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Impact of drinking water treatment processes on the residues of plant protection products for consumer and aquatic risk assessment: theoretical and experimental studies

Angela Mari, Elena Alonso-Prados, Juan José Villaverde, Jose Luis Alonso-Prados and Pilar Sandín-España

Unit of Plant Protection Products, National Institute for Agricultural and Food Research and Technology, INIA-CSIC, Ctra. La Coruña, km 7.5, 28040, Madrid, Spain

Abstract

Pesticides residues can occur in ground and surface waters, and potentially react with chemicals used for water disinfection treatments, such as chlorine. This can lead to the formation of unknown reaction products, which can be more toxic and/or persistent than the active substances themselves, and therefore become a potential risk for human health and environment. Thus, in the framework of the EU Regulation 1107/2009, the identification of these by-products and their potential risk should be assessed. Within the European Food Risk Assessment (EU-FORA) Fellowship Programme, the fellow studied the behaviour of herbicides belonging to the families of imidazolinones and sulfonylureas in waters treated with chlorine disinfectants. Due to their physicochemical properties, these herbicides are susceptible of reaching natural waters. In fact, some of them have been detected in water monitoring programmes. During the experimental part of the present work programme, reactions between the active substances and the most used chlorine disinfecting reactants (hypochlorite and chloramines) were performed. Degradation kinetic parameters such as half-lives and degradation constants were calculated. Results showed that herbicide degradation was both pH and chlorine/chloramines concentration dependent. In order to identify the degradation by-products, high-resolution mass spectrometry experiments were performed, and a possible route of formation of these compounds was proposed. Finally, their risk assessment was carried out by using tox/ecotoxicological properties determined by QSAR methodology and FOCUS modelling for hazard and exposure assessment, respectively. These results will contribute to the definition of a risk assessment scheme for pesticides by-products potentially occurring in drinking water.

Keywords: pesticides, drinking water, risk assessment, chlorine, degradation products, QSAR, FOCUS

Correspondence: eu-fora@efsa.europa.eu

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1. Introduction

The European Food Risk Assessment (EU-FORA) Fellowship Programme is a practical ('training by doing') programme that aims to increase the expertise of early to mid-career scientists in food safety risk assessment at both the European and national levels (Bronzwaer et al., 2016).

The fellow trainership was carried out at the Unit of Plant Protection Products of the National Institute for Agricultural and Food Research and Technology, INIA-CSIC, Madrid, Spain, with a work programme entitled: 'Impact of drinking water treatment processes on the residues of plant protection products for consumer risk assessment. Theoretical and experimental studies'.

The INIA is a public research institute in Spain accredited by the Spanish Ministry of Science and Innovation to perform the evaluation of the substances for which Spain is a Rapporteur Member State. The institute has been involved in the last 25 years in the implementation of the European legislation on plant protection products and has a large experience in the assessment of active substances and plant protection products. The main lines of research of the UPF are:

- Risk assessment of plant protection products in the framework of European Regulation (EC) No 1107/2009.
- Analysis of the strengths and weaknesses of the assessment process to improve the safe use of crop protection tools and to safeguard the competitiveness of European agriculture.
- The study of the environmental behaviour of active substances in terms of degradation studies in waters and soils, and the identification of possible reaction products formed as well as phyto-and eco- toxicological effects on target and non-target organism in laboratory.
- Validation of multiresidue methods for the analytical determination of pesticide residues, and development of computational methodologies for risk assessment of pesticides using statistical modelling methods, quantitative structure–activity relationships (QSARs) models and quantum chemistry.

Pesticide contamination of drinking water is considered a route of major concern. Contamination of tap water supplies by small amounts of pesticides may result in long-term exposure contaminants. However, clear links between individual pesticides and individual health effects can only be shown in animal studies, but the doses used in these studies are far higher than the enforced legally pesticide limits (Damalas and Eleftherohorinos, 2011; Harris and Gaston, 2004). Health risk, for prolonged exposure to very low levels of pesticide, is not always covered by routine toxicological tests performed with regulatory purposes. Therefore, regulation tends to be very conservative with respect to the permitted levels of contaminants in drinking water supplies. For example, EU water and drinking water directives provide that no individual pesticide may exceed 0.1 μg L^{-1} and that the sum of all contaminants present in a drinking water sample may not exceed 0.5 μg L^{-1} (European Commission, 2020).

