

APPROVED: 22 June 2015

PUBLISHED: 06 July 2015

doi:10.2903/j.efsa.2015.4166

Review of the existing maximum residue levels (MRLs) for cinidon-ethyl according to Article 12 of Regulation (EC) No 396/2005

European Food Safety Authority (EFSA)

Abstract

According to Article 12 of Regulation (EC) No 396/2005, the European Food Safety Authority (EFSA) has reviewed the maximum residue levels (MRLs) currently established at European level for the pesticide active substance cinidon-ethyl. Considering that this active substance is no longer authorised within the European Union, that MRLs are not established by the Codex Alimentarius Commission, and that uses authorised in third countries were not reported to EFSA, residues of cinidon-ethyl are not expected to occur in any plant or animal commodity. Nevertheless, available data allowed EFSA to propose a residue definition and limit of quantification (LOQ) for enforcement against potential illegal uses.

© European Food Safety Authority, 2015

Keywords: cinidon-ethyl, MRL review, Regulation (EC) No 396/2005, consumer risk assessment, dicarboximide, herbicide

Requestor: European Commission

Question number: EFSA-Q-2008-511

Correspondence: pesticides.mrl@efsa.europa.eu

Acknowledgement: EFSA wishes to thank the rapporteur Member State, the United Kingdom, for the preparatory work on this scientific output.

Suggested citation: EFSA (European Food Safety Authority), 2015. Reasoned opinion on the review of the existing maximum residue levels (MRLs) for cinidon-ethyl according to Article 12 of Regulation (EC) No 396/2005. EFSA Journal 2015;13(7):4166, 11 pp. doi:10.2903/j.efsa.2015.4166

ISSN: 1831-4732

© European Food Safety Authority, 2015

Reproduction is authorised provided the source is acknowledged.



The EFSA Journal is a publication of the European Food Safety Authority, an agency of the European Union.



Summary

Cinidon-ethyl was included in Annex I to Directive 91/414/EEC on 1 October 2002 by means of Commission Directive 2002/64/EC, and has been deemed to be approved under Regulation (EC) No 1107/2009, in accordance with Commission Implementing Regulation (EU) No 540/2011, as amended by Commission Implementing Regulation (EU) No 541/2011. As the active substance was approved before the entry into force of Regulation (EC) No 396/2005 on 2 September 2008, EFSA is required to provide a reasoned opinion on the review of the existing MRLs for that active substance in compliance with Article 12(2) of the aforementioned regulation. In order to collect the relevant pesticide residues data, EFSA asked the United Kingdom, as the designated rapporteur Member State (RMS), to complete the Pesticide Residues Overview File (PROFile) for this active substance. This PROFile was submitted to EFSA on 25 February 2011.

Meanwhile, the approval of cinidon-ethyl, which was initially foreseen to be reviewed by 30 September 2012, was not renewed by means of Regulation (EC) No 1134/2011. European authorisations reported in the PROFile were therefore no longer considered relevant but a request for additional information was still addressed to the Member States in the framework of a completeness check period which was initiated by EFSA on 23 December 2014 and finalised on 24 February 2015. Member States did not contest the proposal of EFSA to disregard the European authorisations reported by the RMS and no further information was provided. EFSA prepared a completeness check report which was made available to all Member States on 11 March 2015.

Considering that the use of cinidon-ethyl is no longer authorised within the EU (authorisations for emergency situations in plant protection granted in application of Article 53 of Regulation (EC) No 1107/2009 are not considered in the context of this reasoned opinion), that codex maximum residue limits (CXLs) are not available for this active substance and that uses authorised in third countries were not reported to EFSA, European consumers are not expected to be exposed to residues of this active substance. In order to assist risk managers in applying the most appropriate enforcement measures (against potential illegal uses), EFSA assessed the available data with particular attention to the analytical methods and the nature of residues in plants and livestock. Based on the data reported in the framework of Directive 91/414/EEC, EFSA prepared in May 2015 a draft reasoned opinion, which was circulated to Member States for consultation via a written procedure. Comments received by 29 May 2015 were considered during the finalisation of this reasoned opinion. The following conclusions are derived.

