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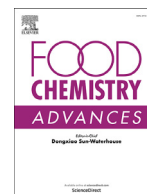
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Thermal degradation of pesticide active substances: Prioritisation list

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ABSTRACT

This study aims at estimating which pesticide active substances (ASs) are the best candidates to study potential further degradation of the AS above 120°C. To achieve this, a prioritisation list was built following five consecutive criteria. This first includes substances that are anthropogenic, have a carbon backbone structure, are authorized in the European Union, and have a defined maximum residue limit (MRL). Then, substances were selected according to their physicochemical and structural properties, MRL in main food commodities, standard price and degradation in hydrolysis studies below 120°C. The results showed that out of the initial 1 478 substances reported in the European pesticide database, 24 ASs were selected as the best candidates to test the assumption of degradation above 120°C. This prioritisation list could be useful for future research studies to build their own list and save time in selecting suitable candidates according to their criteria.

Introduction

Treatment of crops with plant protection products (PPPs) containing active substances (ASs) may leave residues in food and feed commodities in the form of the parent compound (AS), metabolites, and breakdown products (degradation products) (Chun *et al.*, 2003; García *et al.*, 2022; Navarro *et al.*, 2007; Olisah *et al.*, 2020). In the European Union (EU), possible exposure to residues is addressed during the (re-)evaluation of the AS prior to marketing (re-)authorisation under Regulation (EC) No 1107/2009 (EUR-Lex, 2009). For the AS, this scientific evaluation is carried out according to data requirements listed in Regulation (EC) No 283/2013 (EUR-Lex, 2013) and is further described in multiple OECD technical guidelines (OECD, 2007a, 2007b, 2007c, 2008). The evaluations are summarised in assessment reports, both for AS during their (re-)authorisation or for PPPs (re-)approval. To take into account the potential effects of cooking processes, which concerns a large proportion of consumed food, specific experiments were carried out on the degradation of AS residues, according to OECD Guideline Test N° 507 (OECD, 2007c).

Currently, if the use of PPPs lead to significant residue levels in the raw agricultural commodity (RAC), studies are required to investigate the degradation pathway of the residue during processing, known as hydrolysis studies. These studies are performed on buffer solutions spiked with radiolabelled AS (mostly with ¹⁴C) that undergo different hydrolysis conditions (time, temperature, and pH) below 120°C. If degrada-

tion products are produced at significant concentrations in these hydrolysis studies (10% of the total radioactive residue), they are identified and their (geno-)toxic properties are determined in order to assess their relevance for consumer risk assessment. However, certain cooking processes such as oven cooking, grilling or frying (Göckener *et al.*, 2020; Martin *et al.*, 2020) reach temperatures above 120°C and up to 250°C. Since further degradation is expected with increasing temperatures, one can assume that some degradation products may be formed above 120°C.

To verify this assumption, a review was conducted both on academic research literature as well as literature reports submitted by pesticide manufacturers in the framework of regulatory pesticide approval (Dubocq *et al.*, 2022). However, due to the lack of academic studies conducted above 120°C, no conclusion could be drawn about the possible degradation products that could be overlooked when following the EU regulation. As a result, an exploratory evaluation involving thermodegradation studies conducted above 120°C would be of great interest to assess whether the range of temperatures currently required in hydrolysis studies sufficiently elucidates the degradation pathway of the AS as well as its residues during processing.

To achieve this objective, the key question is a matter of prioritisation, i.e., to select, out of the high number of variables, those that suitably answer the scientific question. As research advances, prioritisation is a preliminary but key step when starting scientific studies, especially in the scope of risk assessment, to decide how complex situ-

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ations can be described. Since this clarifies the relevance of the choices behind scientific approaches, but also provides key orientations for research, the number of studies involving a prioritisation step is increasing (Braeuning et al., 2022; Luijten et al., 2022; Sjerps et al., 2021).

Here, prioritisation aims at carefully selecting both the prioritisation parameter to consider (e.g., substances of concern, patterns of exposure, and matrices of interest) and the criteria enabling to build an abbreviated list. Since this work investigates thermodegradation studies, it was decided to conduct prioritisation of AS, with the aim of selecting a limited number of compounds out of the 1 478 ASs listed in the EU Pesticide Database (EUPD). Selection was carried out to reveal compounds that could produce potential degradation products above 120°C that are not observed in the OECD hydrolysis tests (OECD, 2007c) required in the regulatory framework. Here are proposed five prioritisation criteria to select the best candidates to test the assumption of degradation above 120°C. A detailed list was created following each criterion, in the light of other works dealing with prioritisation for risk assessment. As a result, future studies involving prioritisation lists of AS could adapt the criteria proposed in this study to their own objectives.

Prioritisation workflow

a. Step 1: EU regulation

The EUPD, in open access on the European Commission website, reports all the ASs approved and not approved for the EU market. It provides the initial list of ASs with a total of 1 478 records (European Commission, 2023). The EUPD also comprises a list of ASs for which maximum residue limits (MRLs) have been set, with a total of 656 matching records. MRLs can be defined as the highest level of a pesticide residue that is legally tolerated in or on food or feed commodities when pesticides are applied at field levels (European Commission, 2021). This is the amount of pesticide expected to be detected in raw food commodities when the active substance is used according to EU recommendations. These MRL values are set for each food commodity/active substance pair based on the critical intended agricultural use considering the toxicity of the substance and possible human exposure. For some ASs, MRLs were not deemed necessary based on the five criteria described in SANCO/11188/2013 Rev (European Commission, 2015); therefore, these ASs were excluded from the prioritisation list. Among the 656 ASs with MRLs were excluded: (i) non-approved ASs in the EU market as their residues are less likely to be present in food consumed in EU than approved AS, (ii) inorganic ASs (without a carbon backbone structure) and microorganisms as they are not likely to be detected using organic analytical chemistry instruments, and (iii) natural products (such as plant extracts) that are out of scope. At the end of step 1, the initial list dropped down to 232 ASs.

b. Step 2: Physicochemical properties

Physicochemical properties are expected to be key factors in AS degradation during high temperature processes. Thus, four main properties were used to select only ASs based on their predicted degradation pathway and the overall capacity to analyse them.