Environmental contamination of ground and surface natural waters is one of the main route of pesticides contamination. However, before entering the tap water net, water is submitted to physical and chemical treatments for disinfection. The main water disinfection treatments to remove microorganisms for drinking water purposes are chlorine in the form of sodium hypochlorite (NaClO) or chloramines. Chlorine is a potent oxidant that acts as a bactericide. At the same time, chlorine and the other agents are strong oxidants that may react with various organic functional groups of pesticide molecules to form reaction products (Sandín-España et al., 2005). Main degradation processes are hydrolysis, oxidation and chlorination among others (Duirk et al., 2009; Chamberlain et al., 2010). Scientific literature shows that these processes can lead to the formation of a variety of disinfection products (Brix et al., 2009; Quintana et al., 2014; Malato et al., 2014). Many of these are unknown compounds, and their rate of degradation may vary considerably (Sandín-España et al., 2005; Lerch et al., 2007; Vanderford et al., 2008). Information on degradation products and degradation pathways is of utmost importance in understanding the environmental fate of pesticides (Harir et al., 2007). In this regard, (European Commission, 2009) states that for residues (including metabolites, breakdown or reaction products) '(...) which are of toxicological, ecotoxicological, environmental or drinking water relevance, there shall be methods in general use for measuring them' as they can be a potential risk (Boxall et al., 2004; Chen and Young, 2008).

The main concern is that a reaction product 'is deemed relevant if there is a reason to assume that it has intrinsic properties comparable to the parent substance in terms of its biological target activity, or that it poses a higher or comparable risk to organisms than the parent substance or that it has certain toxicological properties that are considered unacceptable' (Regulation 1107/2009/EC). For this reason, the identification of the reaction products, and then the evaluation of their biological activities and tox/ecotoxicological properties are of utmost importance since they might be 'relevant for the overall approval decision or for the definition of risk mitigation measures' (European Commission, 2009).

2. Description of work programme

2.1. Aims and objectives

The aim of this work programme was to investigate the behaviour of selected herbicides in chlorinated/chloraminated waters simulating drinking water treatments, and the study of their reaction products. After evaluating tox/ecotoxicological properties by QSAR methodology, and the exposure assessment by FOCUS modelling, the fellow received training in the aquatic and consumer risk assessment of these by-products.

The main disciplines of interest were analytical chemistry, environmental and agricultural sciences.

The major objectives of this work programme were the following:

Objective 1: general concepts regarding consumer risk assessment of drinking water and aquatic risk assessment.

- Review of EU Regulations and risk assessment guidance documents related to consumer risk assessment of drinking water and environmental exposure assessment.
- Review and selection of the potential active substances for the study.

Objective 2: experimental work.

- Laboratory simulation of the reaction between the selected active substances and different water disinfectants.
- Development of analytical methods.
- Determination of degradation curves.
- Identification of by-products.

Objective 3: theoretical work.

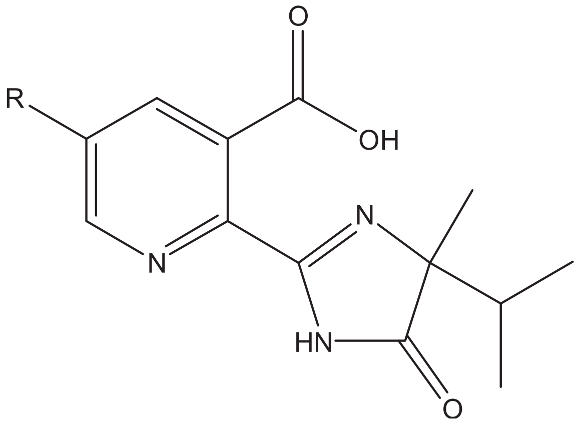
- Prediction of the most probable formation route of nicosulfuron by-products in chlorinated/chloraminated waters.
- Determination of physicochemical and tox/ecotoxicological properties of the potential degradation products by using QSAR methodology.
- Estimation of predicted concentrations of these products in surface and groundwater.