Primary crop metabolism of cinidon-ethyl was investigated in wheat and rotational crop metabolism of cinidon-ethyl was investigated in wheat, beans, carrots and lettuce. Although the available studies provide little information on the nature of cinidon-ethyl residues at harvest, parent compound seems to be the most relevant compound for enforcement against the potential illegal use of cinidon-ethyl in plants. A validated analytical method for enforcement of this compound was reported with a limit of quantification (LOQ) of 0.05 mg/kg in high water content and dry commodities. According to the EURLs, a lower LOQ of 0.01 mg/kg may be achieved in most plant commodities but the supporting data could not be verified by EFSA.

Livestock metabolism of cinidon-ethyl was investigated in goats and hens. These studies indicate that cinidon-ethyl and cinidon acid would be the most relevant compounds for enforcement in livestock. A validated analytical method for enforcement of these compounds was reported with a combined LOQ of 0.05 mg/kg in milk and 0.1 mg/kg in other animal products.

Considering that the enforcement against potential illegal uses falls under the remit of risk managers, EFSA is not in a position to recommend whether the default MRL of 0.01 mg/kg, as defined by Regulation (EC) No 396/2005, or whether the setting of specific LOQ values for plant and animal commodities should apply. It is noted however that specific LOQ values of 0.05 mg/kg for cinidon-ethyl in all plant commodities, 0.05 mg/kg for the sum of cinidon-ethyl and cinidon acid in milk and 0.1 mg/kg for the sum of cinidon-ethyl and cinidon acid in other products of animal origin, would provide a satisfactory level of protection for the European consumers.

Table of contents

| | |
|---|----|
| Abstract..... | 1 |
| Summary..... | 3 |
| Background..... | 5 |
| Terms of reference..... | 6 |
| The active substance and its use pattern | 6 |
| Assessment..... | 7 |
| 1. Residues in plants | 7 |
| 2. Residues in livestock | 7 |
| 3. Consumer risk assessment..... | 8 |
| Conclusions and recommendations | 8 |
| References..... | 9 |
| Abbreviations | 10 |
| Appendix A – List of metabolites and related structural formula | 11 |

Background

Regulation (EC) No 396/2005¹ establishes the rules governing the setting and the review of pesticide maximum residue levels (MRLs) at European level. Article 12(2) of that regulation stipulates that EFSA shall provide by 1 September 2009 a reasoned opinion on the review of the existing MRLs for all active substances included in Annex I to Directive 91/414/EEC² before 2 September 2008. As cinidon-ethyl was included in Annex I to Council Directive 91/414/EEC on 1 October 2002 by means of Commission Directive 2002/64/EC,³ and has been deemed to be approved under Regulation (EC) No 1107/2009,⁴ in accordance with Commission Implementing Regulation (EU) No 540/2011,⁵ as amended by Commission Implementing Regulation (EU) No 541/2011,⁶ EFSA initiated the review of all existing MRLs for that active substance.

According to the legal provisions, EFSA shall base its reasoned opinion in particular on the relevant assessment report prepared under Directive 91/414/EEC. It should be noted, however, that in the framework of Directive 91/414/EEC only a few representative uses are evaluated, while MRLs set out in Regulation (EC) No 396/2005 should accommodate all uses authorised within the EU, and uses authorised in third countries that have a significant impact on international trade. The information included in the assessment report prepared under Directive 91/414/EEC is therefore insufficient for the assessment of all existing MRLs for a given active substance.

In order to gain an overview of the pesticide residues data that have been considered for the setting of the existing MRLs, EFSA developed the Pesticide Residues Overview File (PROFile). The PROFile is an inventory of all pesticide residues data relevant to the risk assessment and MRL setting for a given active substance. This includes data on:

- the nature and magnitude of residues in primary crops;
- the nature and magnitude of residues in processed commodities;
- the nature and magnitude of residues in rotational crops;
- the nature and magnitude of residues in livestock commodities and;
- the analytical methods for enforcement of the proposed MRLs.

The United Kingdom, the designated rapporteur Member State (RMS) in the framework of Directive 91/414/EEC, was asked to complete the PROFile for cinidon-ethyl. This PROFile was submitted to EFSA on 25 February 2011.