Molar mass of the substance: Only ASs having a mass between 250 and 600 g/mol were retained. Small active substances (< 250 g/mol) were excluded for analytical reasons because their degradation products are expected to be smaller molecules (< 50 g/mol) that are difficult to detect and analyse with mass spectrometers. The higher threshold of 600 g/mol was selected: (i) for analytical reasons, since the analytical parameters would need to be modified in order to optimize the detection of higher masses, and (ii) since most of the active substances have a molar mass below this threshold. Analysing compounds in a narrow range of masses makes it possible to obtain higher accuracy during instrument calibration and chemical analysis, facilitating the identification of degradation products following thermodegradation studies.

Log Kow value: The octanol/water partition coefficient (ratio between molecule concentrations in octanol and in water) provides information on the water affinity of an AS. It also gives information about the polarity and the volatility of the analysed compound. Different chromatography techniques are used depending on the log Kow value of the analysed substances. The two main analytical techniques are: (i) liquid chromatography, used to analyse polar to mid-polar compounds, and (ii) gas chromatography, used to analyse mid-polar to non-polar compounds (Brack et al., 2016). ASs with a log Kow < 0 were excluded as they are difficult to detect in traditional reversed-phase liquid chromatography and gas chromatography analytical methods.

Chemical structure: The degradation of a compound can be predicted by looking at its chemical structure, meaning the atoms, the chemical bonds between atoms, and the functional groups (Fenner et al., 2013; Gangola et al., 2022). To keep in the prioritisation list compounds that are more likely to degrade with increasing temperatures, retained ASs were the ones that have: (i) heteroatoms such as nitrogen, oxygen, sulphur, fluorine, chlorine, or bromine, (ii) at least one ring, containing heteroatoms or not, (iii) specific groups such as carboxylic acid, cetone, aldehyde, ester, amine, amide, or cyano, and (iv) carbon/heteroatom or heteroatom/heteroatom bonds that are expected to break easily when increasing the temperature (Hoang et al., 2014; Tsugawa et al., 2016). When an AS does not fulfil all these criteria, it was not included in the final prioritisation list. Despite other parameters that have defined threshold values (e.g., mass between 250 and 600, log kow > 0), this step was conducted according to author appreciation (selecting compounds according to their general structure). To mitigate exclusion of ASs based on subjective criteria, a supplementary list was reported and marked as “Possibly” in Table 2 (detailed list of substances that passed “Step 1”). This supplementary list was further refined with the following criteria to include compounds widely monitored in scientific literature (e.g., pyrethroids) that could still be of interest for further thermodegradation studies. This step enabled us to reduce the list to 120 ASs in the main list, and 44 ASs in the supplementary list.

c. Step 3: Presence in main food commodities

The MRLs for the 120 ASs selected in step 2 were checked for 8 RACs (wheat, apple, milk, olive oil, potato, rapeseed, sunflower and tomato). These RACs were selected because: (i) they are often ingested following thermal treatments such as frying, boiling or microwaving (Deak et al., 2023), and (ii) they are widely consumed in the European diet and contribute strongly to human exposure (European Food Safety Authority (EFSA), 2011). From all substances were retained those with MRLs above the limit of quantification (LOQ) on at least five of the eight RACs (presence in most of the food commodities), or one of the eight if previously monitored by the Laboratory for Food Safety at the French Agency for Food, Environmental and Occupational Health & Safety (ANSES) (already studied in the laboratory). Following step 3, 32 ASs were kept for further investigation in the main list, and 10 ASs in the supplementary list.

d. Step 4: Price of the analytical standard

Six ASs (benzovindiflupyr, cyantraniliprole, fenpyrazamine, fluopyram, penthiopyrad and sulfoxaflor) were excluded from the list since the price of the analytical standard exceeded € 200 for 100 mg. This parameter was selected to match the budget of the overall project. It can be considered as a limitation of the project, but can be adapted for other studies that can increase this price threshold.

e. Step 5: Degradation studies at temperatures below 120°C

In the framework of AS authorisation, hydrolysis studies are conducted up to 120°C to mimic pasteurisation (90°C, pH=4, 20'), baking/boiling, brewing (100°C, pH=4, 60') and sterilisation (120°C, pH=6, 20') (OECD, 2007c). During hydrolysis studies, the total radioactive residue is monitored to ensure that no loss of radioactivity is observed