Objective 4: conclusions

- Comparing of the experimental and theoretical results.
- Environmental and risk assessment of the degradation by-products.

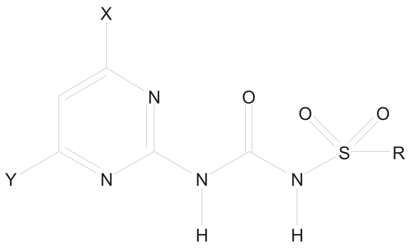
2.2. Activities/methods

In the frame of the present project, active substances considered susceptible to polluting surface and groundwater were selected on basis of their physical–chemical properties. At the same time, a bibliographic research on pesticides found in natural waters was carried out. According to this, five herbicides were selected: three belonging to the family of pyridine imidazolinones (imazamox, imazapyr and imazethapyr, Figure 1) and two to the family of sulfonylureas (azimsulfuron and nicosulfuron, Figure 2).



Active substance	**R**
Imazamox	$-CH_2-O-CH_3$
Imazapyr	-H
Imazethapyr	$-CH_2-CH_3$

Figure 1: Molecular structure of pyridine imidazolinones herbicides



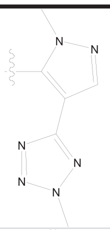
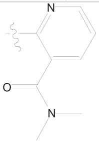
Active substance	**R**	**X**	**Y**
Azimsulfuron		$-OCH_3$	$-OCH_3$
Nicosulfuron		$-OCH_3$	$-OCH_3$

Figure 2: Molecular structure of sulfonylurea herbicides

2.2.1. Degradation kinetic experiments

In order to simulate the reactions between the selected herbicides and sodium hypochlorite (NaClO), different molar concentration ratios of active substance/disinfection chemical were used for the experiments at different pHs.

The exact concentration of NaClO in the stock solution was quantified using I 4500 Cl B – method, according to the iodometric titration standard method guidance (American Public Health Association APHA, 1999).

Chloramines solutions were prepared using different herbicide to disinfectant molar ratios. An appropriate mixture of sodium hypochlorite (NaClO)/ammonium chloride (NH_2Cl) was prepared for each pH. The hypochlorite solution was added drop by drop to ammonium chloride, and left stirring in darkness. Finally, NH_2Cl solution was added to a solution of active substance (a.s.) at a known concentration.

For all the experiments (chlorination and chloramination), blank samples containing only the a.s. were used to ensure that no degradation or hydrolysis occurred. The reaction was quenched with sodium thiosulfate at scheduled time intervals.

A reversed-phase high-performance liquid chromatography with diode array detector (HPLC-DAD) procedure was developed to evaluate the kinetic evolution and the half-lives of the a.s. A 1260 Infinity HPLC model equipped with a diode array detector (Agilent Technologies, Inc., Palo Alto, CA, USA) was employed for analysis. For the a.s., a calibration plot was built for concentration ranging between 0.1 and 10 μg mL^{-1}. A good linearity was always observed. Pseudo–first-order kinetic was assumed in order to calculate the corresponding degradation rate constant (k):

$$C = C_0 \cdot e^{-kt},$$

where C_0 and C are the concentrations (mg L^{-1}) of the a.s. at t_0 and at a given time t, respectively, and k is the first-order degradation rate constant.

Half-life ($t_{1/2}$) was calculated from k using the following equation:

$$t_{1/2} = \ln 2/k.$$

Origin85 Software program was used to obtain non-linear least squares regression fit for the a.s. degradation data to the first-order model.

2.2.2. By-products identification and degradation fitting model

In order to identify the by-products deriving from the degradation of the a.s. in chlorinated/chloraminated water, liquid chromatography–electrospray-quadrupole time of flight-mass spectrometry (LC-ESI-QToF-MS) experiments were performed.

An HPLC coupled with a mass spectrometer equipped with a Q-ToF hybrid analyser model MAXIS II (Bruker) was used for the analysis. The chromatographic separations were achieved by 1100 HPLC model (Agilent Technologies, Inc., Palo Alto, CA, USA).

The analysis were carried out in positive ion mode by monitoring both $[M + H]^+$ and $[M + Na]^+$ ions, in a mass range of m/z: 50–3,000 a.m.u. A mass tolerance of maximum 5 ppm error was allowed.

