Bayer CropScience

M-542456-01-3

Document Title

# Summary of the fate and behaviour in the environment Prothioconazole FS 100 (100 g/L)

Data Requirements

## EU Regulation 1107/2009 & EU Regulation 284/2013
## Document MCP
## Section 9: Fate and behaviour in the environment

**According to the guidance document, SANCO 10181/2013, for preparing dossiers for the approval of a chemical active substance**

**Date**

**2015-12-07**

**Author(s)**

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# OWNERSHIP STATEMENT

# Version history

| Date | Data points containing amendments or additions[1] and brief description | Document identifier and version number |
|---|---|---|
| | | |
| | | |
| | | |

[1] It is suggested that applicants adopt a similar approach to showing revisions and version history as outlined in SANCO/10180/2013 Chapter 4 How to revise an Assessment Report

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# CP 9 FATE AND BEHAVIOUR IN THE ENVIRONMENT

## Introduction

A dossier on prothioconazole (CAS No. 178928-70-6) was submitted February 2002 by Bayer CropScience to the EU RMS United Kingdom for agricultural use as a fungicide. Prothioconazole was included into Annex I of the Council Directive 91/414/EEC by the Commission Directive 2008/44/EC published 4 April 2008, with an entry into force by 1 August 2008.

This Supplemental Dossier contains only detailed summaries of studies, which were not part of the dossier during the first Annex I inclusion of prothioconazole and were, therefore, not evaluated during the first EU review of this compound. In order to facilitate discrimination between new and old information, the new information is written in black letters whereas *grey letters describe the old information.*

All studies, which have been already submitted by Bayer CropScience for the first Annex I inclusion, are contained in the Monograph and its Addenda and are included in the Baseline dossier provided by Bayer CropScience. The summaries on the different endpoints were taken from the Monograph and its Addenda and supplemented with new information (new studies, references, further comments).

A synonymous name for prothioconazole used at several locations in this supplementary dossier is JAU 6476.

The representative formulation (spray use) submitted in the first Annex I listing process is no longer considered as a representative formulation for the renewal of approval of prothioconazole. One of the representative formulations used for the submission of the renewal of the approval of prothioconazole is the seed treatment formulation Prothioconazole FS 100. The summaries of formulation studies and the risk assessment will be presented in this Dossier.

In this Dossier only endpoints used for the risk assessment are presented. For an overview of all available endpoints for prothioconazole and its metabolites please refer to the respective section of the MCA document. In order to facilitate discrimination between new and information submitted during the Annex I inclusion process, the previously evaluated information is written in grey letters.

## Use pattern considered in the environmental exposure and risk assessment

**Table CP 9- 1: Intended application pattern**

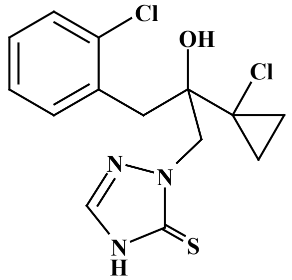
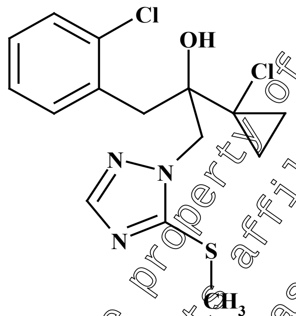
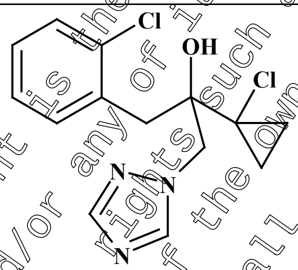
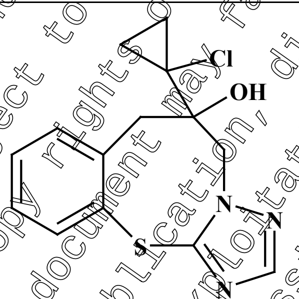
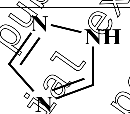
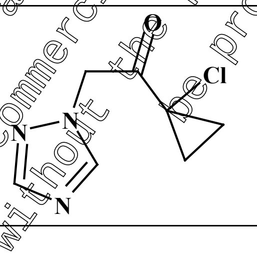
| Crop | Timing of application | Number of applications | Max. application rate, individual treatment [g a.s./ha] Prothioconazole* |
|---|---|---|---|
| Wheat (spring, winter), Barley (spring, winter), Oat, Spelt, Triticale | Seed treatment BBCH 00 | 1 | 18 |

* Maximum label rate: 0.180 L prod./ha; seeding rate: 180 kg seeds/ha; 0.100 L product/100 kg seeds (i.e. 10 g a.s./100 kg seeds)

## Compounds addressed in this document

In addition to the active substance prothioconazole, the degradation products summarised in Table 9- 2 were addressed in this document as they have to be considered for exposure assessments.

**Table CP 9- 2: Active substance and degradation products addressed in this document**

| Compound / Codes | Chemical structure | Considered for |
|---|---|---|
| **Prothioconazole (JAU 6476)** |  | $PEC_{soil}$<br>$PEC_{gw}$<br>$PEC_{sw}$ & $PEC_{sed}$ |
| JAU 6476-S-methyl (M01) |  | $PEC_{soil}$<br>$PEC_{gw}$<br>$PEC_{sw}$ & $PEC_{sed}$ |
| JAU 6476-desthio (M04) |  | $PEC_{soil}$<br>$PEC_{gw}$<br>$PEC_{sw}$ & $PEC_{sed}$ |
| JAU 6476-thiazocine (M12) |  | $PEC_{sw}$ & $PEC_{sed}$ |
| 1,2,4-triazole (M13) |  | $PEC_{sw}$ & $PEC_{sed}$ |
| JAU 6476-triazolylketone (M42) |  | $PEC_{sw}$ & $PEC_{sed}$ |

A list of metabolites, which contains the structures, the synonyms and code numbers attributed to the compound prothioconazole, is presented in Document N3 of this dossier.