Meanwhile, the approval of cinidon-ethyl, which was initially foreseen to be reviewed by 30 September 2012, was not renewed by means of Regulation (EC) No 1134/2011⁷. European authorisations reported in the PROFile were therefore no longer considered relevant but a request for additional information was still addressed to the Member States in the framework of a completeness check period which was initiated by EFSA on 23 December 2014 and finalised on 24 February 2015. Member States did not contest the proposal of EFSA to disregard the European authorisations reported by the RMS and no further information was provided. EFSA prepared a completeness check

¹ Regulation (EC) No 396/2005 of the European Parliament and of the Council of 23 February 2005 on maximum residue levels of pesticides in or on food and feed of plant and animal origin and amending Council Directive 91/414/EEC. OJ L 70, 16.3.2005, p. 1-16.

² Council Directive 91/414/EEC of 15 July 1991 concerning the placing of plant protection products on the market. OJ L 230, 19.8.1991, p. 1-32. Repealed by Regulation (EC) No 1107/2009.

³ Commission Directive 2002/64/EC of 15 July 2002 amending Council Directive 91/414/EEC to include cinidon-ethyl, cyhalofop butyl, famoxadone, florasulam, metalaxyl-M and picolinafen as active substances. OJ No L 189, 18.7.2002, p. 27-32.

⁴ 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 L 309, 24.11.2009, p. 1-50.

⁵ Commission Implementing Regulation (EU) No 540/2011 of 25 May 2011 implementing Regulation (EC) No 1107/2009 of the European Parliament and of the Council as regards the list of approved active substances. OJ L 153, 11.6.2011, p.1-186.

⁶ Commission Implementing Regulation (EU) No 541/2011 of 1 June 2011 amending Implementing Regulation (EU) No 540/2011 implementing Regulation (EC) No 1107/2009 of the European Parliament and of the Council as regards the list of approved active substances. OJ L 153, 11.6.2011, p.187-188.

⁷ Commission Implementing Regulation (EU) No 1134/2011 of 9 November 2011 concerning the non-renewal of the approval of the active substance cinidon-ethyl, in accordance with Regulation (EC) No 1107/2009 of the European Parliament and of the Council concerning the placing of plant protection products on the market, and amending Commission Implementing Regulation (EU) No 540/2011. OJ L 292, 10.11.2011, p. 1-3.

report which was made available to all Member States on 11 March 2015, and no further clarifications were sought from Member States.

Based on the data reported in the framework of Directive 91/414/EEC, EFSA prepared in May 2015 a draft reasoned opinion, which was submitted to Member States for commenting via a written procedure. All comments received by 29 May 2015 were considered by EFSA during the finalisation of the reasoned opinion.

In addition, key supporting documents to this reasoned opinion are the completeness check report (EFSA, 2015a) and the Member States consultation report (EFSA, 2015b). These reports are developed to address all issues raised in the course of the review, from the initial completeness check to the reasoned opinion.

Considering the importance of the completeness check and consultation report, all documents are considered as background documents to this reasoned opinion and, thus, are made publicly available.

Terms of reference

According to Article 12 of Regulation (EC) No 396/2005, EFSA shall provide a reasoned opinion on:

- the inclusion of the active substance in Annex IV to the Regulation, when appropriate;
- the necessity of setting new MRLs for the active substance or deleting/modifying existing MRLs set out in Annex II or III of the Regulation;
- the inclusion of the recommended MRLs in Annex II or III to the Regulation;
- the setting of specific processing factors as referred to in Article 20(2) of the Regulation.

The active substance and its use pattern

Cinidon-ethyl is the ISO common name for ethyl (Z)-2-chloro-3-[2-chloro-5-(cyclohex-1-ene-1,2-dicarboximido)phenyl]acrylate (IUPAC).

Cinidon-ethyl belongs to the group of dicarboximide compounds which are used as herbicide. It acts by the inhibition of protoporphyrinogen oxidase. Through a series of effects, this quickly leads to cell death and tissue desiccation. The compound was mainly developed to control a wide range of annual dicotyledonous seed propagated weeds at a post-emergence stage.

The chemical structure of the active substance and its main metabolites are reported in Appendix A.