CAKE Software (version 3.5) was used to estimate kinetic fits of the a.s. and their by-products, in order to determine their possible route of degradation in chlorinated/chloraminated water.

2.2.3. QSAR modelling

The key physicochemical, environmental and ecotoxicological properties of the by-products were estimated by computational-based models based on quantitative structure–activity/structure–property relationship (QSAR/QSPR) tools. To perform this task, Toxicity Estimation Software Tool (T.E.S.T.) and the EPI Suite™ software (United States Environmental Protection Agency – USEPA) were used. The models and the software were developed with the aim of regulatory use in line with strict quality criteria according to OECD guidelines (OECD, 2014).

2.2.4. Environmental exposure, aquatic and consumer risk assessment

Predicted environmental concentrations in surface water

The predicted environmental concentrations in surface water (PEC_{sw}) and sediment (PEC_{sed}) were calculated using the FOCUS simulation models Steps 1–2 v. 3.2, Focus SWASH v. 5.3 (PRZM v. 4.3.1, MACRO v. 5.5.4, TOXWA v. 5.5.3) and SWAN v. 5.0.1 (FOCUS, 2015) (Tables 1 and 3).

Table 1: Input parameters related to nicosulfuron application for $PEC_{sw/sed}$ calculations

	Input parameters
Crop	Maize
Application rate (g/ha)	62.0 g/ha
Application window	Steps 1–2: maize: Mar-May Steps 3–4: Default (post-emergence)
Application method	Steps 1–2: – Steps 3–4: ground spray
CAM (Chemical Application Method)	Steps 1–2: – Steps 3–4: CAM1
Soil depth (cm)	Steps 1–2: – Steps 3–4: 4 cm

Predicted environmental concentrations in groundwater

Predicted environmental concentrations in groundwater (PEC_{gw}) at a soil depth of 1 m, were calculated for the active substance nicosulfuron for its uses on maize, with simulation models FOCUS PELMO 6.6.4 and FOCUS PEARL 5.5.5 (FOCUS, 2021) (Tables 2 and 3).

Table 2: Application scenarios for nicosulfuron PEC_{gw} calculations

	Input parameters
Crop	Maize
Application rate (g/ha)	62.0 g/ha
Number of application	1
Crop interception (%)	0
Frequency of application	Annual
Application timing	From 2 to 4 leaves – BBCH 12

Table 3: Application generic nicosulfuron input parameters for $PEC_{sw/sed}$ calculations (STEP 1–4) and for PEC_{gw} leaching simulation (FOCUS PELMO/PEARL)

	Nicosulfuron	**References**
Molecular weight (g/mol)	410.4	EFSA Scientific Report 120 (2007)
Water solubility (mg/L)	9,500 (20°C)	EFSA Scientific Report 120 (2007)
Saturated water pressure (Pa)	8 E-10 (20°C)	EFSA Scientific Report 120 (2007)
DT_{50} in soil (day)	16.4	EFSA Scientific Report 120 (2007)
DT_{50} in water (day)	42.3	EFSA Scientific Report 120 (2007)
DT_{50} in sediment (day)	1,000	Worst case
DT_{50} in whole system (day)	42.3	EFSA Scientific Report 120 (2007)
Activation energy (KJ/mol)	54,5	FOCUS recommendation
K_{foc} (mL/g)/K_{fom}	15.34/8.9 (geomean)	EFSA Scientific Report 120 (2007)
Freundlich exponent (L/n)	0.94	EFSA Scientific Report 120 (2007)
Plant uptake factor	0	FOCUS recommendation
Diffusion coefficient in water (m^2/day)	Steps 1–2: – Steps 3–4: 4.3×10^{-5}	FOCUS recommendation
Diffusion coefficient in air (m^2/day)	Steps 1–2: – Steps 3–4: 0.43	FOCUS recommendation
Wash-off factor from crop (L/mm)	Steps 1–2: – Steps 3–4: 1×10^{-7} (MACRO) 0 (PRZM)	FOCUS recommendation

Aquatic risk assessment

The aquatic risk assessment was conducted by estimating the regulatory acceptable concentration in surface water ($RAC_{sw;ac}$) of nicosulfuron by-products, on the basis of ecotoxicological data for aquatic target organisms predicted by QSAR modelling. $RAC_{sw;ac}$ values were compared to PEC_{sw} calculated for each by-product by FOCUS surface water modelling.

