FSA Journal

REASONED OPINION

APPROVED: 9 March 2020 doi: 10.2903/j.efsa.2020.6060

Evaluation of confirmatory data following the Article 12 MRL review for sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate (sodium nitrocompounds)

European Food Safety Authority (EFSA),

Maria Anastassiadou, Giovanni Bernasconi, Alba Brancato, Luis Carrasco Cabrera, Luna Greco, Samira Jarrah, Aija Kazocina, Renata Leuschner, Jose Oriol Magrans, Ileana Miron, Stefanie Nave, Ragnor Pedersen, Hermine Reich, Alejandro Rojas, Angela Sacchi, Miguel Santos, Alois Stanek, Anne Theobald, Benedicte Vagenende and Alessia Verani

Abstract

The applicant Asahi Chemical Europe s.r.o. submitted a request to the competent national authority in the Netherlands to evaluate the confirmatory data that were identified for the pesticide active substances sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate (sodium nitrocompounds) in the framework of the maximum residue level (MRL) review under Article 12 of Regulation (EC) No 396/2005 as not available. To address the data gap related to validated analytical enforcement method, the validation data of a method for the determination of sodium nitrocompounds in high acid content commodities, dry commodities and hops (dried) was submitted. The data gap was considered satisfactorily addressed. The risk assessment performed for the three active substances sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate in the framework of the MRL review remains valid.

© 2020 European Food Safety Authority. *EFSA Journal* published by John Wiley and Sons Ltd on behalf of European Food Safety Authority.

Keywords: sodium nitrocompounds, sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate, confirmatory data, pesticide, MRL review, risk assessment

Requestor: European Commission

Question numbers: EFSA-Q-2019-00545

Correspondence: pesticides.mrl@efsa.europa.eu

Acknowledgements: EFSA wishes to thank the following for the support provided to this scientific output: Silvia Ruocco, Laszlo Bura, Georgios Chatzisotiriou, and Viktor Toth.

Amendment: The corrigendum concerns a correction of the MRL proposal in hops which is proposed at the new LOQ of 0.3 mg/kg. To avoid confusion, the older version has been removed from the EFSA Journal but is available on request.

Suggested citation: EFSA (European Food Safety Authority), Anastassiadou M, Bernasconi G, Brancato A, Carrasco Cabrera L, Greco L, Jarrah S, Kazocina A, Leuschner R, Magrans JO, Miron I, Nave S, Pedersen R, Reich H, Rojas A, Sacchi A, Santos M, Stanek A, Theobald A, Vagenende B and Verani A, 2020. Reasoned opinion on the evaluation of confirmatory data following the Article 12 MRL review for sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate (sodium nitrocompounds). EFSA Journal 2020;18(4):6060, 14 pp. https://doi.org/10.2903/j.efsa.2020.6060

ISSN: 1831-4732

© 2020 European Food Safety Authority. *EFSA Journal* published by John Wiley and Sons Ltd on behalf of European Food Safety Authority.

This is an open access article under the terms of the Creative Commons Attribution-NoDerivs License, which permits use and distribution in any medium, provided the original work is properly cited and no modifications or adaptations are made.



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



Summary

In 2015, when the European Food Safety Authority (EFSA) reviewed the existing maximum residue levels (MRLs) for sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate (sodium nitrocompounds) according to Article 12 of Regulation (EC) No 396/2005, EFSA identified some information as unavailable (data gaps) and derived tentative MRLs for those uses which were not fully supported by data but for which no risk to consumers was identified. The following data gaps were noted:

- 1) a validated analytical method for monitoring in high acid content commodities, dry commodities and hops (dried);
- 2) a detailed evaluation of all northern residue trials reported by the RMS in this review;
- 3) additional residue trials supporting authorisations on olives (table and oil).

Tentative MRL proposals have been implemented in the MRL legislation by Commission Regulation (EU) No 2016/1785, including footnotes related to data gap 1, indicating the type of confirmatory data that should be provided by a party having an interest in maintaining the proposed tentative MRLs by 8 October 2018. The data gaps number 2 and 3 were not implemented in the MRL Regulation because risk managers decided to set the MRLs at the level of a combined limit of quantification (LOQ) of 0.03 mg/kg for the related commodities.