### Definition of the residue for risk assessment

Justification for the residue definition for risk assessment is provided by MCA Section 7.

**Table CP 9- 3: Definition of the residue for risk assessment**

| Compartment | Residue definition for risk assessment |
|---|---|
| Soil | Prothioconazole,<br>JAU 6476-S-methyl *(M01)* and<br>JAU 6476-desthio *(M04)* |
| Groundwater | Prothioconazole,<br>JAU 6476-S-methyl *(M01)* and<br>JAU 6476-desthio *(M04)* |
| Surface water | Prothioconazole,<br>JAU 6476-S-methyl *(M01)*,<br>JAU 6476-desthio *(M04)*,<br>JAU 6476-thiazocine *(M12)*,<br>1,2,4-triazole *(M13)* and<br>JAU 6476-triazolylketone *(M42)* |
| Sediment | Prothioconazole,<br>JAU 6476-S-methyl *(M01)*,<br>JAU 6476-desthio *(M04)*,<br>JAU 6476-thiazocine *(M12)*,<br>1,2,4-triazole *(M13)* and<br>JAU 6476-triazolylketone *(M42)* |
| Air | Prothioconazole and<br>JAU 6476-desthio *(M04)* |

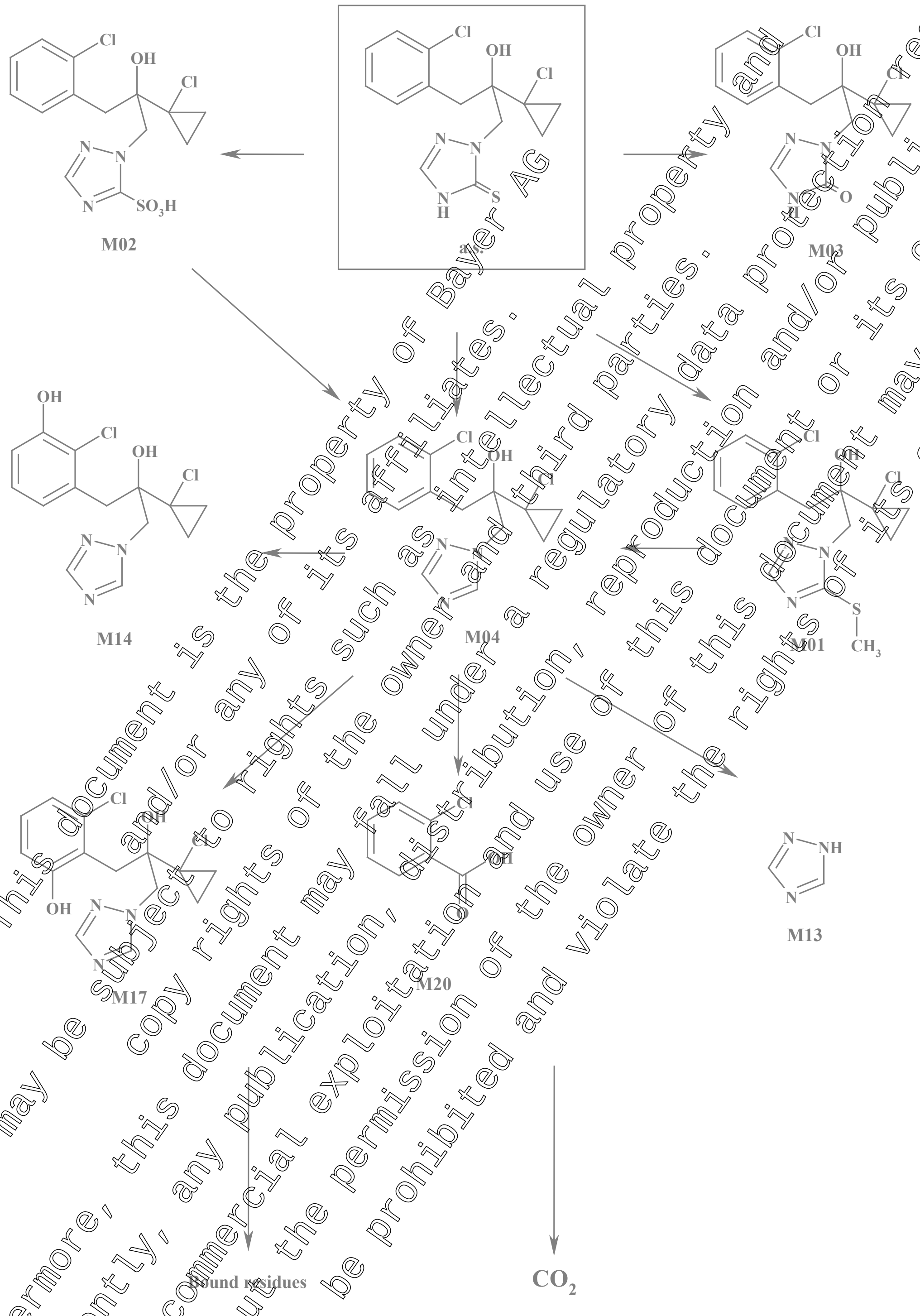
*Justification for the residue definition for risk assessment is provided in MCA Sec.7, Point 7.4.1

## CP 9.1 Fate and behaviour in soil

For information on the fate and behaviour in soil please refer to MCA Section 7, data point 7.1.