Consumer risk assessment

The consumer risk assessment was conducted by estimating the maximum allowable concentration (MAC) of nicosulfuron by-products for infants, toddlers and adults. By-products were considered 100 times more toxic than the parent compound. Finally, MAC values were compared to PEC_{gw} calculated for each by-product by FOCUS groundwater modelling.

3. Conclusions

3.1. Conclusion regarding herbicides behaviour in disinfected water and risk assessment of their by-products

Within the EU-FORA Fellowship Programme, the fellow carried out the study of the behaviour of selected active substances in chlorinated/chloraminated waters. The subsequent formation of their reaction products under specific experimental conditions was evaluated. In particular, nicosulfuron degradation increased with the concentration of chlorine/chloramines following a first order kinetic equation, and it proved to be pH sensitive as well. In agreement with the stronger oxidising potential of hypochlorite vs. chloramines (Reckhow and Singer, 1990), degradation rate of nicosulfuron/chloramines was slower than nicosulfuron/hypochlorite. In addition, the chemical structures of the by-products generated by the reaction of nicosulfuron and the disinfectants were tentatively identified by LC-HR-MS. Their amount increased while that of nicosulfuron decreased over time. A possible route of degradation for these by-products was proposed by means of CAKE kinetic degradation fitting model.

In the last part of the work programme, the estimation of the RACs and the MAC of nicosulfuron residues was performed by means of FOCUS surface water and groundwater scenarios, respectively. The acute aquatic toxicity of the degradation products for *Daphnia magna* and fathead minnow, was predicted by QSAR models. These data were employed to estimate the RAC in surface water. As reported in the EFSA Scientific opinion on Plant Protection Products and their Residues (PPR) (EFSA PPR Panel, 2013), $RAC_{sw;ac}$ (RAC in surface water – SW – for adverse effects of pesticide exposure occurring within a relatively short period after exposure) is always compared with the $PEC_{sw;max}$ (the maximum PEC in surface water) derived from the predicted exposure profile of the active substance. In this study, in no cases the PEC_{sw} of nicosulfuron by-products was higher than the $RAC_{sw;ac,}$ thus indicating that they can be classified as a low risk. Regarding the environmental exposure risk assessment, the PEC of nicosulfuron in groundwater showed to be above the regulatory threshold of 0.1 μg/L at 1 m depth in three out of the eight scenarios considered in the FOCUS groundwater modelling. In no case, the PEC_{gw} of nicosulfuron by-products was higher than the MAC for adults, toddlers and infants in drinking waters. To the best of our knowledge, this is the first time that the behaviour of imazamox, imazapic and imazethapyr and nicosulfuron in chlorinated/chloraminated waters was studied. These results will contribute to supporting more complete risk assessment of the studied active substances, especially for nicosulfuron and its by-products potentially occurring in drinking water.

3.2. Conclusion regarding the participation to the EU-FORA programme

The hands-on training carried out during this year allowed the fellow to gain experience in the field of pesticide risk assessment. In particular, the fellow received training in generating data on pesticides residues and their degradation products, and in analysing these data in order to perform the environmental exposure assessment and risk assessment of the selected active substances and their by-products. Finally, participation in the EFSA EU-FORA work programme provided a valuable opportunity for the fellow to become part of a strong professional network that will provide basis for future collaborations in the field of food safety and risk assessment.

3.3. Additional scientific activities

During the EU-FORA programme, the fellow was presenting author of the poster entitled 'Behaviour of nicosulfuron herbicide in chlorinated drinking water. By-products identification and risk assessment', at the 11th European Conference on Pesticides and Related Organic Micropollulants in the Environment and the 17th Symposium on Chemistry and Fate of Modern Pesticides – Ioannina (Greece), June 23–26, 2022. (Annex A).