In accordance with the agreed procedure set out in the working document SANTE/10235/2016, Asahi Chemical Europe s.r.o. submitted an application to the competent national authority in the Netherlands (rapporteur Member State (RMS)) to evaluate the confirmatory data identified during the MRL review. The RMS assessed the new information in an evaluation report, which was submitted to the European Commission and forwarded to EFSA on 20 August 2019.

The summary table below provides an overview of the assessment of confirmatory data and the recommended MRL modifications to Regulation (EU) No 396/2005.

| Code ^(a) | Commodity | Existing MRL ^(b) | Proposed MRL | Conclusion/recommendation | | |
|--|---|--------------------------------|-----------------|---|--|--|
| p-nitropher | Enforcement residue definition: Sodium 5-nitroguaiacolate, sodium <i>o</i> -nitrophenolate and sodium <i>p</i> -nitrophenolate (sum of sodium 5-nitroguaiacolate, sodium <i>o</i> -nitrophenolate and sodium <i>p</i> -nitrophenolate, expressed as sodium 5-nitroguaiacolate) | | | | | |
| 0151000 0151010 0151020 0152000 0153030 0154030 0500030 0500030 0500060 0500090 | a) Grapes Table grapes Wine grapes b) Strawberries Raspberries (red and yellow) Currents (black, red and white) Maize/corn Rice Wheat | 0.03* (ft 1) | 0.03* | The data gap identified by EFSA concerning a validated analytical method for enforcement in high acid content commodities and dry commodities has been addressed. The MRL is confirmed and the footnote can be deleted. The previous consumer risk assessment remains valid | | |
| 0700000 | Hops | 0.03* (ft 1) | 0.3* | The data gap identified by EFSA concerning a validated analytical method for enforcement in hops (dried) has been addressed. Based on the new information, the MRL is proposed at the new LOQ of 0.3 mg/kg and the footnote can be deleted. The previous consumer risk assessment remains valid | | |

MRL: maximum residue level.

(a): Commodity code number according to Annex I of Regulation (EC) No 396/2005.

(b): Existing EU MRL and corresponding footnote on confirmatory data.

^{*:} Indicates that the MRL is set at the limit of analytical quantification (LOQ).

Ft.1: The European Food Safety Authority identified some information on analytical methods as unavailable. When re-viewing the MRL, the Commission will take into account the information referred to in the first sentence, if it is submitted by 8 October 2018, or, if that information is not submitted by that date, the lack of it. (Footnote related to data gap No 1).

Table of contents

| Abstrac | t | 1 | | | |
|---------|---|----|--|--|--|
| Summa | iry | 3 | | | |
| | nent | 5 | | | |
| 1. | Residues in plants | 5 | | | |
| 1.1. | Nature of residues and methods of analysis in plants | 5 | | | |
| 1.1.1. | Nature of residues in primary crops | 5 | | | |
| 1.1.2. | Nature of residues in rotational crops | 6 | | | |
| 1.1.3. | Nature of residues in processed commodities | 6 | | | |
| 1.1.4. | Methods of analysis in plants | 6 | | | |
| 1.1.5. | Stability of residues in plants | 6 | | | |
| 1.1.6. | Proposed residue definitions | | | | |
| 1.2. | Magnitude of residues in plants | 6 | | | |
| 2. | Residues in livestock | 6 | | | |
| 3. | Consumer risk assessment | 6 | | | |
| 4. | Conclusion and Recommendations | 6 | | | |
| Referer | nces | 7 | | | |
| Abbrevi | iations | 7 | | | |
| Append | lix A – Summary of GAPs assessed in the evaluation of confirmatory data | 8 | | | |
| Append | lix B – List of end points | 9 | | | |
| Append | lix C – Pesticide Residue Intake Model (PRIMo) | 12 | | | |
| Append | lix D – Input values for the exposure calculations | 13 | | | |
| Append | Appendix E – Used compound codes | | | | |

Assessment

The review of existing maximum residue levels (MRLs) for the active substances sodium 5nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate (sodium nitrocompounds) according to Article 12 of Regulation (EC) No $396/2005^1$ (MRL review) has been performed in 2015 (EFSA, 2015). The European Food Safety Authority (EFSA) identified some information as unavailable (data gaps) and derived tentative MRLs for those uses not fully supported by data but for which no risk to consumers was identified.

Following the review of existing MRLs, the relevant legal limits have been modified by Commission Regulation (EU) No 2016/1785², including footnotes for tentative MRLs specifying the type of information that was identified as missing. Any party having an interest in maintaining the proposed tentative MRLs was requested to address the confirmatory data by 8 October 2018.