Cinidon-ethyl was evaluated in the framework of Directive 91/414/EEC with the United Kingdom designated as RMS. The representative uses supported for the peer review process included a post-harvest application on cereals. Following the peer review, a decision on inclusion of the active substance in Annex I to Directive 91/414/EEC was published by means of Commission Directive 2002/64/EC, which entered into force on 1 October 2002. According to Regulation (EU) No 540/2011, cinidon-ethyl was deemed to have been approved under Regulation (EC) No 1107/2009. This approval was restricted to uses as herbicide only. Meanwhile, the approval of cinidon-ethyl, which was initially foreseen to be reviewed by 30 September 2012, was not renewed by means of Regulation (EC) No 1134/2011. According to this regulation, any period of grace granted by a Member State for plant protection products containing cinidon-ethyl should have on 31 March 2013 at the latest for the sale and distribution and on 31 March 2014 at the latest for the disposal, storage, and use of existing stocks. As EFSA was not yet involved in the peer review of cinidon-ethyl, an EFSA Conclusion on this active substance is not available.

The EU MRLs for cinidon-ethyl are established in Annexes II and IIIB of Regulation (EC) No 396/2005. Changes of these MRLs did not occur since the entry into force of that regulation.

According to the expiry of the approval under Regulation (EC) No 1107/2009, plant protection products containing cinidon-ethyl are no longer authorised in EU Member States (authorisations for emergency situations in plant protection granted in application of Article 53 of Regulation (EC) No 1107/2009 are not considered in the context of this reasoned opinion). For the purpose of this MRL

review, Member States did not report any use authorised in third countries that might have a significant impact on international trade.

Assessment

Considering that the use of cinidon-ethyl is no longer authorised within the EU, that codex maximum residue limits (CXLs) are not available for this active substance and that uses authorised in third countries were not reported to EFSA, European consumers are not expected to be exposed to residues of this active substance. A consumer risk assessment is therefore, in principle, not required.

Risk managers might need however to enforce against the potential illegal use of cinidon-ethyl within the EU as well as the presence of illegitimate residue levels in imported products. In order to assist risk managers in applying the most appropriate enforcement measures, EFSA assessed the available data with particular attention to the analytical methods and the nature of residues in plants and livestock. EFSA mainly bases its assessment on the draft assessment report (DAR) prepared under Council Directive 91/414/EEC (United Kingdom, 1998).

1. Residues in plants

Primary crop metabolism of cinidon-ethyl in wheat was investigated in the framework of Directive 91/414/EEC (United Kingdom, 1998). The active substance (labelled on both the phenyl- and indolyl-rings) was applied once or twice to the plants at BBCH growth stage 31, at a rate of 0.1 kg a.s./ha. Parent compound was found to be the main component of the residue in forage sampled 7-14 days after treatment (up to 51 % of the TRR) but declined to very low levels in straw at harvest (<1 % of the TRR). Formation of the E-isomer of cinidon-ethyl (metabolite 615M00; see Appendix A) was also observed up to 8 % of the TRR in forage, most likely due to the influence of light. Although this isomer was considered relevant in the framework of the peer review, it is present in lower amounts compared to the parent compound and therefore considered of less importance within this framework, in view of identifying indicators for enforcement against potential illegal uses.

The main component of the residue in straw was attributed to a broad fraction of residues which could not be clearly identified. Further attempts to identify this fraction were not successful but severe chemical treatments of this fraction revealed a complex mixture of compounds, some of which were found to be similar to lignin. This unknown fraction was therefore attributed to bound residues or conjugates, which are unlikely to be bioavailable. Residues in grain were generally found to be low (0.01-0.09 mg eq/kg) and to consist of numerous polar compounds.

Rotational crop metabolism of cinidon-ethyl was also investigated in the framework of Directive 91/414/EEC (United Kingdom, 1998). Following treatment of a bare soil at 0.1 kg a.s./ha, residues in rotational crops (wheat, beans, carrots and lettuce at different plant-back intervals) were generally found to be below 0.005 mg eq/kg, except in wheat straw and husk where residues amounted to 0.022 and 0.01 mg eq/kg, respectively. Further investigation of the residues was therefore not carried out and it is concluded that no significant uptake from soil residues is expected.