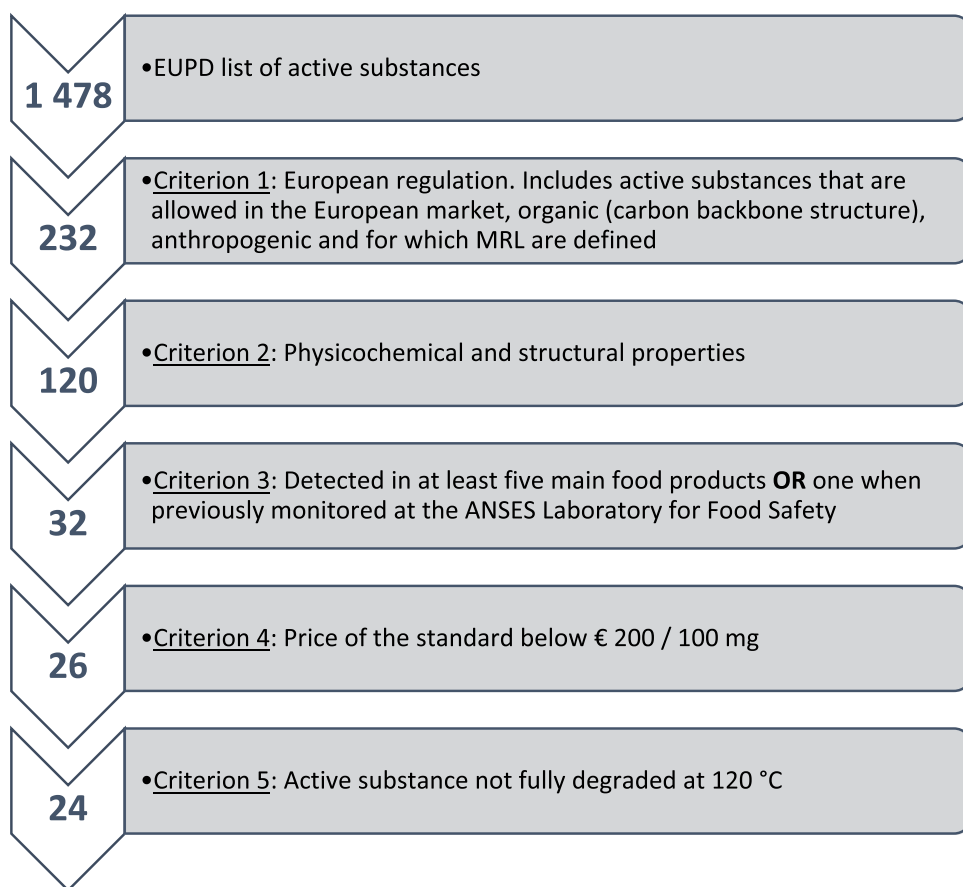


Fig. 1. Summary of the overall prioritisation workflow

during the process. If total radioactivity remains stable while radioactivity specific to the AS decreases, this means that there is degradation of the AS. Since the aim of the project was to select the best AS candidates to conduct thermodegradation studies above 120°C, AS that were found to be fully degraded in hydrolysis studies below 120°C (no radioactivity corresponding to the AS at the end of the process) were considered to be not relevant. In their respective assessment reports, based on hydrolysis studies, out of the 26 ASs, 14 are reported to be stable up to 120°C, 7 are partly degraded into degradation products, 2 are fully degraded into degradation products, and 3 were not investigated for thermal degradation. The two fully degraded ASs (captan and folpet) were removed from the list since their degradation products during hydrolysis (tetrahydrophthalimide for captan and phthalimide and phthalimic acid for folpet) were small molecules: (i) not expected to further degrade at temperatures above 120°C and (ii) difficult to analyse using mass spectrometry. The main prioritisation list consists of 24 ASs with their chemical properties shown in Table 1, and their formula and structure presented in Fig. 2.

Prioritisation list

The prioritisation approach developed here is required since it is not feasible as a research study to conduct thermodegradation for all ASs, and applying it randomly to some substances could induce bias in the overall methodology. As such, the overall workflow proposed here and described in Fig. 1 enabled to select 24 ASs out of the initial 1 478 initial ASs reported in the EUPD. Moreover, Table 2 lists the 232 ASs selected following step 1, as well as details on their exclusion/inclusion from steps 2 to 5. Further studies could thus use the proposed workflow to adapt selected ASs to their specific objectives. For instance, if the price of the analytical standard is not a limitation in other studies, they could include the six ASs removed during this step to their final prioritisation

list. This is possible since, according to the Table 2, all these six ASs also pass all other steps including the “Step 5”.

This prioritisation is based on previous works conducted in air (Hulin et al., 2021) and aquatic environment (Guillén et al., 2012), which show how important it is to select relevant compounds to conduct monitoring and risk assessment. However, to the best of our knowledge, this prioritisation list is the first one to consider thermodegradation studies to estimate active substances that need to be further evaluated. This investigation could help to estimate the risk exposure to consumers or to the person cooking contaminated food commodities.

The novelty of this study is also the use of regulatory studies conducted for each AS before marketing authorisation to build prioritisation list. Information required to build regulatory studies are rarely mentioned in research studies and their accessibility was difficult, even if it has greatly been improved nowadays. Hydrolysis studies, that are part of regulatory studies, are thus not often considered to evaluate degradation of ASs at higher temperatures even if they can be a foundation to estimate the behaviour of ASs during heating treatment. Here, consideration of hydrolysis studies enabled to use key parameters from the regulation point of view that are often not investigated from scientific researches, especially above 120°C. Moreover, the possible exposure to degradation and volatilisation products from contaminated food commodities following thermal treatments above 120°C is not yet well known and need further investigation.

All 24 ASs in the prioritisation list are authorised in the EU. Table 1 reports the countries where the ASs are marketed. Among these 24 ASs, 14 are fungicides, 6 are insecticides, 3 are herbicides, 2 are acaricides, and 1 is a plant growth regulator. The AS m/z values (mass to charge ratio, utilised in mass spectrometry following ionisation of the compounds) range from 253 to 502, and the AS log Kow values range from 1.36 to 7.02. These properties allow analysis of the AS by either liquid chromatography or gas chromatography, but also of their

Table 1
 Prioritisation list (FU = Fungicide, AC = Acaricide, IN = Insecticide, HB = Herbicide, PG = Plant growth regulator, ND = not determined, † according to Dr. Ehrenstorfer supplier and “> Dec” means that the product is decomposed before the boiling temperature)