In accordance with the specific provisions set out in the working document of the European Commission SANTE/10235/2016 (European Commission, 2016) the applicant, Asahi Chemical Europe s.r.o., submitted an application to the competent national authority in the Netherlands (designated rapporteur Member State (RMS)) to evaluate the confirmatory data identified during the MRL review. To address the data gaps identified by EFSA, the applicant provided validation data for the determination of residues of sodium nitrocompounds in high acid content commodities, dry commodities and hops (dried).

The RMS assessed the new information in an evaluation report, which was submitted to the European Commission and forwarded to EFSA on 20 August 2019 (Netherlands, 2019). EFSA assessed the application as requested by the European Commission in accordance with Article 9 of Regulation (EC) No 396/2005.

EFSA based its assessment on the evaluation report submitted by the RMS (Netherlands, 2019³) and the reasoned opinion on the MRL review according to Article 12 of Regulation (EC) No 396/2005.

For this application, the data requirements established in Regulation (EU) No 544/2011⁴ and the relevant guidance documents at the date of implementation of the confirmatory data requirements by Regulation (EU) No 2016/1785 are applicable. The assessment is performed in accordance with the legal provisions of the Uniform Principles for the Evaluation and the Authorisation of Plant Protection Products adopted by Commission Regulation (EU) No 546/2011⁵.

An updated list of end points, including the end points of relevant studies assessed previously and the confirmatory data evaluated in this application, is presented in Appendix B.

The evaluation report submitted by the RMS (Netherlands, 2019) is considered a supporting document to this reasoned opinion and, thus, is made publicly available as a background document to this reasoned opinion.

1. Residues in plants

1.1. Nature of residues and methods of analysis in plants

1.1.1. Nature of residues in primary crops

Not relevant for the current assessment.

¹ Regulation (EC) No 396/2005 of the 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 Commission Regulation (EU) 2016/1785 of 7 October 2016 amending Annexes II and III to Regulation (EC) No 396/2005 of the European Parliament and of the Council as regards maximum residue levels for cymoxanil, phosphane and phosphide salts and sodium 5-nitroguaiacolate, sodium o-nitrophenolate and sodium p-nitrophenolate in or on certain products. OJ L 273, 8.10.2016, p. 10–30.

³ The evaluation report submitted in support of the application on the confirmatory data requested in the framework of the EFSA MRL review (EFSA-Q-2019-00545), covers also the assessment of data submitted in support of a request for the modification of MRLs of sodium nitrocompounds in cucurbits with inedible peel (EFSA-Q-2019-00544); this MRL application will be assessed in a separate reasoned opinion.

⁴ Commission Regulation (EU) No 544/2011 of 10 June 2011 implementing Regulation (EC) No 1107/2009 of the European Parliament and of the Council as regards the data requirements for active substances. OJ L 155, 11.6.2011, p. 1–66.

⁵ Commission Regulation (EU) No 546/2011 of 10 June 2011 implementing Regulation (EC) No 1107/2009 of the European Parliament and of the Council as regards uniform principles for evaluation and authorisation of plant protection products. OJ L 155, 11.6.2011, p. 127–175.

1.1.2. Nature of residues in rotational crops

Not relevant for the current assessment.

1.1.3. Nature of residues in processed commodities

Not relevant for the current assessment.

1.1.4. Methods of analysis in plants

In order to address data gap number $1,^6$ the applicant provided validation data for the determination of residues of sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate in high acid content commodities (strawberries), dry commodities (peas) and hops (dried) (Netherlands, 2019). Residues of free phenol (5-nitroguaiacol, *o*-nitrophenol and *p*-nitrophenol) are determined and expressed as sodium 5–nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate. The quantification is done by high-performance liquid chromatography with mass spectrometric detection (HPLC–MS/MS). The quantification is realised with the free phenol reference item all expressed as the sodium salt (Netherlands, 2019). The validated limit of quantifications (LOQs) were at the level of 0.01 mg/kg per each active substance in high acid content matrices and dry matrices. In hops (dried), an LOQ of 0.1 mg/kg per active substance was sufficiently validated. An independent laboratory validation (ILV) was provided.