During the peer review under Directive 91/414/EEC, the RMS also reported an analytical method for enforcement of the parent compound in plants, which uses GC-MS (United Kingdom, 1998). This method was validated for three different fragment ions in two different laboratories with a limit of quantification (LOQ) of 0.05 mg/kg in wheat forage, wheat grain and wheat straw. During the consultation of Member States, EURLs commented that a lower LOQ of 0.01 mg/kg may be achieved in most plant commodities but the supporting data could not be verified by EFSA.

Hence, although the above studies provide little information on the nature of cinidon-ethyl residues at harvest, parent compound seems to be the most relevant compound for enforcement against the potential illegal use of cinidon-ethyl in plants. A validated analytical method for enforcement of this compound was reported with an LOQ of 0.05 mg/kg in high water content and dry commodities.

2. Residues in livestock

Livestock metabolism of cinidon-ethyl was investigated in the framework of Directive 91/414/EEC (United Kingdom, 1998). Goats were dosed for five consecutive days with 5 mg/kg diet or 250-300 mg/kg diet of active substance (labelled on both the phenyl- and indolyl-rings). Hens were dosed for

seven or eight consecutive days with 8 mg/kg diet or 333 mg/kg diet of active substance (also labelled on both rings). Total radioactive residues in the low dose groups were too low for further investigation, except in goat liver and kidney where metabolites 614M37 and 615M39 (see Appendix A) were identified as the major compounds. In the high dose groups, all relevant matrices were investigated and different metabolites were observed at significant levels, depending on the matrix. Cinidon acid (metabolite 615M01; see Appendix A) was the only metabolite to be retrieved in all matrices and parent compound was also recovered at significant levels in poultry fat. Cinidon-ethyl and its acid metabolite are therefore considered to be the most relevant indicator compounds in livestock.

During the peer review under Directive 91/414/EEC, the RMS also reported an analytical method for enforcement of cinidon-ethyl and cinidon acid in livestock, which uses GC-MS (United Kingdom, 1998). This method was validated for three different fragment ions in two different laboratories with, for each analyte, an LOQ of 0.05 mg/kg in muscle, fat, liver, kidney and eggs and an LOQ of 0.025 mg/kg in milk.

Hence, cinidon-ethyl and cinidon acid are considered to be the most relevant compounds for tracing potential illegal use of cinidon-ethyl in feed production. A validated analytical method for enforcement of these compounds was reported with a combined LOQ of 0.05 mg/kg in milk and 0.1 mg/kg in other animal products.

3. Consumer risk assessment

The toxicological assessment of cinidon-ethyl was peer reviewed under Directive 91/414/EEC, which resulted in an acceptable daily intake (ADI) of 0.01 mg/kg bw per day being established by the European Commission (2002). An acute reference dose (ARfD) was not considered necessary for this compound. Although cinidon acid was not identified as a major metabolite in rats, it is expected that cinidon acid is a precursor metabolite for a wide range of other metabolites identified in the rat metabolism. It is therefore considered appropriate to apply the ADI derived for cinidon ethyl to its acid metabolite as well.

In the framework of the current MRL review, exposure of European consumers to residues of cinidon-ethyl is in principle not expected because the use of cinidon-ethyl is no longer authorised within the EU, CXLs are not available and uses authorised in third countries were not reported to EFSA. Nevertheless, in order to assess whether the reported LOQ values are sufficiently protective for European consumers, chronic intake calculations were performed using revision 2 of the EFSA PRIMo (EFSA, 2007). These calculations were carried out assuming an LOQ of 0.05 mg/kg for all plant commodities and milk and a combined LOQ of 0.1 mg/kg for all other products of animal origin. Acute intake calculations were not carried out because an ARfD was not considered necessary for this compound.

The calculated exposures were compared with the toxicological reference value for cinidon-ethyl, derived by the European Commission under Directive 91/414/EEC. The highest chronic exposure was calculated for French toddlers, representing 40 % of the ADI. EFSA highlights that this calculation does not reflect real exposure of consumers to cinidon-ethyl residues. This theoretical calculation only indicates that a specific LOQ of 0.05 mg/kg in plants and milk and a specific LOQ of 0.1 mg/kg in other animal products would provide a satisfactory level of protection for the European consumers.

