16$	0.9998	0.71	366.55
Quinoclamine	$y = 335.21x + 5235.3$	0.9993	0.87	385.04
Quinoxifen	$y = 996.03x - 2935.8$	0.9997	0.72	1377.6
Quizalofop-p-ethyl	$y = 563.61x - 223.08$	1.0000	0.72	785.9
Rotenone	$y = 194.39x + 236.74$	1.0000	0.67	291.48
Secbumeton	$y = 38395x - 22068$	0.9999	0.58	66332
Sethoxydim	$y = 7311.3x + 122137$	0.9996	0.26	28078
Siduron isomer 1	$y = 18756x + 32664$	1.0000	0.88	21282
Siduron isomer 2	$y = 3995.6x + 8442.3$	1.0000	0.97	4139.9
Simazine	$y = 43.826x - 19.123$	1.0000	0.34	129.66
Spinosyn A	$y = 9430.1x + 30545$	0.9975	0.71	13303
Spinosyn D	$y = 1290.6x + 5421.7$	0.9994	0.58	2228.5
Spiromesifen	$y = 1607.1x - 3350.2$	1.0000	0.57	2809.3
Spirotetramat	$y = 7454.6x + 121775$	0.9998	1.16	6444
Sulcotrione	$y = 2875.3x - 46809$	0.9992	0.68	4204.4
Sulfometuron methyl	$y = 919.84x - 4129.1$	0.9999	0.55	1664.7

Sulfotep	$y = 214.57x - 258.9$	0.9994	0.89	240.13
Sulprofos	$y = 563.19x + 10133$	1.0000	0.41	1362.1
Tau-fluvalinate	$y = 280.21x - 10969$	0.9999	0.77	365.75
TCPP	$y = 685.65x + 11938$	0.9999	0.64	1074.2
Tebuconazole	$y = 5222.8x - 25719$	0.9996	0.68	7678
Tebufenpyrad	$y = 1248.6x - 3129.2$	0.9997	0.70	1778
Tebutam	$y = 36277x + 656464$	0.9999	0.59	61878
Tebuthiuron	$y = 29288x + 157299$	0.9991	0.61	48046
Teflubenzuron	$y = 10.051x + 229.46$	0.9986	1.05	9.5612
Tembotrione	$y = 110.75x - 194.11$	1.0000	0.83	133.67
Temephos	$y = 35.522x + 4057$	0.9996	0.39	90.74
Tepraloxymid	$y = 495.31x - 2530.7$	0.9993	0.35	1432.3
Terbacil	$y = 26.157x - 602.23$	0.9998	0.34	76.296
Terbufos	$y = 90.523x - 140.56$	0.9998	0.39	232.83
Terbumeton	$y = 20747x + 110836$	1.0000	0.33	63250
Terbutylazine	$y = 3328.3x + 6484.2$	0.9997	0.51	6528.5
Terbutryn	$y = 9128.8x - 16145$	0.9999	0.47	19417
Tetrachovinphos	$y = 68.846x + 2023.8$	0.9999	0.49	141.31
Thiabendazole	$y = 6581.5x + 29673$	0.9991	0.81	8099.8
Thiacloprid	$y = 529.46x - 3074.1$	0.9999	0.84	628.60
Thiamethoxam	$y = 39.415x - 155.9$	0.9998	0.71	55.155
Thidiazuron	$y = 3568.1x - 19611$	0.9997	0.88	4036.7
Thiocyclam	$y = 450.49x - 5645.8$	0.9999	1.27	354.81
Thiodicarb	$y = 3059.1x + 33713$	0.9999	1.79	1708.3
Thiofanox	$y = 1142.4x + 55154$	0.9976	0.70	1626.1
Thiophanate methyl	$y = 176.33x - 134.75$	0.9994	0.86	204.41
Tolclofos methyl	$y = 502.75x + 2625.1$	1.0000	0.58	865.9
Tolyfluanid	$y = 130.22x + 1343.9$	0.9965	1.98	65.822
Tralkoxidym	$y = 13633x + 8846.3$	0.9996	0.35	38803
Transfluthrin	$y = 5.1721x + 52.055$	1.0000	0.90	5.7751
Triadimefon	$y = 1267.4x - 2385.6$	0.9998	0.63	2021
Triadimenol	$y = 68.661x + 2210.4$	0.9999	0.67	102.1
Triallat	$y = 107.56x + 1871.5$	1.0000	0.85	126.52
Triasulfuron	$y = 4320.9x - 48130$	0.9998	0.79	5457.3
Triazophos	$y = 2998x + 9374.5$	1.0000	0.54	5515.2
Triazoxid	$y = 6764x - 5914.9$	0.9999	0.75	9078.8
Trichlorfon	$y = 68.146x - 276$	0.9992	0.98	69.79
Triclocarban	$y = 159.51x + 137.96$	0.9999	0.63	251.89
Tridemorph	$y = 8978.7x - 26813$	0.9999	0.67	13438