The analytical method can be considered to be fully validated as enforcement method in terms of specificity, linearity, accuracy and precision based on the provisions of the SANCO/825/00 rev 8.1 guidance document (European Commission, 2010). Details on the analytical method are presented in Appendix B.1.1.1.

EFSA concluded that the data gap identified in the framework of the MRL review is sufficiently addressed.

1.1.5. Stability of residues in plants

Not relevant for the current assessment.

1.1.6. Proposed residue definitions

The previously derived residue definitions are still applicable.

1.2. Magnitude of residues in plants

Not relevant for the current assessment.

2. Residues in livestock

The confirmatory data assessed in this evaluation do not have an impact on pesticide residues expected in livestock. Thus, the previous assessment of residues in livestock (EFSA, 2015) is still valid.

3. Consumer risk assessment

The submitted confirmatory data did not trigger a modification of the most recent consumer risk assessment which was performed in the framework of the MRL review (EFSA, 2015) and the conclusions derived therein are still valid.

4. Conclusion and Recommendations

To address the data gap identified in the framework of the MRL review (EFSA, 2015), validation data for the determination of sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate residues in high acid content commodities, dry commodities and hops (dried) were submitted by the applicant. The submitted analytical method is sufficiently validated to be proposed as enforcement method in plant matrices with high acid content, dry matrices and hops (dried). The data gap is therefore sufficiently addressed.

⁶ A validated analytical method for monitoring in high acid content commodities, dry commodities and hops (dried).

The overview of the assessment of confirmatory data and the recommended MRL modifications are summarised in Appendix B.4.

References

- EFSA (European Food Safety Authority), 2009. Conclusion regarding the peer review of the pesticide risk assessment of the active substances sodium 5-nitroguaiacolate, sodium o-nitrophenolate and sodium p-nitrophenolate. EFSA Journal 2009;7(4):RN-191, 130 pp. https://doi.org/10.2903/j.efsa.2009.191r
- EFSA (European Food Safety Authority), 2015. Review of the existing maximum residue levels for sodium 5nitroguaiacolate, sodium o-nitrophenolate and sodium p-nitrophenolate according to Article 12 of Regulation (EC) No 396/2005. EFSA Journal 2015;13(12):4356, 39 pp. https://doi.org/10.2903/j.efsa.2015.4356
- European Commission, 2010. Guidance document on pesticide residue analytical methods. SANCO/825/00 rev. 8.1, 16 November 2010.
- European Commission, 2016. Commission staff working document on the evaluation of data submitted to confirm MRLs following the review of existing MRLs Finalised in the Standing Committee on Plants, Animals, Food and Feed at its meeting on 17 June 2016. SANTE/E4/VW 10235/2016 Rev. 2, 3 pp. Brussels, 17 June 2016.
- Greece, 2007. Draft assessment report on the active substance sodium 5-nitroguaiacolate, sodium onitrophenolate and sodium p-nitrophenolate, prepared by the rapporteur Member State Greece in the framework of Council Directive 91/414/EEC, September 2007. Available online: www.efsa.europa.eu
- Greece, 2008. Final addendum to the draft assessment report on the active substance sodium 5-nitroguaiacolate, sodium o-nitrophenolate and sodium p-nitrophenolate, compiled by EFSA, September 2008. Available online: www.efsa.europa.eu
- Netherlands, 2019. MRL application on the setting of an MRL in melons, and evaluation of confirmatory data following review according to Article 12 of Regulation (EC) No 396/2005. July, 2019, 93 pp.

Abbreviations

| a.s. | active substance |
|------------------|--|
| DAT | days after treatment |
| DT ₉₀ | period required for 90% dissipation (define method of estimation) |
| GAP | Good Agricultural Practice |
| HPLC-MS/MS | high-performance liquid chromatography with tandem mass spectrometry |
| ILV | independent laboratory validation |
| LOQ | limit of quantification |
| MRL | maximum residue level |
| PBI | plant-back interval |
| PRIMO | (EFSA) Pesticide Residues Intake Model |
| RA | risk assessment |
| RD | residue definition |
| RMS | rapporteur Member State |
| SANCO | Directorate-General for Health and Consumers |
| SANCO | Directorate-General for Health and Consumers |