The fellow was invited by the Spanish Agency for Food Safety and Nutrition (AESAN) – Madrid (Spain) February 23–25, 2022, as speaker presenting her work programme, to attend seminars on AESAN's activities on risk assessment, management and communication, and, finally, to visit the laboratories of the National Centre for Food, located in Majadahonda (Madrid – Spain).

References

APHA (American Public Health Association), 1999. Standard methods for the examination of water and wastewater, 20th Edition. APHA, Washington, DC, 1268 pp.

Boxall ABA, Sinclair CI, Fenner K, Kolpin DW and Maund SJ, 2004. When synthetic chemicals degrade in the environment. Environmental Science and Technology, 1, 369A–375A.

Brix R, Bahi N, Alda MJL, Farré M, Fernandez J-M and Barceló D, 2009. Identification of disinfection by-products of selected triazines in drinking water by LC-Q-ToF-MS/MS and evaluation of their toxicity. Journal of Mass Spectrometry, 44, 330–337.

Bronzwaer S, Le Gourierec N and Koulouris S, 2016. Editorial: The European Food Risk Assessment Fellowship Programme (EU-FORA). EFSA Journal 2016;14(11), e14111, 2.

Chamberlain EF, Wang CA, Shi HL, Adams CD and Ma YF, 2010. Oxidative removal and kinetics of fipronil in various oxidation systems for drinking water treatment. Journal of Agricultural and Food Chemistry, 58, 6895–6899.

Chen WH and Young TM, 2008. NDMA formation during chlorination and chloramination of aqueous diuron solutions. Environmental Science and Technology, 42, 1072–1077.

Damalas CA and Eleftherohorinos IG, 2011. Pesticide exposure, safety issues, and risk assessment indicators. International Journal of Environmental Research and Public Health, 8, 1402–1419.

Duirk SE, Desetto LM and Davis GM, 2009. Transformation of organophosphorus pesticides in the presence of aqueous chlorine: kinetics, pathways, and structure-activity relationships. Environmental Science and Technology, 43, 2335–2340.

EFSA PPR Panel (EFSA Panel on Plant Protection Products and their Residues), 2013. Guidance on tiered risk assessment for plant protection products for aquatic organisms in edge-of-field surface waters. EFSA Journal 2013;11(7):3290, 268 pp. https://doi.org/10.2903/j.efsa.2013.3290

EFSA Scientific Report 120, 2007. Conclusion regarding the peer review of the pesticide risk assessment of the active substance nicosulfuron, 29.11.2007, 1–91.

European Commission, 2009. Regulation (EC) No 1107/2009 of the European Parliament and of the Council of 21 October 2009 concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/414/EEC. OJ L309, 24.11.2009, EC (European Commission), 2009. 1–50.

European Commission, 2020. Directive (EC) No 2020/2184 of the European Parliament and of the Council of 16 Dicember 2020, concerning the quality of water intended for human consumption, EC (European Commission). OJ L 435, 23.12.2020, 1–62.

FOCUS, 2015. Generic Guidance (version 1.4) for surface water scenarios: document based on official guidance document of FOCUS surface water scenarios in the context of 91/414/EEC and Regulation (EC) No 1107/2009.

FOCUS, 2021. Generic Guidance (version 2.3) for Tier 1 FOCUS groundwater assessments: document based on the reports of the FOCUS groundwater scenarios workgroup, 2000.

Harir M, Frommberger M, Gaspar A, Martens D, Kettrupp A, El Azzouzi M and Schmitt-Kopplin P, 2007. Characterization of Imazamox degradation by-products by using liquid chromatography mass spectrometry and high-resolution Fourier transform ion cyclotron resonance mass spectrometry. Analytical and Bioanalytical Chemistry, 389, 1459–1467.

Harris C and Gaston CP, 2004. Effects of refining predicted chronic dietary intakes of pesticide residues: a case study using glyphosate. Food Additives & Contaminants, 21, 857–864.

Lerch RN, Lin CH and Leigh ND, 2007. Reaction pathways of the diketonitrile degradate of isoxaflutole with hypochlorite in water. Journal of Agricultural and Food Chemistry, 55, 1893–1899.