Trifloxystrobin	$y = 357.16x + 881.18$	0.9999	0.70	507.21
Triflumizole	$y = 137.14x + 3.5$	0.9999	0.54	251.91
Triflumuron	$y = 42.8x - 216$	0.9997	0.78	54.73
Trinexapac-ethyl	$y = 357.91x + 1570.7$	0.9991	0.62	575.98
Triticonazole	$y = 502.75x + 2625.1$	1.0000	0.03	19597
XMC (3,5-xylmethylcarbamate)	$y = 33.039x + 3007.3$	1.0000	0.44	74.586
Zoxamide	$y = 3294.6x - 1410.3$	0.9999	0.76	4345.4
α -Cypermethrin	$y = 13.812x - 898.25$	0.9997	1.03	13.351



Conclusiones

IV. Conclusiones

En la presente Tesis se ha evaluado la potencialidad de la cromatografía de líquidos-espectrometría de masas con analizador de tiempo de vuelo para el análisis de contaminantes orgánicos en alimentos, a través del empleo de bases de datos de masas exactas de iones. Del trabajo realizado se pueden obtener las siguientes conclusiones generales:

1.- Se ha encontrado que la separación cromatográfica (UHPLC) es clave para poder resolver la mayoría de las coeluciones que se han presentado en el estudio debido al elevado número de analitos incluidos. Por este motivo, para la creación de una base de datos con más de 600 compuestos es crucial estudiar detalladamente la cromatografía, que todavía juega un papel fundamental en este tipo de metodologías, al permitir la separación e identificación de prácticamente todos los analitos en un único análisis, con la excepción de algunos compuestos que ni siquiera empleando fragmentación CID en celda de colisión podían ser resueltos.

2.- Por lo que respecta a la capacidad de identificación empleando fragmentación, se ha observado tras un estudio exhaustivo de la fragmentación tanto en la fuente (*in source CID fragmentation*) como empleando celda de colisión (*all ion mode CID MS/MS fragmentation*), que el primer tipo de experimento ofrece información para un número limitado de compuestos (85% aproximadamente). Para los casos restantes y salvo contadas excepciones de moléculas de bajo peso molecular, la aproximación MS/MS en celda de colisión sin aislamiento de ion precursor (*all ion mode*) es la más adecuada para este tipo de metodologías de screening, aportando información específica que permite la identificación inequívoca de las especies incluidas en la base de datos.

IV. CONCLUSIONES

3. Las principales limitaciones encontradas en la metodología propuesta son la limitada sensibilidad del equipo para un determinado número de compuestos, entorno al 10 %, que presentan baja respuesta por su dificultad de ser ionizados en la fuente *electrospray* y además, otros aspectos de tipo práctico, como la efectividad limitada del software actualmente disponible para este tipo de métodos de *screening*, dada la dificultad de gestionar tanta información.

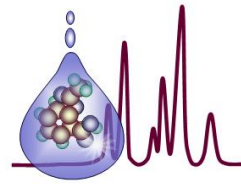
4.- El método de *screening* propuesto ha sido aplicado a la determinación de más de 600 contaminantes orgánicos en muestras de alimentos. Se examinó la linealidad, efectos matriz y límites de cuantificación en diferentes matrices (tomate, naranja y potitos obtenidos a base de carne y pescado). Se encontró que los valores de los límites de detección empeoran conforme la matriz es más compleja, de forma que para un porcentaje de entre el 10 y el 15 % de los compuestos no se llega al nivel de los valores de límite máximo de residuos (LMRs) establecidos para las combinaciones pesticida/matriz estudiadas. Éste hecho se agudizaba para el caso de la matriz de naranja, mucho más compleja y que presentaba efectos matriz mucho más significativos. La sensibilidad es quizás la principal debilidad del método propuesto, ya que es difícil que ésta pueda alcanzarse de manera satisfactoria absolutamente para todos los compuestos bajo unas condiciones instrumentales concretas (ionización mediante *electrospray*). El empleo de instrumentación con transmisión de iones y fuentes de ionización asistidas, térmicamente optimizadas, podría mejorar esta situación aunque es difícil, en cualquier caso, para aquellos analitos que por su naturaleza presentan unas características incompatibles con la ionización mediante *electrospray*.