The proposed degradation pathway of prothioconazole in soil is shown in Figure CP 9.1- 1.

**Figure CP 9.1- 1: Proposed degradation pathway of prothioconazole in soil under laboratory conditions considering all routes of soil degradation and lysimeter studies.**




a.s. = prothioconazole
M01 = JAU 6476-S-methyl
M02 = JAU 6476-sulfonic acid
M03 = JAU 6476-triazolinone
M04 = JAU 6476-desthio

M13 = 1,2,4-triazole
M14 = JAU 6476-desthio-3-hydroxy
M17 = JAU 6476-desthio-6-hydroxy
M20 = 2-chlorobenzoic acid

## CP 9.1.1 Rate of degradation in soil

No specific studies with the formulation are required. For further information on the fate and behaviour in soil please refer to MCA Section 7, data points 7.1.1 and 7.1.2.

### CP 9.1.1.1 Laboratory studies

For information on laboratory studies please refer to MCA Section 7, data point 7.1.2.1.

### CP 9.1.1.2 Field studies

For information on field studies please refer to MCA Section 7, data point 7.1.2.2.

#### CP 9.1.1.2.1 Soil dissipation studies

For information on field dissipation studies please refer to MCA Section 7, data point 7.1.2.2.1.

#### CP 9.1.1.2.2 Soil accumulation studies

For information on field accumulation studies please refer to MCA Section 7, data point 7.1.2.2.2.

## CP 9.1.2 Mobility in the soil

For information on mobility studies please refer to MCA Section 7, data point 7.1.4.

### CP 9.1.2.1 Laboratory studies

For information on laboratory studies please refer to MCA Section 7, data point 7.1.4.1

### CP 9.1.2.2 Lysimeter studies

For information on lysimeter studies please refer to MCA Section 7, data point 7.1.4.2.

### CP 9.1.2.3 Field leaching studies

For information on field leaching studies please refer to MCA Section 7, data point 7.1.4.3.

## CP 9.1.3 Estimation of concentrations in soil

New calculations were performed to reflect findings from new studies presented in the active substance dossier, section 7 "Fate and behaviour in the environment". In addition these calculations considered the most recent guidance documents for exposure calculations. Calculations of predicted environmental concentrations in soil ($PEC_{soil}$) are presented below.

### Predicted environmental concentrations in soil ($PEC_{soil}$)

### Endpoints for $PEC_{soil}$

For deriving the respective end points please refer to MCA Section 7, data point 7.1.

**Table CP 9.1.3- 1: Key modelling input parameters for prothioconazole and its metabolites**

| Compound | Worst case $DT_{50}$ non-normalised [days] | Maximum occurrence in soil [%] | Molar mass [g/mol] | Molar mass correction factor |
|---|---|---|---|---|
| Prothioconazole | 1.6 | 100 | 344.3 | 1 |
| JAU 6476-S-methyl | 280 | 14.2 | 358.3 | 1.0407 |
| JAU 6476-desthio | 63.4 | 56 | 312.2 | 0.9068 |

| | |
|---|---|
| **Report:** | KCP 9.1.3/03 [redacted]Ä; 2015; M-536053-01-1 |
| Title: | Prothioconazole (PTZ) and metabolites: PECsoil EUR - Use in cereals as spray application and as seed treatment in Europe |
| Report No.: | EnSa-15-0492 |
| Document No.: | M-536053-01-1 |
| Guideline(s): | not applicable |
| Guideline deviation(s): | not applicable |
| **GLP/GEP:** | **no** |

**Methods and Materials:** The predicted environmental concentrations in soil ($PEC_{soil}$) of prothioconazole and its metabolites were estimated based on a first tier approach using a Microsoft® Excel spreadsheet. A bulk density of 1.5 kg/L and a soil mixing depths of 5 cm were used as recommended by FOCUS (1997) and EU Commission (1995, 2000). The accumulation potential of prothioconazole and metabolites after long term use was also assessed, employing the mixing depth of 20 cm for the calculation of the background concentration.
Detailed application data used for simulation of $PEC_{soil}$ were compiled in Table CP 9.1.3- 2.

**Table CP 9.1.3- 2: Application pattern used for $PEC_{soil}$ calculations of prothioconazole**

| Individual crop | FOCUS crop used for interception | Application | | | | Amount reaching soil per season application [g a.s./ha] |
|---|---|---|---|---|---|---|
| | | Rate per season [g a.s. /ha] | Interval [days] | Plant interception [%] | BBCH stage | |
| Winter & spring cereals (seed treatment), GAP | - | 1 × 18 | - | - | 00 | - |
| Winter cereals (seed treatment), simulation | Winter cereals | 1 × 18 | - | - | 00 | 1 × 18.0 |
| Spring cereals (seed treatment), simulation | Spring cereals | 1 × 18 | - | - | 00 | 1 × 18.0 |

**Substance Specific Parameters:** The compound specific input parameters (end points for $PEC_{soil}$ calculations) are summarized in Table CP 9.1.3- 1.

**Findings:** The maximum $PEC_{soil}$ values for prothioconazole and its metabolites are summarised in Table CP 9.1.3- 3. The maximum, short-term and long-term $PEC_{soil}$ values and the time weighted average values ($TWAC_{soil}$) are provided thereafter.