CAS No.	Name	Formula	Detected in X main food products	Authorised in X countries in Europe	Category	Log Kow (*pubchem, **IUPAC)	Degraded < 120°C?	Previously analysed in the laboratory?	Price for 100 mg (€)†	Melting T° (°C)	Boiling T° (°C)	Decomposition T° (°C)
131860-33-8	Azoxystrobin	C ₂₂ H ₁₇ N ₃ O ₅	5	25	FU	2.50*	No	Yes	77	116	ND	345
149877-41-8	Bifenazate	C ₁₇ H ₂₀ N ₂ O ₃	2	23	AC	3.40*	No	Yes	192	122	> Dec	240
581809-46-3	Bixafen	C ₁₈ H ₁₂ Cl ₂ F ₃ N ₃ O	3	24	FU	3.3**	No	Yes	96	147	> Dec	250
188425-85-6	Boscalid	C ₁₈ H ₁₂ Cl ₂ N ₂ O	7	28	FU	2.96*	No	No	70	145	> Dec	300
500008-45-7	Chlorantraniliprole	C ₁₈ H ₁₄ BrCl ₂ N ₅ O ₂	7	23	IN	2.76*	Partly	Yes	104	210	> Dec	330
101205-02-1	Cycloxydim	C ₁₇ H ₂₇ NO ₃ S	5	27	HB	1.36**	Partly	No	59	40	> Dec	200
119446-68-3	Difenoconazole	C ₁₉ H ₁₇ Cl ₂ N ₃ O ₃	6	28	FU	4.40*	No	No	28	82	> Dec	337
110488-70-5	Dimethomorph	C ₂₁ H ₂₂ ClNO ₄	2	27	FU	2.68*	No	Yes	77	135	> Dec	280
149961-52-4	Dimoxystrobin	C ₁₉ H ₂₂ N ₂ O ₃	2	16	FU	3.59**	No	Yes	57	139	> Dec	300
3347-22-6	Dithianon	C ₁₄ H ₄ N ₂ O ₂ S ₂	6	27	FU	2.84*	Partly	Yes	23.6	215	> Dec	222
126833-17-8	Fenhexamid	C ₁₄ H ₁₇ Cl ₂ NO ₂	1	24	FU	3.51*	No	Yes	77	153	> Dec	230
113158-40-0	Fenoxaprop-P	C ₁₆ H ₁₂ ClNO ₅	8	25	HB	1.83**	Not investigated	No	72	87	> Dec	330
69377-81-7	Fluroxypyr	C ₇ H ₅ Cl ₂ FN ₂ O ₃	2	28	HB	2.20*	Not investigated	Yes	70	232	ND	ND
907204-31-3	Fluxapyroxad	C ₁₈ H ₁₂ F ₅ N ₃ O	7	26	FU	3.13**	No	No	83	157	> Dec	230
78587-05-0	Hexythiazox	C ₁₇ H ₂₁ ClN ₂ O ₂ S	7	23	AC, IN	5.57*	Partly	Yes	59	105	222	> 300
91465-08-6	Lambda-cyhalothrin	C ₂₃ H ₁₉ ClF ₃ NO ₃	7	27	IN	5.5**	Partly	No	96	49	> Dec	275
67747-09-5	Prochloraz	C ₁₅ H ₁₆ Cl ₃ N ₃ O ₂	3	25	FU	3.5**	No	Yes	20.8	135	> Dec	185-450
178928-70-6	Prothioconazole	C ₁₄ H ₁₅ Cl ₂ N ₃ OS	3	27	FU	3.82*	No	Yes	194	140	> Dec	220
175013-18-0	Pyraclostrobin	C ₁₉ H ₁₈ ClN ₃ O ₄	5	28	FU, PG	3.99*	No	Yes	57	65	> Dec	200
102851-06-9	Tau-Fluvalinate	C ₂₆ H ₂₂ ClF ₃ N ₂ O ₃	6	25	IN	7.02**	Partly	No	58	-14	> Dec	> 200
112410-23-8	Tebufenozide	C ₂₂ H ₂₈ N ₂ O ₂	3	12	IN	4.25*	No	Yes	155	200	> Dec	200-300
79538-32-2	Tefluthrin	C ₁₇ H ₁₄ ClF ₇ O ₂	7	24	IN	6.40*	Not investigated	No	155	45	156	295
112281-77-3	Tetraconazole	C ₁₃ H ₁₁ Cl ₂ F ₄ N ₃ O	5	19	FU	3.56*	No	No	155	6	> Dec	>235
141517-21-7	Trifloxystrobin	C ₂₀ H ₁₉ F ₃ N ₂ O ₄	5	25	FU	4.50*	Partly	Yes	77	73	> Dec	285

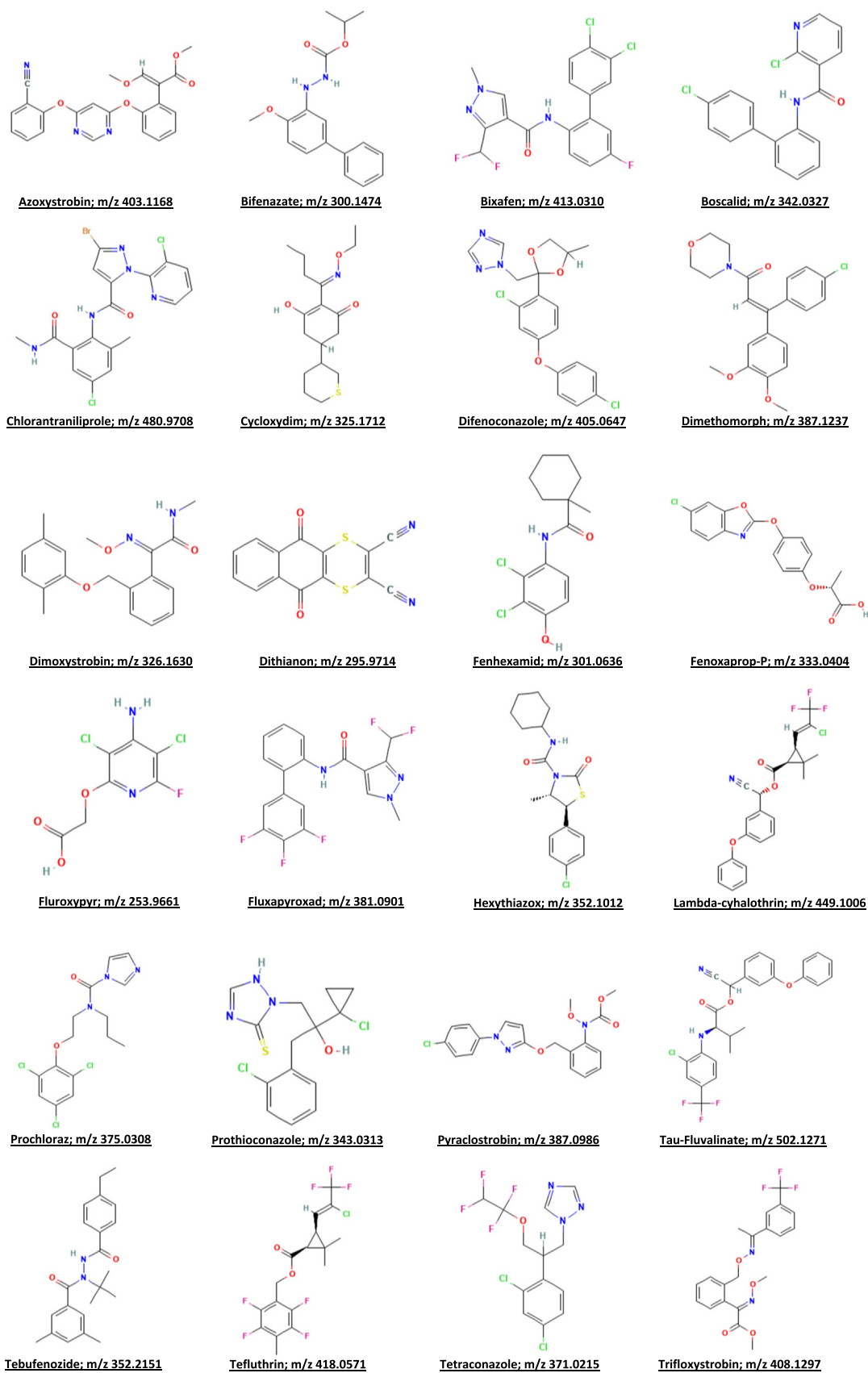


Fig. 2. Structure and monoisotopic mass of the 24 active substances obtained from the prioritisation list