Conclusions and recommendations

Considering that the use of cinidon-ethyl is no longer authorised within the EU, that CXLs are not available for this active substance and that uses authorised in third countries were not reported to EFSA, European consumers are not expected to be exposed to residues of this active substance. In order to assist risk managers in applying the most appropriate enforcement measures (against potential illegal uses), EFSA assessed the available data with particular attention to the analytical methods and the nature of residues in plants and livestock.

Primary crop metabolism of cinidon-ethyl was investigated in wheat and rotational crop metabolism of cinidon-ethyl was investigated in wheat, beans, carrots and lettuce. Although the available studies provide little information on the nature of cinidon-ethyl residues at harvest, parent compound seems to be the most relevant compound for enforcement against the potential illegal use of cinidon-ethyl in

plants. A validated analytical method for enforcement of this compound was reported with an LOQ of 0.05 mg/kg in high water content and dry commodities. According to the EURLs, a lower LOQ of 0.01 mg/kg may be achieved in most plant commodities but the supporting data could not be verified by EFSA.

Livestock metabolism of cinidon-ethyl was investigated in goats and hens. These studies indicate that cinidon-ethyl and cinidon acid would be the most relevant compounds for enforcement in livestock. A validated analytical method for enforcement of these compounds was reported with a combined LOQ of 0.05 mg/kg in milk and 0.1 mg/kg in other animal products.

Considering that the enforcement against potential illegal uses falls under the remit of risk managers, EFSA is not in a position to recommend whether the default MRL of 0.01 mg/kg, as defined by Regulation (EC) No 396/2005, or whether the setting of specific LOQ values for plant and animal commodities should apply. It is noted however that specific LOQ values of 0.05 mg/kg for cinidon-ethyl in all plant commodities, 0.05 mg/kg for the sum of cinidon-ethyl and cinidon acid in milk and 0.1 mg/kg for the sum of cinidon-ethyl and cinidon acid in other products of animal origin, would provide a satisfactory level of protection for the European consumers.

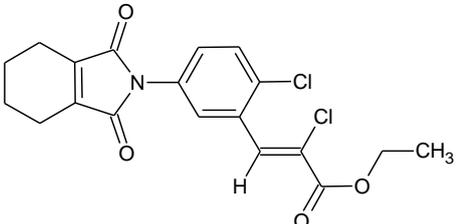
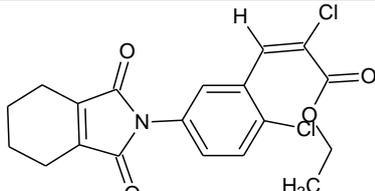
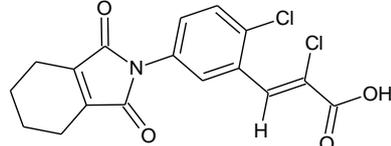
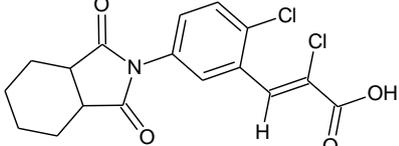
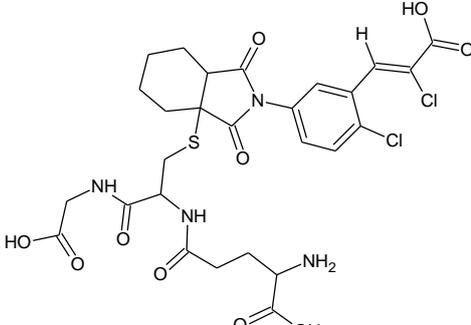
References