**Table CP 9.1.3- 3: Maximum $PEC_{soil}$ of prothioconazole and its metabolites for the uses assessed**

| | Prothioconazole | S-methyl | Desthio |
|---|---|---|---|
| Use Pattern | $PEC_{soil}$ [mg/kg] | $PEC_{soil}$ [mg/kg] | $PEC_{soil}$ [mg/kg] |
| Winter and spring cereals Seed treatment | 0.024 | 0.004 | 0.012 |

**Table CP 9.1.3- 4: $PEC_{soil}$ (actual) ofprotioconazoleand its metabolites**

| | Time [days] | Winter and spring cereals (seed treatment) 1×18 g a.s./ha, 0% interception | | |
|---|---|---|---|---|
| | | Prothioconazole $PEC_{soil}$ [mg/kg] | S-methyl $PEC_{soil}$ [mg/kg] | Desthio $PEC_{soil}$ [mg/kg] |
| Initial | 0 | 0.024 | 0.004 | 0.012 |
| Short term | 1 | 0.016 | 0.004 | 0.012 |
| | 2 | 0.010 | 0.004 | 0.012 |
| | 4 | 0.004 | 0.004 | 0.012 |
| Long term | 7 | 0.001 | 0.003 | 0.011 |
| | 14 | <0.001 | 0.003 | 0.010 |
| | 21 | <0.001 | 0.003 | 0.010 |
| | 28 | <0.001 | 0.003 | 0.009 |
| | 42 | <0.001 | 0.003 | 0.008 |
| | 50 | <0.001 | 0.003 | 0.007 |
| | 100 | <0.001 | 0.003 | 0.004 |

**Table CP 9.1.3- 5: TWAC$_{soil}$ of prothioconazole and its metabolites**

| | | Winter and spring cereals (seed treatment) 1×18 g a.s./ha, 0% interception | | |
|---|---|---|---|---|
| | | Prothioconazole | S-methyl | Desthio |
| | Time [days] | TWAC$_{soil}$ [mg/kg] | TWAC$_{soil}$ [mg/kg] | TWAC$_{soil}$ [mg/kg] |
| Initial | 0 | --- | --- | --- |
| Short term | 1 | 0.019 | 0.004 | 0.012 |
| | 2 | 0.016 | 0.004 | 0.012 |
| | 4 | 0.011 | 0.004 | 0.012 |
| Long term | 7 | 0.008 | 0.004 | 0.012 |
| | 14 | 0.004 | 0.003 | 0.011 |
| | 21 | 0.003 | 0.003 | 0.011 |
| | 28 | 0.002 | 0.003 | 0.011 |
| | 42 | 0.001 | 0.003 | 0.010 |
| | 50 | 0.001 | 0.003 | 0.009 |
| | 100 | <0.001 | 0.003 | 0.007 |

**Potential accumulation in soil:**

The accumulation potential after long term use was also assessed. The results for a standard-mixing depth of 20 cm for an arable crop with tillage are presented in Table CP 9.1.3- 6.

**Table CP 9.1.3- 6: PEC$_{soil}$ of prothioconazoleand its metabolites taking the effect of accumulation into account (mixing (tillage) depth of 20 cm)**

| Use Pattern | PEC$_{soil}$ | Prothioconazole [mg/kg] | S-methyl [mg/kg] | Desthio [mg/kg] |
|---|---|---|---|---|
| Winter and spring cereals (seed treatment), 1×18 g a.s./ha, 0% interception | plateau | <0.001 | <0.001 | <0.001 |
| | total* | 0.024 | 0.004 | 0.012 |