Table 2

Detailed list of substances that passed “Step 1” and the filtering steps conducted to build the prioritisation list (a: the active substance has an MRL above the LOD in at least five main food products, b: the active substance has an MRL above the LOD in one to four main food products and was previously monitored by the Laboratory for Food Safety at ANSES)

CAS No.	Pesticide residue	Step 1	Step 2	Step 3	Step 4	Step 5	Included in the prioritisation list
131860-33-8	Azoxystrobin	Yes	Yes	Yes ^a	Yes	Yes	Yes
149877-41-8	Bifenazate	Yes	Yes	Yes ^b	Yes	Yes	Yes
581809-46-3	Bixafen	Yes	Yes	Yes ^b	Yes	Yes	Yes
188425-85-6	Boscalid	Yes	Yes	Yes ^a	Yes	Yes	Yes
500008-45-7	Chlorantraniliprole	Yes	Yes	Yes ^a	Yes	Yes	Yes
101205-02-1	Cycloxydim	Yes	Yes	Yes ^a	Yes	Yes	Yes
119446-68-3	Difenoconazole	Yes	Yes	Yes ^a	Yes	Yes	Yes
110488-70-5	Dimethomorph	Yes	Yes	Yes ^b	Yes	Yes	Yes
149961-52-4	Dimoxystrobin	Yes	Yes	Yes ^b	Yes	Yes	Yes
3347-22-6	Dithianon	Yes	Yes	Yes ^a	Yes	Yes	Yes
126833-17-8	Fenhexamid	Yes	Yes	Yes ^b	Yes	Yes	Yes
113158-40-0	Fenoxaprop-P	Yes	Yes	Yes ^a	Yes	Yes	Yes
69377-81-7	Fluroxypyr	Yes	Yes	Yes ^b	Yes	Yes	Yes
907204-31-3	Fluxapyroxad	Yes	Yes	Yes ^a	Yes	Yes	Yes
78587-05-0	Hexythiazox	Yes	Yes	Yes ^a	Yes	Yes	Yes
91465-08-6	Lambda-cyhalothrin	Yes	Yes	Yes ^a	Yes	Yes	Yes
67747-09-5	Prochloraz	Yes	Yes	Yes ^b	Yes	Yes	Yes
178928-70-6	Prothioconazole	Yes	Yes	Yes ^b	Yes	Yes	Yes
175013-18-0	Pyraclostrobin	Yes	Yes	Yes ^a	Yes	Yes	Yes
102851-06-9	Tau-Fluvalinate	Yes	Yes	Yes ^a	Yes	Yes	Yes
112410-23-8	Tebufozozide	Yes	Yes	Yes ^b	Yes	Yes	Yes
79538-32-2	Tefluthrin	Yes	Yes	Yes ^a	Yes	Yes	Yes
112281-77-3	Tetraconazole	Yes	Yes	Yes ^a	Yes	Yes	Yes
141517-21-7	Trifloxystrobin	Yes	Yes	Yes ^a	Yes	Yes	Yes
52315-07-8	Cypermethrin	Yes	Possibly	Yes ^a	Yes	Yes	Possibly
52918-63-5	Deltamethrin	Yes	Possibly	Yes ^a	Yes	Yes	Possibly
143390-89-0	Kresoxim-methyl	Yes	Possibly	Yes ^a	Yes	Yes	Possibly
94-81-5	MCPB	Yes	Possibly	Yes ^a	Yes	Yes	Possibly
40487-42-1	Pendimethalin	Yes	Possibly	Yes ^b	Yes	Yes	Possibly
118134-30-8	Spiroxamine	Yes	Possibly	Yes ^b	Yes	Yes	Possibly
107534-96-3	Tebuconazole	Yes	Possibly	Yes ^a	Yes	Yes	Possibly
55335-06-3	Triclopyr	Yes	Possibly	Yes ^b	Yes	Yes	Possibly
1072957-71-1	Benzovindiflupyr	Yes	Yes	Yes ^a	No	Yes	No
133-06-2	Captan	Yes	Yes	Yes ^b	Yes	No	No
736994-63-1	Cyantraniliprole	Yes	Yes	Yes ^a	No	Yes	No
473798-59-3	Fenpyrazamine	Yes	Yes	Yes ^b	No	Yes	No
658066-35-4	Fluopyram	Yes	Yes	Yes ^a	No	Yes	No
133-07-3	Folpet	Yes	Yes	Yes ^b	Yes	No	No
183675-82-3	Penthiopyrad	Yes	Yes	Yes ^a	No	Yes	No
946578-00-3	Sulfoxaflor	Yes	Yes	Yes ^a	No	Yes	No
99129-21-2	Clethodim	Yes	Possibly	Yes ^a	No	No	No
83066-88-0	Fluazifop-P	Yes	Possibly	Yes ^a	No	Yes	No
74070-46-5	Aclonifen	Yes	Yes	No	-	-	No
101007-06-1	Acrinathrin	Yes	Yes	No	-	-	No
865318-97-4	Ametoctradin	Yes	Yes	No	-	-	No
120923-37-7	Amidosulfuron	Yes	Yes	No	-	-	No
348635-87-0	Amisulbrom	Yes	Yes	No	-	-	No
120162-55-2	Azimsulfuron	Yes	Yes	No	-	-	No
113614-08-7	Beflubutamid	Yes	Yes	No	-	-	No
98243-83-5	Benalaxyl-M	Yes	Yes	No	-	-	No
1861-40-1	Benfluralin	Yes	Yes	No	-	-	No
83055-99-6	Bensulfuron	Yes	Yes	No	-	-	No
413615-35-7	Benthiavalicarb	Yes	Yes	No	-	-	No
42576-02-3	Bifenox	Yes	Yes	No	-	-	No
125401-92-5	Bispyribac	Yes	Yes	No	-	-	No
116255-48-2	Bromuconazole	Yes	Yes	No	-	-	No
41483-43-6	Bupirimate	Yes	Yes	No	-	-	No
128639-02-1	Carfentrazone-ethyl	Yes	Yes	No	-	-	No
105512-06-9	Clodinafop	Yes	Yes	No	-	-	No
74115-24-5	Clofentezine	Yes	Yes	No	-	-	No
120116-88-3	Cyazofamid	Yes	Yes	No	-	-	No
180409-60-3	Cyflufenamid	Yes	Yes	No	-	-	No
122008-85-9	Cyhalofop-butyl	Yes	Yes	No	-	-	No
257-141-8	Diclofop	Yes	Yes	No	-	-	No
83164-33-4	Diflufenican	Yes	Yes	No	-	-	No
153233-91-1	Etoxazole	Yes	Yes	No	-	-	No
134098-61-6	Fenpyroximate	Yes	Yes	No	-	-	No
104040-78-0	Flazasulfuron	Yes	Yes	No	-	-	No
145701-23-1	Florasulam	Yes	Yes	No	-	-	No
1390661-72-9	Florpyrauxifen-benzyl	Yes	Yes	No	-	-	No