5.- Se obtuvieron resultados muy satisfactorios en lo que respecta al método de extracción en fase sólida con cartuchos poliméricos desarrollado para el

IV. CONCLUSIONES

tratamiento de muestra genérico empleado en la determinación simultánea de pesticidas y micotoxinas en muestras de vino. El método desarrollado permitía detectar la mayoría de los analitos estudiados a niveles de concentración muy bajos, presentando efecto matriz relativamente reducido para la mayoría de éstos.

6.- Finalmente, los métodos desarrollados fueron aplicados a más de 80 muestras de alimentos de diferentes tipos (mermeladas y vinos). Los resultados obtenidos mostraron que en la mayoría de las muestras se encontraron pesticidas (y micotoxinas en el caso de las muestras de vino), aunque el contenido de los pesticidas detectados era inferiores a los límites máximos de residuos (LMRs) para los productos de los que estos alimentos se derivan. Esto puede indicar que no constituye un gran riesgo el consumo de productos derivados, pero sí pone de manifiesto la necesidad de establecer LMRs que regulen su contenido de pesticidas, para así garantizar que su consumo es seguro.



Contribuciones Científicas

V. CONTRIBUCIONES CIENTÍFICAS.

La información incluida en la presente Tesis Doctoral ha formado parte de un capítulo de libro, un artículo de investigación publicado en una revista de ámbito internacional (Journal of Chromatography A) y 3 artículos, pendientes de publicar en revistas científicas también de amplia importancia (Journal of Chromatography A and Food Chemistry).

Las contribuciones científicas son:

A) Publicaciones.

1. Título: Bases de datos para el estudio de residuos de pesticidas (Capítulo de libro (Introducción)).

Autores: Juan F. García-Reyes, Patricia Pérez-Ortega, Bienvenida Gilbert-López and Antonio Molina-Díaz

In: L.M. Nollet, H. Heinzen, A.R. Fernández-Alba (Ed). Multiresidue methods for Pesticide Trace Analysis in Food. Ed. CRC Press, **2015**.

2. Título: Estudio de las principales ventajas e inconvenientes de la cromatografía de líquidos de ultraelevada eficacia acoplada con espectrometría de masas de tiempo de vuelo (UHPLC-TOFMS) para el desarrollo de métodos de *screening* para la detección de más de 600 contaminantes orgánicos (Artículo de Investigación).

Autores: Patricia Pérez-Ortega, Felipe J. Lara-Ortega, Juan F. García-Reyes and Antonio Molina-Díaz

Revista: Pendiente de publicación en Journal of Chromatography A, February 2015.

3. Título: Desarrollo de un método para la detección de más de 600 contaminantes (pesticidas, productos veterinarios, micotoxinas y otras

especies) en alimentos mediante cromatografía de líquidos de alto rendimiento y espectrometría de masas de tiempo de vuelo (UHPLC-TOFMS). (Artículo de investigación).

Autores: Patricia Pérez-Ortega, Juan F. García-Reyes and Antonio Molina-Díaz.

Revista: Pendiente de publicación en Journal of Chromatography A, February 2015.

4. Título: Método genérico de tratamiento de muestra para la determinación simultánea de pesticidas y micotoxinas en vino mediante cromatografía de líquidos-espectrometría de masas (Artículo de Investigación).

Autores: Patricia Pérez-Ortega, Bienvenida Gilbert-López, Juan F. García-Reyes, Natividad Ramos-Martos and Antonio Molina-Díaz

Revista: Journal of Chromatography A 1249 (2012) 83-91.

5. Título: Determinación de más de 350 pesticidas multiclase en mermeladas obtenidas a base de frutas mediante cromatografía de líquidos de alta resolución-tiempo de vuelo-espectrometría de masas (UHPLC-TOFMS). (Artículo de Investigación).

Autores: Patricia Pérez-Ortega, Felipe J. Lara-Ortega, Juan F. García-Reyes and Antonio Molina-Díaz.

Revista: Pendiente de publicación en Food Chemistry, February 2015.

(B) COMUNICACIONES A CONGRESOS

1. Título: "Development of a multiclass method for the determination of pesticides and micotoxins in red wines by HPLC-TOFMS"

Autores: P. Pérez-Ortega, J.C. Domínguez-Romero, B. Gilbert-López, J.F. García-Reyes, N. Ramos-Martos, A. Molina-Díaz

Participación: Tipo Póster.