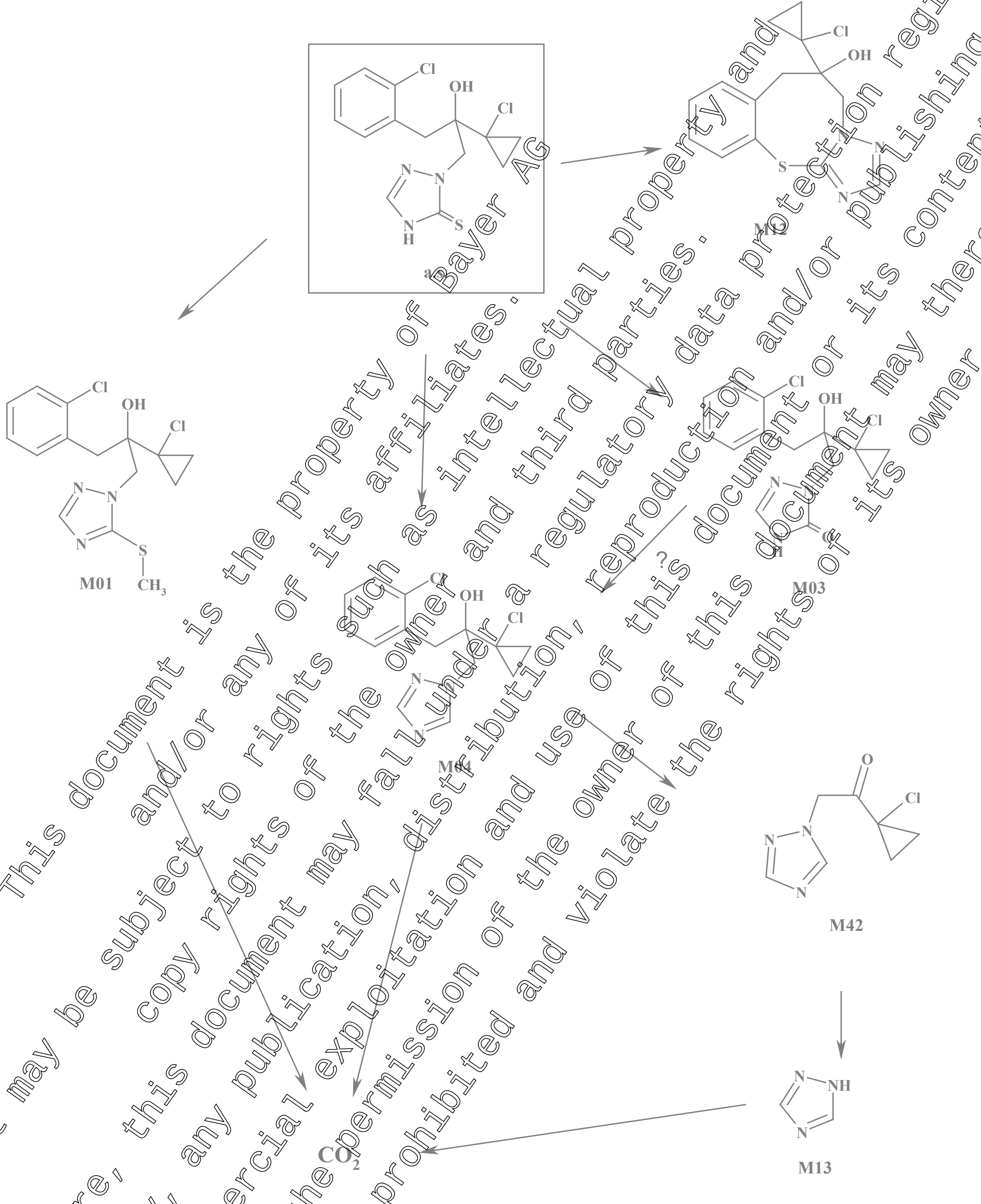
* total = plateau (background concentration after multi-year use) + max. PEC$_{soil}$ (see Table CP 9.1.3- 3)

## CP 9.2 Fate and behaviour in water and sediment

The proposed degradation pathway of prothioconazole in water and sediment is shown in Figure CP 9.2-1.

Specific studies with the formulation have not been performed and are not required. For information on the fate and behaviour in water and sediment please refer to MCA Section 7, data point 7.2.

**Figure CP 9.2- 1:** **Proposed bio-degradation pathway of prothioconazole (JAU 6476-desthio) in water and sediment (major degradation products)**




a.s. = prothioconazole
M01 = JAU 6476-S-methyl
M03 = JAU 6476-triazolinone
M04 = JAU 6476-desthio

M12 = JAU 6476-thiazocine
M13 = 1,2,4-triazole
M42 = JAU 6476-triazolylketone

## CP 9.2.1 Aerobic mineralisation in surface water

For information on aerobic mineralisation in surface water studies please refer to MCA Section 7, data point 7.2.2.2.

## CP 9.2.2 Water/sediment study

For information on water/sediment studies please refer to MCA Section 7, data point 7.2.2.3.

## CP 9.2.3 Irradiated water/sediment study

For information on irradiated water/sediment studies please refer to MCA Section 7, data point 7.2.2.4.

## CP 9.2.4 Estimation of concentrations in groundwater

Calculations were performed, to reflect findings from new studies presented in the active substance dossier, section 7 “Fate and behaviour in the environment”. In addition these calculations consider the most recent guidance documents for exposure calculations.
Calculations of predicted environmental concentrations in groundwater ($PEC_{gw}$) are presented below.

**Endpoints for $PEC_{gw}$**

For deriving the respective end points please refer to MCA Section 7, data point 7.1.

**Table CP 9.2.4.1- 1: Compound input parameters for prothioconazole and its metabolites**

| Parameter | Unit | Prothioconazole | S-methyl | Desthio |
|---|---|---|---|---|
| **Common** | | | | |
| Molar Mass | [g/mol] | 344.3 | 358.3 | 312.2 |
| Solubility | [mg/L] | 22.5 | 4.6 | 50.6 |
| Vapour Pressure | [Pa] | 1.00E-10 | 8.20E-06 | 1.00E-10 |
| Freundlich Exponent | | 1.000 | 0.880 | 0.810 |
| Plant Uptake Factor | | 0.0 | 0.0 | 0.0 |
| Walker Exponent | | 0.7 | 0.7 | 0.7 |
| **PEARL Parameters** | | | | |
| Substance Code | | PTZ | Smet | Des |
| $DT_{50}$ | [days] | 0.90 | 46.4 | 24.7 |
| Molar Activ. Energy | [kJ/mol] | 65.4 | 65.4 | 65.4 |
| $K_{om}$ | [mL/g] | 1024.0 | 1465.0 | 332.7 |
| **PELMO Parameters** | | | | |
| Substance Code | | AS | A1 | B1 |
| Rate Constant | [1/day] | 0.77009 | 0.02806 | 0.01494 |
| $Q_{10}$ | | 2.58 | 2.58 | 2.58 |
| $K_{oc}$ | [mL/g] | 1765.0 | 2526.0 | 573.5 |

**Table CP 9.2.4.1- 2: Degradation pathway related parameters for prothioconazole and its metabolites**

| | |
|---|---|
| Degradation fraction from → to (FOCUS PEARL) | 0.11 PTZ -> Smet<br>0.49 PTZ -> Des<br>1 Smet -> Des |
| Degradation rate from → to (FOCUS PELMO) | 0.3773080 Active Substance -> A1<br>0.0847180 Active Substance -> B1<br>0.3080650 Active Substance -> <BR/$CO_2$<br>0.0280630 A1 -> B1<br>0.0149390 B1 -> <BR/$CO_2$ |