- European Commission, 2002. Review report for the active substance cinidon-ethyl. Finalised in the Standing Committee on the Food Chain and Animal Health at its meeting on 19 April 2002 in view of the inclusion of active substance in Annex I of Council Directive 91/414/EEC. SANCO/6498/VI/99-Final, 18 September 2002.
- EFSA (European Food Safety Authority), 2007. Reasoned opinion on the potential chronic and acute risk to consumers' health arising from proposed temporary EU MRLs according to Regulation (EC) No 396/2005 on Maximum Residue Levels of Pesticides in Food and Feed of Plant and Animal Origin. 15 March 2007. The EFSA Journal 2007, 32r, 1-1141. doi:10.2903/j.efsa.2007.32r
- EFSA (European Food Safety Authority), 2015a. Completeness check report on the review of the existing MRLs of cinidon-ethyl prepared by EFSA in the framework of Article 12 of Regulation (EC) No 396/2005, 11 March 2015. Available online: www.efsa.europa.eu
- EFSA (European Food Safety Authority), 2015b. Member States consultation report on the review of the existing MRLs of a cinidon-ethyl prepared by EFSA in the framework of Article 12 of Regulation (EC) No 396/2005, 16 June 2015. Available online: www.efsa.europa.eu
- United Kingdom, 1998. Draft assessment report on the active substance cinidon-ethyl prepared by the rapporteur Member State the United Kingdom in the framework of Council Directive 91/414/EEC, October 1998.

Abbreviations

| | |
|---------|---|
| a.s. | active substance |
| ADI | acceptable daily intake |
| ARfD | acute reference dose |
| BBCH | growth stages of mono- and dicotyledonous plants |
| bw | body weight |
| CXL | codex maximum residue limit |
| DAR | Draft Assessment Report (prepared under Council Directive 91/414/EEC) |
| eq | residue expressed as a.s. equivalent |
| EURLs | EU Reference Laboratories (former CRLs) |
| GC-MS | gas chromatography with mass spectrometry |
| ISO | International Organisation for Standardization |
| IUPAC | International Union of Pure and Applied Chemistry |
| LOQ | limit of quantification |
| MRL | maximum residue level |
| PRIMo | (EFSA) Pesticide Residues Intake Model |
| PROFile | (EFSA) Pesticide Residues Overview File |
| RMS | rapporteur Member State |
| TRR | total radioactive residue |

Appendix A – Used compound codes

| Code/trivial name | Chemical name/SMILES notation ^(a) | Structural formula ^(a) |
|-----------------------|---|--|
| cinidon-ethyl | ethyl (Z)-2-chloro-3-[2-chloro-5-(cyclohex-1-ene-1,2-dicarboximido)phenyl]acrylate <chem>O=C(OCC)C(\Cl)=C\c1cc(ccc1Cl)N3C(=O)C=2CCCC=2C3=O</chem> |  |
| E-isomer (615M00) | ethyl (E)-2-chloro-3-[2-chloro-5-(cyclohex-1-ene-1,2-dicarboximido)phenyl]acrylate <chem>O=C(OCC)C(\Cl)=C/c1cc(ccc1Cl)N3C(=O)C=2CCCC=2C3=O</chem> |  |
| cinidon acid (615M01) | (2Z)-2-chloro-3-[2-chloro-5-(1,3-dioxo-1,3,4,5,6,7-hexahydro-2H-isoindol-2-yl)phenyl]acrylic acid <chem>O=C(O)C(\Cl)=C\c1cc(ccc1Cl)N3C(=O)C=2CCCC=2C3=O</chem> |  |
| 614M37 | (2Z)-2-chloro-3-[2-chloro-5-(1,3-dioxooctahydro-2H-isoindol-2-yl)phenyl]acrylic acid <chem>O=C(O)C(\Cl)=C\c1cc(ccc1Cl)N3C(=O)C2CCCC2C3=O</chem> |  |
| 615M39 | γ-glutamyl-S-(2-{3-[(Z)-2-carboxy-2-chlorovinyl]-4-chlorophenyl}-1,3-dioxooctahydro-3aH-isoindol-3a-yl)cysteinylglycine <chem>O=C(O)C(N)CCC(=O)NC(CSC3CCCC3C(=O)N(C1=O)c2cc(\C=C(/Cl)C(=O)O)c(Cl)c2)C(=O)NCC(=O)O</chem> |  |

(a): ACD/ChemSketch, Advanced Chemistry Development, Inc., ACD/Labs Release: 12.00 Product version: 12.00 (Build 29305, 25 Nov 2008).