Congreso: XIII International Conference of Instrumental Analysis, Barcelona, España, 14-16 Noviembre 2011.

2. Título: “Desarrollo de una base de datos de masas exactas de iones para la detección de 600 contaminantes orgánicos en alimentos de origen vegetal mediante cromatografía de líquidos/espectrometría de masas de alta resolución”

Autores: P. Pérez-Ortega, J.F. García-Reyes, N. Ramos-Martos, A. Molina-Díaz.

Participación: Tipo Póster.

Congreso: XIII Reunión del Grupo Regional Andaluz de la Sociedad Española de Química Analítica, Málaga, España, 7-8 Junio 2012.

3. Título: “Screening of 400 multiclass pesticides in fruit jam by ultrahigh pressure liquid chromatography-time-of-flight mass spectrometry”

Autores: F.J. Lara-Ortega, P. Pérez-Ortega, J.F. García-Reyes, N. Ramos-Martos, A. Molina-Díaz

Participación: Tipo Póster.

Congresos: XIII Reunión del Grupo Regional Andaluz de la Sociedad Española de Química Analítica, Málaga, España, 7-8 de Junio de 2012/ XVIII Reunión de la Sociedad Española de Química Analítica/ VI Reunión de la Sociedad Española de Espectrometría de Masas, Úbeda, España, 16-19 Junio 2013.

4. Título: “Performance of a screening method for the detection of 600 multiclass contaminants in food by liquid chromatography-high resolution mass spectrometry”

Autores: P. Pérez-Ortega, J.F. García-Reyes, A. Molina-Díaz

Participación: Tipo Póster.

Congreso: XVIII Reunión de la Sociedad Española de Química Analítica/ VI Reunión de la Sociedad Española de Espectrometría de Masas, Úbeda , España, 16-19 Junio 2013.

5. Título: “Performance of a screening method for the detection of 600 multiclass contaminants in food by liquid chromatography-high resolution mass spectrometry”

Autores: P. Pérez Ortega, J.F. García Reyes, A. Molina Díaz

Participación: Tipo Póster.

Congreso: XIV Reunión del Grupo GRASEQA de la Sociedad Española de Química Analítica, Baeza, España, 26-27 Junio 2014.

6. Título: “Parameters affecting the performance of LC-HRMS Screening methods for multiclass screening of 600 organic contaminants in food base on accurate mass database”

Autores: P. Pérez-Ortega, J.F. García-Reyes, A. Molina-Díaz

Participación: Tipo Póster. (ISBN: 978-80-7080-861-0).

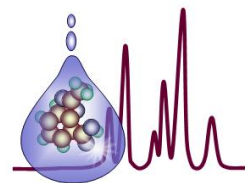
Congreso: 6th International Symposium on Recent Advances in Food Analysis (RAFA 2013), Praga (Czech Republic), 5-8 Noviembre 2013.

7. Título: “Parameters affecting the performance of LC-HRMS Screening methods for multiclass screening of 600 organic contaminants in food based on accurate mass database”

Autores: P. Pérez-Ortega, J.F. García-Reyes, A. Molina-Díaz

Participación: Tipo Póster.

Congreso: 65th Pittsburg Conference on Analytical Chemistry and Applied Spectroscopy (PITTCO 2014), Chicago (USA), Marzo 2014.



Acrónimos

ACRÓNIMOS

Acronimo	Definición
A	
AECOSAN	<i>Agencia Española de Consumo, Seguridad Alimentaria y Nutrición</i>
AFB ₁	Aflatoxina B ₁
AFB ₂	Aflatoxina B ₂
AFG ₁	Aflatoxina G ₁
AFG ₂	Aflatoxina G ₂
AFM ₁	Aflatoxina M ₁
AFM ₂	Aflatoxina M ₂
C	
CCAH	Comité Científico de la Alimentación Humana
CONTAM	Panel de Contaminantes de la Cadena Alimentaria
CID	<i>Collision-induced dissociation</i> . Disociación inducida por colisión
D	
DEHP	Di (2-etilhexil) ftalato
DINP	Di (iso-nonil) ftalato
DI-SPME	<i>Direct inmersión SPME</i> . Microextracción en fase sólida por inmersión directa
DLLME	<i>Dispersive liquid-liquid microextraction</i> . Microextracción líquido-líquido dispersiva
DON	Deoxinivalenol
E	
ECD	<i>Electron Capture Detector</i> . Detector de Captura electrónica
EFSA	<i>European Food Safety Authority</i> . Autoridad Europea de Seguridad Alimentaria
EI	<i>Electron impact</i> . Impacto electrónico
EIC	<i>Extracted Ion chromatogram</i> . Cromatograma del ión extraído
EMA	Agencia Europea de Medicamentos
ESI	<i>Electrospray Ionization</i> . Ionización por Electrospray
F	
FID	<i>Flame Ionization Detector</i> . Detector de ionización de llama
FB1	Fumonisina B ₁
G	
GC	<i>Gas chromatography</i> . Cromatografía de gases
GCB	<i>Graphitized carbon black</i> . Carbón grafitizado
GPC	<i>Gel permeation chromatography</i> . Cromatografía de permeación en gel
H	
HLB	<i>Hydrophilic lipophilic balanced copolymer</i> . Copolímero de balance hidrofílico-lipofílico