## CP 9.2.4.1 Calculation of concentrations in groundwater

### Predicted environmental concentrations in soil ($PEC_{GW}$)

| | |
|---|---|
| **Report:** | KCP 9.2.4.1/02 [redacted].; 2015; M-536056-01-1 |
| Title: | Prothioconazole (PTZ) and metabolites: PECgw FOCUS PEARL, PELMO EUR - Use in cereals as spray application and as seed treatment in Europe |
| Report No.: | EnSa-15-0491 |
| Document No.: | M-536056-01-1 |
| Guideline(s): | not applicable |
| Guideline deviation(s): | not applicable |
| **GLP/GEP:** | **no** |

The predicted environmental concentrations in groundwater ($PEC_{gw}$) for prothioconazole and its metabolites were calculated using the simulation model FOCUS PEARL (version 4.4.4) and FOCUS PELMO (version 5.5.3). Crop interception was taken into account according to the BBCH growth stage, as recommended by FOCUS (2014). Application dates for the simulation runs were defined following the crop event dates of the respective crop and scenario as given by FOCUS (2000, 2009).

Detailed application data used for simulation of $PEC_{gw}$ were compiled in the following table.

**Table CP 9.2.4.1- 3: Application pattern used for $PEC_{gw}$ calculations**

| Individual crop | FOCUS crop used for interception | Application | | | | Amount reaching soil per season application [g a.s./ha] |
|---|---|---|---|---|---|---|
| | | Rate per season [g a.s. /ha] | Interval [days] | Plant interception [%] | BBCH stage | |
| Winter & spring cereals (seed treatment), GAP | - | 1 × 18 | - | - | 00 | - |
| Winter cereals (seed treatment), simulation | Winter cereals | 1 × 18 | | 0 | 00 | 1 × 18 |
| Spring cereals (seed treatment), simulation | Spring cereals | 1 × 18 | - | 0 | 00 | 1 × 18 |

For cereal applications, absolute dates were derived for the simulation runs. All application dates are summarised in the table below.

**Table CP 9.2.4.1- 4: First application dates and related information for prothioconazole as used for the simulation runs**

| Individual crop | **Winter cereals** | **Spring cereals** |
|---|---|---|
| Repeat Interval for App. Events | Every Year | Every Year |
| Application Technique | Incorp. [4 cm] | Incorp. [4 cm] |
| Absolute / Relative to | Planting | Planting |
| Scenario | 1st App. Date/(Julian day) | 1st App. Date/(Julian day) |
| Chateaudun | 20 Oct/(293) | 20 Feb/(51) |
| Hamburg | 12 Oct/(285) | 10 Mar/(69) |
| Jokioinen | 10 Sep/(253) | 07 May/(127) |
| Kremsmuenster | 25 Oct/(298) | 10 Mar/(69) |
| Okehampton | 07 Oct/(280) | 25 Mar/(84) |
| Piacenza | 25 Nov/(329) | - |
| Porto | 15 Nov/(319) | 20 Feb/(51) |
| Sevilla | 15 Nov/(319) | - |
| Thiva | 15 Nov/(319) | - |

**Findings:** $PEC_{GW}$ were evaluated as the 80th percentile of the mean annual leachate concentration at 1 m soil depth. FOCUS PEARL and PELMO $PEC_{gw}$ results for prothioconazole and its metabolites after application to winter cereals and spring cereals are given in Table CP 9.2.4.1- 5

**Table CP 9.2.4.1- 5: Winter & spring cereals: FOCUS PEARL & PELMO $PEC_{gw}$ results of prothioconazole and its metabolites**

| **Use Pattern** | **Winter cereals (seed treatment), 1 × 18 g a.s./ha** | | | **Spring cereals (seed treatment), 1 × 18 g a.s./ha** | | |
|---|---|---|---|---|---|---|
| | **PTZ*** | **S-methyl** | **Desthio** | **PTZ*** | **S-methyl** | **Desthio** |
| **FOCUS PEARL** | **$PEC_{gw}$ [µg/L]** | **$PEC_{gw}$ [µg/L]** | **$PEC_{gw}$ [µg/L]** | **$PEC_{gw}$ [µg/L]** | **$PEC_{gw}$ [µg/L]** | **$PEC_{gw}$ [µg/L]** |
| Chateaudun | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Hamburg | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Jokioinen | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Kremsmuenster | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Okehampton | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Piacenza | <0.001 | <0.001 | <0.001 | - | - | - |
| Porto | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Sevilla | <0.001 | <0.001 | <0.001 | - | - | - |
| Thiva | <0.001 | <0.001 | <0.001 | - | - | - |
| **FOCUS PELMO** | **$PEC_{gw}$ [µg/L]** | **$PEC_{gw}$ [µg/L]** | **$PEC_{gw}$ [µg/L]** | **$PEC_{gw}$ [µg/L]** | **$PEC_{gw}$ [µg/L]** | **$PEC_{gw}$ [µg/L]** |
| Chateaudun | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Hamburg | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Jokioinen | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Kremsmuenster | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Okehampton | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Piacenza | <0.001 | <0.001 | <0.001 | - | - | - |
| Porto | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| Sevilla | <0.001 | <0.001 | <0.001 | - | - | - |
| Thiva | <0.001 | <0.001 | <0.001 | - | - | - |

* PTZ = prothioconazole

**Conclusion:** There are no concerns for groundwater from the use of prothioconazole in accordance with the use pattern for the representative formulation.