Appendix A – Summary of GAPs assessed in the evaluation of confirmatory data

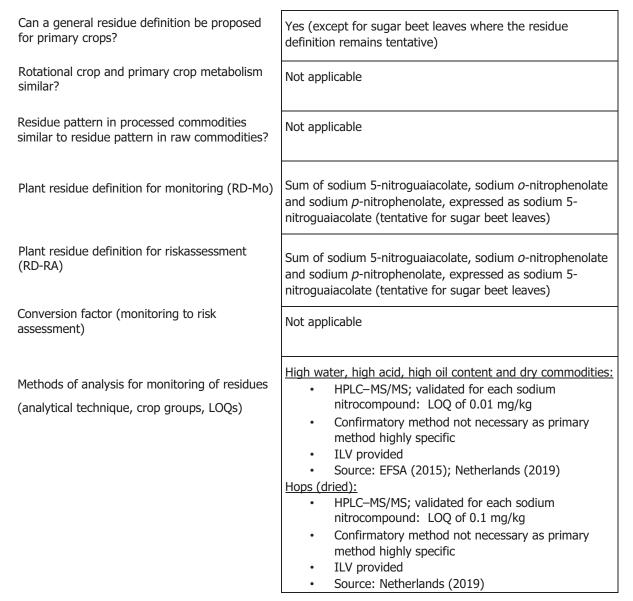
Not applicable.

Appendix B – List of end points

B.1. Residues in plants

- **B.1.1.** Nature of residues and methods of analysis in plants
- **B.1.1.1.** Metabolism studies, methods of analysis and residue definitions in plants

| Primary crops (available studies) | Crop groups | Crop(s) | Application(s) | Sampling (DAT) |
|---|--|---------------|---------------------------------|---|
| I | Fruit crops | Tomatoes | Foliar, 3 $	imes$ 60 g a.s./ha | 6 |
| | Root crops | Sugar beet | Foliar, 2×60 g a.s./ha | 90 |
| | Pulses/oilseeds | Rape seed | Foliar, 2 $	imes$ 60 g a.s./ha | 60 |
| Studies performed with a mixture of sodium 5-nitroguaiacolate, sodium <i>o</i> -nitrophenolate and sodium <i>p</i> -nitrophenolate in the respective concentrations of 0.1%, 0.2% and 0.3° representative of the authorised formulations (Greece, 2007, 2008). The EFSA peer reconcluded that, at the authorised application rates, significant residues are not expect edible parts of the investigated crops. In sugar beet leaves, however, two major compounds remain unidentified and further information on their possible structure wa requested by EFSA. Meanwhile, in the absence of this information, the residue definiti sugar beet leaves is deemed tentative (EFSA, 2009, 2015) | | | | b, 0.2% and 0.3%, the EFSA peer review as are not expected in two major ble structure was |
| Rotational crops (available studies) | l crops Crop groups Crop(s) Application(s) PBI (D | | | |
| Not available and not required as residues not exactly $(DT_{90} = 7.5 \text{ days} \ll 100 \text{ days} = \text{trigger value})$ (f | | | | crops |
| Processed Conditions I commodities Conditions I | | Investigated? | | |
| 1 | Pasteurisation (20 min, 90°C, pH 4)NoBaking, brewing and boiling (60 min, 100°C, pH 5)No | | | No |
| | | | | No |
| | Sterilisation (20 min, 120°C, pH 6) No | | | |
| | Not available and not required as a no-residue situation is expected in fruit crops, root crops and pulses/oilseeds (EFSA, 2015) | | | |



a.s.: active substance; DAT: days after treatment; PBI: plant-back intervals; DT90: period required for 90% dissipation; HPLC–MS/MS: high-performance liquid chromatography with tandem mass spectrometry; LOQ: limit of quantification; ILV: independent laboratory validation.

B.1.1.2. Storage stability of residues in plants

| Plant products (available studies) | Category | Commodity | T (°C) | Stability (Months/years) | |
|---------------------------------------|---|--------------|--------------|--------------------------------|--|
| | High water content | Cucumbers | Not reported | \leq 3 month ^(a) | |
| | High oil content | Oilseed rape | Not reported | 9 months | |
| | Dry | Maize grain | Not reported | 9 months | |
| | High acid content | Strawberries | Not reported | \leq 3 months ^(a) | |
| | (a): Critical storage period was observed for sodium o-nitrophenolate which showed significant degradation after 3 months while sodium 5-nitroguaiacolate and sodium p-nitrophenolate were stable for a longer period (9-10 months) (EFSA, 2015). | | | | |

EFSA Journal

B.1.2. Magnitude of residues in plants

Not relevant. No residue trials were submitted in support of the confirmatory data request of the MRL review.