(continued on next page)

Table 2 (continued)

CAS No.	Pesticide residue	Step 1	Step 2	Step 3	Step 4	Step 5	Included in the prioritisation list
79622-59-6	Fluazinam	Yes	Yes	No	-	-	No
142459-58-3	Flufenacet	Yes	Yes	No	-	-	No
62924-70-3	Flumetralin	Yes	Yes	No	-	-	No
103361-09-7	Flumioxazin	Yes	Yes	No	-	-	No
239110-15-7	Fluopicolide	Yes	Yes	No	-	-	No
361377-29-9	Fluoxastrobin	Yes	Yes	No	-	-	No
951659-40-8	Flupyradifurone	Yes	Yes	No	-	-	No
136426-54-5	Fluquinconazole	Yes	Yes	No	-	-	No
958647-10-4	Flutianil	Yes	Yes	No	-	-	No
66332-96-5	Flutolanil	Yes	Yes	No	-	-	No
173159-57-4	Foramsulfuron	Yes	Yes	No	-	-	No
98886-44-3	Fosfiazate	Yes	Yes	No	-	-	No
943831-98-9	Halauxifen-methyl	Yes	Yes	No	-	-	No
100784-20-1	Halosulfuron - methyl	Yes	Yes	No	-	-	No
35554-44-0	Imazalil	Yes	Yes	No	-	-	No
114311-32-9	Imazamox	Yes	Yes	No	-	-	No
173584-44-6	Indoxacarb	Yes	Yes	No	-	-	No
144550-36-7	Iodosulfuron	Yes	Yes	No	-	-	No
125225-28-7	Ipconazole	Yes	Yes	No	-	-	No
140923-17-7	Iprovalicarb	Yes	Yes	No	-	-	No
875915-78-9	Isofetamid	Yes	Yes	No	-	-	No
82558-50-7	Isoxaben	Yes	Yes	No	-	-	No
141112-29-0	Isoxaflutole	Yes	Yes	No	-	-	No
374726-62-2	Mandipropamid	Yes	Yes	No	-	-	No
1417782-03-6	Mefentrifluconazole	Yes	Yes	No	-	-	No
208465-21-8	Mesosulfuron	Yes	Yes	No	-	-	No
139968-49-3	Metaflumizone	Yes	Yes	No	-	-	No
74223-64-6	Metsulfuron-methyl	Yes	Yes	No	-	-	No
111991-09-4	Nicosulfuron	Yes	Yes	No	-	-	No
1003318-67-9	Oxathiapiprolin	Yes	Yes	No	-	-	No
42874-03-3	Oxyfluorfen	Yes	Yes	No	-	-	No
219714-96-2	Penoxsulam	Yes	Yes	No	-	-	No
13684-63-4	Phenmedipham	Yes	Yes	No	-	-	No
732-11-6	Phosmet	Yes	Yes	No	-	-	No
137641-05-5	Picolinafen	Yes	Yes	No	-	-	No
243973-20-8	Pinoxaden	Yes	Yes	No	-	-	No
139001-49-3	Profoxydim	Yes	Yes	No	-	-	No
181274-15-7	Propoxycarbazono	Yes	Yes	No	-	-	No
23950-58-5	Propyzamide	Yes	Yes	No	-	-	No
94125-34-5	Prosulfuron	Yes	Yes	No	-	-	No
129630-19-9	Pyraflufen-ethyl	Yes	Yes	No	-	-	No
96489-71-3	Pyridaben	Yes	Yes	No	-	-	No
179101-81-6	Pyridalyl	Yes	Yes	No	-	-	No
422556-08-9	Pyroxulam	Yes	Yes	No	-	-	No
122931-48-0	Rimsulfuron	Yes	Yes	No	-	-	No
874967-67-6	Sedaxane	Yes	Yes	No	-	-	No
130561-48-7	Sintofen	Yes	Yes	No	-	-	No
141776-32-1	Sulfosulfuron	Yes	Yes	No	-	-	No
119168-77-3	Tebufenpyrad	Yes	Yes	No	-	-	No
335104-84-2	Tembotrione	Yes	Yes	No	-	-	No
79277-27-3	Thifensulfuron-methyl	Yes	Yes	No	-	-	No
101200-48-0	Tribenuron	Yes	Yes	No	-	-	No
126535-15-7	Triflusulfuron	Yes	Yes	No	-	-	No
142469-14-5	Tritosulfuron	Yes	Yes	No	-	-	No
283159-90-0	Valifenalate	Yes	Yes	No	-	-	No
156052-68-5	Zoxamide	Yes	Yes	No	-	-	No
57960-19-7	Acequinocyl	Yes	Possibly	No	-	-	No
953030-84-7	Buprofezin	Yes	Possibly	No	-	-	No
143807-66-3	Chromafenozide	Yes	Possibly	No	-	-	No
400882-07-7	Cyflumetofen	Yes	Possibly	No	-	-	No
50563-36-5	Dimethachlor	Yes	Possibly	No	-	-	No
26225-79-6	Ethofumesate	Yes	Possibly	No	-	-	No
131807-57-3	Famoxadone	Yes	Possibly	No	-	-	No
120928-09-8	Fenazaquin	Yes	Possibly	No	-	-	No
67306-00-7	Fenpropidin	Yes	Possibly	No	-	-	No
61213-25-0	Flurochloridone	Yes	Possibly	No	-	-	No
881685-58-1	Isopyrazam	Yes	Possibly	No	-	-	No
173662-97-0	Mandestrobip	Yes	Possibly	No	-	-	No
6119-92-2	Meptyldinocap	Yes	Possibly	No	-	-	No
104206-82-8	Mesotrione	Yes	Possibly	No	-	-	No
70630-17-0	metalaxy-M	Yes	Possibly	No	-	-	No
67129-08-2	Metazachlor	Yes	Possibly	No	-	-	No
125116-23-6	Metconazole	Yes	Possibly	No	-	-	No
161050-58-4	Methoxyfenozide	Yes	Possibly	No	-	-	No