## CP 9.2.4.2 Additional field tests

No additional field studies were performed or required due to low $PEC_{gw}$ values calculated (see CP 9.2.4.1).

## CP 9.2.5 Estimation of concentrations in surface water and sediment

Calculations were performed considering the most recent guidance documents for exposure calculations and taking into account the residue definition derived from the environmental fate studies on MCA Section 7.
Calculations of predicted environmental concentrations in surface water ($PEC_{sw}$) for prothioconazole and its metabolites are presented below.

**Table CP 9.2.5- 1: Key modelling input parameters for prothioconazole and its metabolites at Steps 1/2 level PEC calculations**

| Parameter | Unit | Prothioconazole | JAU 6476-Desthio | JAU 6476 S-Methyl | 1,2,4-Triazole | Triazocine | Triazolylketone |
|---|---|---|---|---|---|---|---|
| Molar Mass | g/mol | 344.26 | 312.2 | 358.3 | 69.1 | 307.8 | 185.7 |
| Water Solubility | mg/L | 22.5 | 50.6 | 4.6 | 700000 | 20 | 1000000 |
| Koc | mL/g | 1765 | 573.5 | 2526 | 83 | 165 | 1 |
| Degradation | | | | | | | |
| Soil | days | 1.4 | 39.6 | 62.6 | 1000 | 1000 | 1000 |
| Total System | days | 14.2 | 55.6 | 80.7 | 1000 | 1000 | 1000 |
| Water | days | 1.2 | 20 | 10.4 | 1000 | 122.1 | 1000 |
| Sediment | days | 80.1 | 57 | 53.6 | 1000 | 1000 | 1000 |
| Max Occurrence | | | | | | | |
| Water / Sediment | % | 100 | 54.5 | 12.7 | 41.8 | 15.2 | 9.1 |
| Soil | % | 100 | 56.2 | 14.2 | 0.0001 | 0.0001 | 0.0001 |

**Table CP 9.2.5- 2: Additional modelling input parameters for prothioconazole and its metabolites at Steps 3/4 level PEC calculations**

| Parameter | Unit | Prothioconazole | JAU 6476-desthio |
|---|---|---|---|
| SWASH code | | PTZ | Des |
| **General** | | | |
| Molar mass | g/mol | 344.3 | 312.2 |
| Water solubility (temp.) | mg/L | 22.5 (20 °C) | 50.6 (20 °C) |
| Vapour pressure (temp.) | Pa | 1E-10 (20 °C) | 1E-10 (20 °C) |
| **Crop processes** | | | |
| Coefficient for uptake by plant (TSCF) | - | 0 | 0 |
| Wash-off factor | 1/m | 50 | 50 |
| **Sorption** | | | |
| KOC | mL/g | 1765.38 | 573.57 |
| KOM | mL/g | 1024 | 332.7 |
| Freundlich exponent (1/n) | - | 1 | 0.81 |
| **Transformation** | | | |
| DT50 in soil | days | 0.9 | 24.7 |
| temperature | °C | 20 | 20 |
| moisture content (relative to) | % | - | - |
| pF | log(cm) | 2 | 2 |
| formation fraction in soil | - | | 0.6 |
| DT50 in water | days | 14.2 | 55.6 |
| temperature | °C | 20 | 20 |
| formation fraction in water | - | | 0.638 |
| DT50 in sediment | days | 1000 | 1000 |
| temperature | °C | 20 | 20 |
| formation fraction in sediment | - | | 0.638 |
| DT50 on canopy | days | 10 | 4 |
| **Exponent for the effect of moisture** | | | |
| PRZM and TOXSWA (Walker exp.) | - | 0.7 | 0.7 |
| MACRO (calibrated value) | - | 0.49 | 0.49 |
| **Effect of temperature** | | | |
| TOXSWA (molar activation energy) | kJ/mol | 65.4 | 65.4 |
| MACRO (effect of temperature) | 1/K | 0.0948 | 0.0948 |
| PRZM (Q10) | - | 2.58 | 2.58 |

## Predicted environmental concentrations in water ($PEC_{sw}$) and sediment ($PEC_{sed}$)

| | |
|---|---|
| **Report:** | KCP 9.2.5/08 [redacted]; 2015; M-536157-01-1 |
| Title: | Prothioconazole (PTZ) and metabolites: PECsw,sed FOCUS EUR - Use in winter and spring cereals in Europe |
| Report No.: | EnSa-15-0840 |
| Document No.: | M-536157-01-1 |
| Guideline(s): | not applicable |
| Guideline deviation(s): | not applicable |
| **GLP/GEP:** | **no** |

**Materials and Methods:** Predicted environmental concentrations in surface water and sediment ($PEC_{sw}$ and $PEC_{sed}$) of prothioconazole and its metabolites have been calculated for the use in winter and spring cereals in Europe. The relevant entry paths can differ based on the intended application type, e.g., spray drift is not relevant for seed treatments.

At FOCUS Step 2 the application period was set to October to February for winter cereals and to March to May for spring cereals. Additioanlly, the use in Northern and Southern Europe was considered. Details of the application pattern used in the Step 2 calculations are summarised in Table CP 9.2.5- 3.