B.1.2.1. Residues in rotational crops

| Residues in rotational and succeeding crops expected based on confined rotational crop study? | Not triggered | Residues not expected in rotational crops $(DT_{90} = 7.5 \text{ days})$ (EFSA, 2009) |
|---|---------------|---|
| Residues in rotational and succeeding crops expected based on field rotational crop study? | Not triggered | See above |

 DT_{90} : period required for 90% dissipation.

B.1.2.2. Processing factors

Not available and not required; a no-residue situation is expected in fruit crops, root crops and pulses/oilseeds (EFSA, 2015).

B.2. Residues in livestock

Not relevant to the current assessment.

B.3. Consumer risk assessment

The previous most recent consumer risk assessment remains valid (EFSA, 2015).

B.4. Recommended MRLs

| Code ^(a) | Commodity | Existing MRL ^(b) | Proposed MRL | Conclusion/recommendation | | |
|--|---|--------------------------------|-----------------|---|--|--|
| <i>p</i> -nitroph | Enforcement residue definition: Sodium 5-nitroguaiacolate, sodium <i>o</i> -nitrophenolate and sodium <i>p</i> -nitrophenolate (sum of sodium 5-nitroguaiacolate, sodium <i>o</i> -nitrophenolate and sodium <i>p</i> -nitrophenolate, expressed as sodium 5-nitroguaiacolate) | | | | | |
| 0151000 0151010 0151020 0152000 0153030 0154030 0500030 0500030 0500060 0500090 | Wine grapes b) Strawberries Raspberries (red and yellow) Currents (black, red and white) Maize/corn Rice | 0.03* (ft 1) | 0.03* | The data gap identified by EFSA concerning a validated analytical method for enforcement in high acid content commodities and dry commodities has been addressed. The MRL is confirmed and the footnote can be deleted. The previous consumer risk assessment remains valid | | |
| 0700000 | Hops | 0.03* (ft 1) | 0.3* | The data gap identified by EFSA concerning a validated analytical method for enforcement in hops (dried) has been addressed. Based on the new information, the MRL is proposed at the new LOQ of 0.3 mg/kg and the footnote can be deleted. The previous consumer risk assessment remains valid | | |

MRL: maximum residue level.

*: Indicates that the MRL is set at the limit of analytical quantification (LOQ).

(a): Commodity code number according to Annex I of Regulation (EC) No 396/2005.

(b): Existing EU MRL and corresponding footnote on confirmatory data.

.....

Ft.1: The European Food Safety Authority identified some information on analytical methods as unavailable. When re-viewing the MRL, the Commission will take into account the information referred to in the first sentence, if it is submitted by 8 October 2018, or, if that information is not submitted by that date, the lack of it. (Footnote related to data gap No 1).

Appendix C – Pesticide Residue Intake Model (PRIMo)

The previous most recent exposure assessment remains valid (EFSA, 2015).

Appendix D – Input values for the exposure calculations

The previous most recent exposure assessment remains valid (EFSA, 2015).

| Code/trivial name | Chemical name/SMILES notation ^(a) | Structural formula ^(a) |
|---------------------------------|--|-----------------------------------|
| Sodium 5- nitroguaiacolate | sodium 2-methoxy-5-nitrophenolate [Na+].[O-]c1cc(ccc1OC)[N+]([O-])=O KBRKFTKQRMYINW-UHFFFAOYSA-M | |
| Sodium <i>o</i> -nitrophenolate | sodium 2-nitrophenolate [Na+].O=[N+]([O-])c1ccccc1[O-] AXKBOWBNOCUNJL-UHFFFAOYSA-M | |
| Sodium <i>p</i> -nitrophenolate | sodium 4-nitrophenolate [Na+].O=[N+]([O-])c1ccc([O-])cc1 CURNJKLCYZZBNJ-UHFFFAOYSA-M | |

Appendix E – Used compound codes

SMILES: simplified molecular-input line-entry system.

(a): The metabolite name in bold is the name used in the conclusion.

(b): ACD/Name 2015 ACD/Labs 2015 Release (File version N20E41, Build 75170, 19 December 2014).

(c): ACD/ChemSketch 2015 ACD/Labs 2015 Release (File version C10H41, Build 75059, 17 December 2014).