(continued on next page)

Table 2 (continued)

CAS No.	Pesticide residue	Step 1	Step 2	Step 3	Step 4	Step 5	Included in the prioritisation list
51596-10-2	Milbemectin	Yes	Possibly	No	-	-	No
15299-99-7	Napropamide	Yes	Possibly	No	-	-	No
66246-88-6	Penconazole	Yes	Possibly	No	-	-	No
106700-29-2	Pethoxamid	Yes	Possibly	No	-	-	No
29232-93-7	Pirimiphos-methyl	Yes	Possibly	No	-	-	No
189278-12-4	Proquinazid	Yes	Possibly	No	-	-	No
52888-80-9	Prosulfocarb	Yes	Possibly	No	-	-	No
55512-33-9	Pyridate	Yes	Possibly	No	-	-	No
688046-61-9	Pyriofenone	Yes	Possibly	No	-	-	No
95737-68-1	Pyriproxyfen	Yes	Possibly	No	-	-	No
87392-12-9	S-metolachlor	Yes	Possibly	No	-	-	No
283594-90-1	Spiromesifen	Yes	Possibly	No	-	-	No
203313-25-1	Spirotetramat	Yes	Possibly	No	-	-	No
99105-77-8	Sulcotrione	Yes	Possibly	No	-	-	No
57018-04-9	Tolclofos-methyl	Yes	Possibly	No	-	-	No
131983-72-7	Triticonazole	Yes	Possibly	No	-	-	No
571-58-4	1,4-Dimethylnaphthalene	Yes	No	-	-	-	No
3100-04-7	1-methylcyclopropene	Yes	No	-	-	-	No
86-87-3	1-Naphthylacetamide and 1-naphthylacetic acid	Yes	No	-	-	-	No
94-75-7	2,4-D	Yes	No	-	-	-	No
94-82-6	2,4-DB	Yes	No	-	-	-	No
2905-69-3	2,5-dichlorobenzoic acid methylester	Yes	No	-	-	-	No
90-43-7	2-Phenylphenol	Yes	No	-	-	-	No
148-24-3	8-Hydroxyquinoline incl. oxyquinoleine	Yes	No	-	-	-	No
71751-41-2	Abamectin	Yes	No	-	-	-	No
135410-20-7	Acetamiprid	Yes	No	-	-	-	No
135158-54-2	Acibenzolar-S-methyl	Yes	No	-	-	-	No
150114-71-9	Aminopyralid	Yes	No	-	-	-	No
11141-17-6	Azadirachtin	Yes	No	-	-	-	No
25057-89-0	Bentazone	Yes	No	-	-	-	No
999-81-5	Chlormequat	Yes	No	-	-	-	No
15545-48-9	Chlorotoluron	Yes	No	-	-	-	No
81777-89-1	Clomazone	Yes	No	-	-	-	No
1702-17-6	Clopyralid	Yes	No	-	-	-	No
/	Copper compounds	Yes	No	-	-	-	No
57966-95-7	Cymoxanil	Yes	No	-	-	-	No
121552-61-2	Cyprodinil	Yes	No	-	-	-	No
1596-84-5	Daminozide	Yes	No	-	-	-	No
533-74-4	Dazomet	Yes	No	-	-	-	No
1918-00-9	Dicamba	Yes	No	-	-	-	No
1593-77-7	Dodemorph	Yes	No	-	-	-	No
2439-10-3	Dodine	Yes	No	-	-	-	No
155569-91-8	Emamectin	Yes	No	-	-	-	No
16672-87-0	Ethephon	Yes	No	-	-	-	No
80844-07-1	Etofenprox	Yes	No	-	-	-	No
517875-34-2	Fenpicoxamid	Yes	No	-	-	-	No
158062-67-0	Flonicamid	Yes	No	-	-	-	No
272451-65-7	Flubendiamide	Yes	No	-	-	-	No
131341-86-1	Fludioxonil	Yes	No	-	-	-	No
2164-17-2	Fluometuron	Yes	No	-	-	-	No
68157-60-8	Forchlorfenuron	Yes	No	-	-	-	No
22259-30-9	Formetanate	Yes	No	-	-	-	No
39148-24-8	Fosetyl	Yes	No	-	-	-	No
1071-83-6	Glyphosate	Yes	No	-	-	-	No
10004-44-1	Hymexazol	Yes	No	-	-	-	No
133-32-4	Indolylbutyric acid	Yes	No	-	-	-	No
2164-08-1	Lenacile	Yes	No	-	-	-	No
121-75-5	Malathion	Yes	No	-	-	-	No
123-33-1	Maleic hydrazide	Yes	No	-	-	-	No
94-74-6	MCPA	Yes	No	-	-	-	No
110235-47-7	Mepanipyrim	Yes	No	-	-	-	No
24307-26-4	Mepiquat	Yes	No	-	-	-	No
108-62-3	Metaldehyde	Yes	No	-	-	-	No
41394-05-2	Metamitron	Yes	No	-	-	-	No
220899-03-6	Metrafenone	Yes	No	-	-	-	No
21087-64-9	Metribuzin	Yes	No	-	-	-	No
23135-22-0	Oxamyl	Yes	No	-	-	-	No
76738-62-0	Pacllobutrazol	Yes	No	-	-	-	No
/	Phosphane	Yes	No	-	-	-	No
1918-02-1	Picloram	Yes	No	-	-	-	No
23103-98-2	Pirimicarb	Yes	No	-	-	-	No
127277-53-6	Prohexadione	Yes	No	-	-	-	No
24579-73-5	Propamocarb	Yes	No	-	-	-	No
8003-34-7	Pyrethrins	Yes	No	-	-	-	No

(continued on next page)

Table 2 (continued)

CAS No.	Pesticide residue	Step 1	Step 2	Step 3	Step 4	Step 5	Included in the prioritisation list
53112-28-0	Pyrimethanil	Yes	No	-	-	-	No
90717-03-6	Quinmerac	Yes	No	-	-	-	No
175217-20-6	Silthiofam	Yes	No	-	-	-	No
67233-85-6	Sodium 5-nitroguaiacolate	Yes	No	-	-	-	No
935545-74-7	Spinetoram	Yes	No	-	-	-	No
168316-95-8	Spinosad	Yes	No	-	-	-	No
2699-79-8	Sulfuryl fluoride	Yes	No	-	-	-	No
5915-41-3	Terbutylazine	Yes	No	-	-	-	No
148-79-8	Thiabendazole	Yes	No	-	-	-	No
2303-17-5	Tri-allate	Yes	No	-	-	-	No
72459-58-6	Triazoxide	Yes	No	-	-	-	No
143294-89-7	Trinexapac	Yes	No	-	-	-	No
137-30-4	Ziram	Yes	No	-	-	-	No

degradation products that are presumed to have similar physicochemical properties compared to the AS.