ACRÓNIMOS

HPLC	<i>High performance liquid chromatography</i> . Cromatografía de líquidos de alta eficacia
HS-SPME	<i>Headspace-SPME</i> . Microextracción en fase sólida de espacio de cabeza
H-T2	Toxina HT-2
I	
IDA	<i>(ADI-Acceptable daily intake)</i> . Ingesta diaria admisible
IARC	<i>International Agency for Research on Cancer</i> . Agencia Internacional de Investigación sobre el Cáncer
L	
LC	<i>Liquid Chromatography</i> . Cromatografía de líquidos
LC-MS/MS	<i>Liquid Chromatography-tandem mass spectrometry</i> . Cromatografía de líquidos-espectrometría de masas en tándem
LC-TOFMS	<i>Liquid Chromatography-time of flight-mass spectrometry</i> . Cromatografía de líquidos-espectrometría de masas de tiempo de vuelo
LLE	<i>Liquid-liquid extraction</i> . Extracción líquido-líquido
LME	Límite de migración específica
LMG	Límite de migración global
LOD	<i>Limite of detection</i> . Límite de detección
LOQ	<i>Limite of quantification</i> . Límite de cuantificación
M	
MeCN	<i>Acetonitrile</i> . Acetonitrilo
MeOH	<i>Methanol</i> . Metanol
MRM	<i>Multiple reaction monitoring</i>
MRL	<i>Maximum residue level</i> . Límite máximo de residuos permitido
MS	<i>Mass spectrometry</i> . Espectrometría de masas
MS/MS	<i>Tandem mass spectrometry</i> . Espectrometría de masas en tándem
MSPD	<i>Matrix solid phase dispersion</i> . Dispersión de matrix en fase sólida
N	
ND	<i>Non-detected</i> . No detectado
NIV	Nivalenol
NOEL	<i>No observed effective level</i> . Nivel de dosis sin efecto observado
NPD	Nitrogen-phosphorus detector. Detector fósforo-nitrógeno
O	
OTA	Ochratoxina A
P	
PFAS	<i>Perfluoroalkoxy alkanes</i> . Sustancias perfluoroalquiladas
PFOA	<i>Perfluorooctanoic acid</i> . Ácido perfluorooctanoico
PFOS	<i>Perfluorooctanesulfonic acid</i> . Sulfonato de perfluorooctano
PSA	<i>Primary secondary amine</i> . Amina primaria secundaria

ACRÓNIMOS

Q	
QQQ	<i>Triple quadrupole.</i> Triple cuadrupolo
QuEChERS	<i>Quick, Easy, Cheap, Effective, Rugged and Safe.</i> Rápido, fácil, barato, efectivo, robusto y seguro
R	
r	<i>Correlation Coefficient.</i> Coeficiente de Correlación
RSD	<i>Relative Standard Deviation.</i> Desviación estándar relativa
S	
SLE	<i>Solid liquid extraction.</i> Extracción Sólido-Líquido
S/N	<i>Signal-to-noise ratio.</i> Relación señal-ruido
SPE	<i>Solid-phase extraction.</i> Extracción en fase sólida
SPME	<i>Solid-phase microextraction.</i> Microextracción en fase sólida
STE	Esterigmastocistina
T	
T-2	Toxina T-2
TIC	<i>Total ion chromatogram.</i> Cromatograma de iones totales
TOF	<i>Time-of-flight.</i> Tiempo de vuelo
tR	<i>Retention time.</i> Tiempo de retención
U	
UE	<i>European Union.</i> Unión Europea
UV	<i>Ultraviolet.</i> Ultravioleta
W	
WHO	<i>World Health Organization.</i> Organización Mundial de la Salud
Z	
ZEN	<i>Zearalenone</i>