Malato S, Fernández-Ibáñez P, Oller I, Prieto-Rodríguez L, Miralles-Cuevas S and Cabrera-Reina A, 2014. Approaches to water and wastewater treatment for removal of emerging contaminants: in Transformation Products of Emerging Contaminants in the Environment: Analysis. In: Lambropoulou DA and Nollet LML (eds.). Processes, Occurrence, Effects and Risks. John Wiley and Sons Ltd., Chinchester (UK). pp. 161–178.

OECD (Organisation for Economic Co-operation and Development), 2014. Guidance Document on the Validation of (Quantitative) Structure-Activity Relationship [(Q)SAR] Models, OECD Series on Testing and Assessment, No. 69, OECD Publishing, Paris.

Quintana JB, Rodil R and Rodríguez I, 2014. Transformation products of emerging contaminants upon reaction with conventional water disinfection oxidants. In: DA Lambropoulou and LML Nollet (eds). Transformation Products of Emerging Contaminants in the Environment: Analysis, Processes, Occurrence, Effects and Risks. John Wiley and Sons Ltd., Chinchester (UK). pp. 123–160.

Reckhow DA and Singer PC, 1990. The removal of organic halide precursors by preozonation and alum coagulation. Journal of American Water Works Association, 82, 173–180.

Sandín-España P, Santín I, Magrans JO, Alonso-Prados JL and García-Baudín JM, 2005. Degradation of alloxydim in chlorinated water. Agronomy for Sustainable Development, 25, 331–334.

Vanderford BJ, Mawhinney DB, Rosario-Ortiz FL and Snyder SA, 2008. Real-time detection and identification of aqueous chlorine transformation products using QTOF MS. Analytical Chemistry, 80, 4193–4199.

Abbreviations

a.m.u.	atomic mass unit
a.s.	active substance
AESAN	Agencia Española de Seguridad Alimentaria y Nutrición
CSIC	Consejo Superior de Investigaciones Científicas
DT_{50}	degradation time 50
EPI Suite™	Estimation Programs Interface Suite™
EU-FORA	European Food Risk Assessment
FOCUS	FOrum for the Co-ordination of pesticide fate models and their USe
HPLC-DAD	high-performance liquid chromatography with diode array detector
HPLC–MS	high-performance liquid chromatography–mass spectrometry
INIA	Instituto Nacional de Investigación y Tecnología Agraria y Alimentaria
LC–ESI-QToF-MS	liquid chromatography–electrospray-quadrupole time of flight-mass spectrometry
MAC	maximum allowable concentration
OECD	Organisation for Economic Co-operation and Development
PEARL	Pesticide Emission Assessment at Regional and Local scales
PEC	predicted environmental concentration
PELMO	PEsticide Leaching MOdel
PPP	Plant Protection Products
PPR	Plant Protection Residues
PRZM	pesticides root zone model
QSAR/QSPR	quantitative structure–activity/quantitative structure–property relationship
RAC_{sw}	regulatory acceptable concentration in surface water
SWAN	Surface Water Assessment eNabler
SWASH	Surface WAter Scenarios Help
T.E.S.T.	Toxicity Estimation Software Tool
TOXSWA	TOXic substances in Surface WAters
UPF	Unidad de Productos Fitosanitarios
USEPA	United States Environmental Protection Agency

Annex A – Abstract and certificate of attendance to the 11th European Conference on Pesticides and Related Organic Micropollutants in the Environment – Ioannina (Greece), June 23–26, 2022

11th European CONFERENCE on **Pesticides** and Related Organic Micropollutants in the Environment

& 17th Symposium on Chemistry and Fate of Modern Pesticides

www.pesticides2022.gr

June 23-26 2022

Conference center "Karolos Papoulias"
University of Ioannina,
GREECE

CERTIFICATE OF ATTENDANCE

This is to certify that

MARI ANGELA

attended the
11th European Conference on Pesticides and Related Organic Micropollutants in the Environment
&
the 17th Symposium on Chemistry and Fate of Modern Pesticides
which was held in **Ioannina, Greece,** on **June 23-26, 2022.**

The Conference Chair

Prof. Triantafyllos A.D. Almpanis, Rector
Department of Chemistry, University of Ioannina,
Institute of Environment and Sustainable Development,
University Research Center of Ioannina (URCI)

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