Their chemical structures are also diverse (Fig. 2), which is useful to study most of the possible degradation scenarios. Every AS contains both nitrogen and oxygen atoms, except tefluthrin (which contains oxygen but no nitrogen atoms), 18 ASs contain at least 1 halogen atom (16 ASs contain chlorine, 7 ASs contain fluorine, and 1 AS contains bromine), and 4 ASs contain a sulphur atom. Fig. 2 also shows the variability in chemical groups since selected ASs can have various different chemical groups such as heterocycles, ether bonds, amides, esters, nitriles, alcohols, ketones, amines, carboxylic acids, and thioketones.

Lastly, variabilities are observed for the melting (from solid to liquid), boiling (from liquid to vapour) and decomposition temperatures (temperature from which the AS decomposes in its degradation products) for the selected ASs. Most of them are solid at ambient temperatures, except tau-fluvalinate and tetraconazole, which are liquid. The majority of the ASs are decomposed before their boiling point, except hexythiazox and tefluthrin, with boiling points of 222°C and 156°C, respectively. The ASs with a boiling point or decomposition temperature below 240°C can volatilise or can be degraded into products that will be volatilised during processes involving high temperatures.

The high variability between selected ASs in the prioritisation list (category, log Kow, mass, structure, and melting/boiling points) is sufficiently representative of the diversity of ASs to investigate the behaviour of pesticides above 120°C. This investigation above 120°C would be necessary in the future to increase knowledge, as mentioned in the review conducted by Dubocq et al. (2022), about the behaviour of ASs at high temperatures. So far, investigation are only conducted between 90 and 120°C for regulatory studies. Most of the research studies are thus following this range of temperature and investigate about removing the analysed active substance and calculating processing factors (Jankowska et al., 2019; Shakoori et al., 2018; Yang et al., 2012). However, very few studies are investigating about temperature range above 120°C (Chavarri et al., 2005; Huan et al., 2015; Mekonen et al., 2015) and even less about degradation products of some ASs above 120°C (Göckener et al., 2019; Kontou et al., 2004; Lin et al., 2005; Martin et al., 2020). Potential further degradation studies above 120°C would thus fulfil this gap and are needed in research studies. They could also help to understand if the European regulation hydrolysis studies need to be adapted to request higher temperatures when a new substance wants to be commercialised.

Moreover, investigating both degradation and volatilisation products would be useful to study the behaviour of AS during thermodegradation studies, mitigating the risk to possibly overlook substances. Further thermodegradation studies could thus be conducted at temperatures above 120°C that are not required yet. Another consideration for further prioritisation studies could be the toxicity of the ASs and the ones of their reported degradation products (from hydrolysis studies or other degradation studies). Investigating selected AS regulatory studies enables to list

each reported degradation product as well as their toxicity and could be a prioritisation criterion to retain only compounds that form most toxic degradation products. This study aims at considering physicochemical properties and analytical chemistry point of view and gave significant and relevant number of selected ASs, but other studies could consider also this toxicological point of view provided by regulatory studies if required.

Conclusion

To define active substance residues following thermal processing, the European Regulation (EC No 1107/2009) requires hydrolysis studies up to 120°C. However, certain cooking processes such as oven cooking, microwaving, grilling or frying reach temperatures up to 250°C. Due to the lack of information in academic studies, no conclusion could be drawn about the potential overlook of degradation products following regulatory hydrolysis studies. In order to address this lack of information, experiments need to be conducted at this range of temperatures. Due to the high number of reported ASs, a prioritisation step was needed to select the compounds that could produce potential degradation products above 120°C and that are not observed in the OECD hydrolysis tests required in the regulatory framework. Therefore, among the 1 478 substances reported in the EUPD, a five-step workflow enabled to build the prioritisation list of 24 compounds that are most likely to be affected by degradation above 120°C. This list was obtained by retaining substances fulfilling following criteria: (i) being anthropogenic, having a carbon backbone structure, authorised in the EU and having a defined MRL (criterion 1, from 1 478 to 232 ASs), (ii) having specific physicochemical and structural properties (criterion 2, from 232 to 120 ASs), (iii) with MRLs higher than the LOQ in the main food commodities (criterion 3, from 120 to 32 ASs), (iv) having a standard price below € 200 / 100 mg (criterion 4, from 32 to 26 ASs), and (v) not being fully degraded in hydrolysis studies of respective AS assessment reports (criterion 5, from 26 to 24 ASs). A detailed list of substances that fulfilled each step is reported to help future research studies to build their own prioritisation list and save time to select the most suitable candidates according to their criteria.

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Declaration of Competing Interest

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

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Pierre L'Yvonnet: Writing – review & editing. **Gaëlle Vial:** Conceptualization, Methodology, Validation, Writing – review & editing. **Xavier Sarda:** Conceptualization, Methodology, Validation, Writing – review & editing. **Arnaud Duboisset:** Conceptualization, Methodology, Validation, Writing – review & editing, Supervision, Funding acquisition, Project administration. **Benjamin Carbonnier:** Conceptualization, Methodology, Validation, Writing – review & editing, Supervision, Funding acquisition, Project administration. **Julien Parinet:** Conceptualization, Methodology, Validation, Writing – review & editing, Supervision, Funding acquisition, Project administration. **Florian Dubocq:** Methodology, Data curation, Formal analysis, Validation, Visualization, Investigation, Writing – original draft, Writing – review & editing.

Data availability

No data was used for the research described in the article.

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