**Table CP 9.2.5- 3: Application pattern used for $PEC_{sw,sed}$ calculations at FOCUS Steps 1&2**

| Crop | Rate [g a.s./ha] | Interval [days] | BBCH stage | FOCUS crop (crop group) | Season | Crop cover |
|---|---|---|---|---|---|---|
| Winter cereals, GAP & simulation | 1 × 18 | - | 00 | no drift (incorp or seed trtmt) (arable crops) | Autumn (Oct. - Feb.) | no interception |
| Spring cereals, GAP & simulation | 1 × 18 | - | 00 | no drift (incorp or seed trtmt) (arable crops) | Spring (Mar. - May) | no interception |

In FOCUS Step 3, the application date for each scenario is determined by the Pesticide Application Timer (PAT), which is part of the FOCUS SW Scenarios. The user may only define an application time window. The actual application date is then set by the PAT in such a way that there are at least 10 mm of rainfall in the first 10 days after application, and at the same time less than 2 mm of rain per day in a five day period around the date of application. If no such date can be found within the application time window, the above rules are step-wise relaxed. Details of the parameters used in the Step 3 calculations are summarised in Table CP 9.2.5- 4.

**Table CP 9.2.5- 4: Application dates of prothioconazole for the FOCUS Step 3 calculations**

| **Parameter** | **Winter cereals** | | **Spring cereals** | |
|---|---|---|---|---|
| PAT start date rel./absolute<br>Appl. method (appl. type)<br>PAT window range | Emergence, -10 days<br>Soil Incorp.<br>(CAM 8 - incorp soil at one depth, 4 cm)<br>30 | | Emergence, -10 days<br>Soil Incorp.<br>(CAM 8 - incorp soil at one depth, 4 cm)<br>30 | |
| Application Details | PAT Start/End Date (Julian Day) | Appl. Date | PAT Start/End Date (Julian Day) | Appl. Date |
| D1 Ditch/Stream | 15-Sep/15-Oct (258/288) | 15.Sep | 25-Apr/25-May (115/145) | 25.Apr |
| D2 Ditch/Stream | 15-Oct/14-Nov (288/318) | 15.Oct | | |
| D3 Ditch | 11-Nov/11-Dec (315/345) | 14.Nov | 22-Mar/21-Apr (81/111) | 04.Apr |
| D4 Pond/Stream | 12-Sep/12-Oct (255/285) | 12.Sep | 16-Apr/16-May (106/136) | 18.Apr |
| D5 Pond/Stream | 31-Oct/30-Nov (304/334) | 27.Nov | 05-Mar/04-Apr (64/94) | 07.Mar |
| D6 Ditch | 20-Nov/20-Dec (324/354) | 06.Dec | | |
| R1 Pond/Stream | 02-Nov/02-Dec (306/336) | 14.Nov | | |
| R3 Stream | 21-Nov/21-Dec (325/355) | 21.Nov | | |
| R4 Stream | 31-Oct/30-Nov (304/334) | 03.Nov | 05-Mar/04-Apr (64/94) | 05.Mar |

Compound input parameters for the Steps 1&2 simulation runs are summarised in Table CP 9.2.5- 1 and for the Steps 3&4 simulation runs in Table CP 9.2.5- 2.

**Findings: Steps 1&2**: The maximum $PEC_{sw}$, $PEC_{sed}$ and 21d-$TWA_{SW}$ values for prothioconazole and its metabolites at Steps 1&2 are summarised in Table CP 9.2.5- 5.

**Table CP 9.2.5- 5: Maximum $PEC_{sw}$ and $PEC_{sed}$ values and 21d-$TWA_{SW}$ values for prothioconazole and its metabolites at Steps 1&2**

| Use pattern | Scenario | Prothioconazole | | | JAU 6476-desthio | | | JAU 6476-S-methyl | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | $PEC_{sw}$ [µg/L] | 21d-TWA [µg/L] | $PEC_{sed}$ [µg/kg] | $PEC_{sw}$ [µg/L] | 21d-TWA [µg/L] | $PEC_{sed}$ [µg/kg] | $PEC_{sw}$ [µg/L] | 21d-TWA [µg/L] | $PEC_{sed}$ [µg/kg] |
| Winter cereals 1 × 18 g a.s./ha | Step 1 | 1.789 | 1.119 | 31.58 | 3.441 | 3.028 | 19.73 | 0.385 | 0.352 | 9.714 |
| | Step 2 | | | | | | | | | |
| | N-EU Single | 0.124 | 0.026 | 2.179 | 0.937 | 0.723 | 5.372 | 0.110 | 0.082 | 2.769 |
| | S-EU Single | 0.099 | 0.021 | 1.743 | 0.749 | 0.578 | 4.298 | 0.088 | 0.066 | 2.216 |
| Spring cereals 1 × 18 g a.s./ha | Step 1 | 1.789 | 1.119 | 31.58 | 3.441 | 3.028 | 19.73 | 0.385 | 0.352 | 9.714 |
| | Step 2 | | | | | | | | | |
| | N-EU Single | 0.049 | 0.010 | 0.872 | 0.375 | 0.289 | 2.149 | 0.044 | 0.033 | 1.108 |
| | S-EU Single | 0.099 | 0.021 | 1.743 | 0.749 | 0.578 | 4.298 | 0.088 | 0.066 | 2.216 |

**Table CP 9.2.5- 6: Maximum $PEC_{sw}$ and $PEC_{sed}$ values and 21d-$TWA_{SW}$ values for prothioconazole and its metabolites at Steps 1&2 (contd.)**

| Use pattern | Scenario | 1,2,4-triazole | | | Thiazocine | | | Triazolylketone | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | $PEC_{sw}$ [µg/L] | 21d-TWA [µg/L] | $PEC_{sed}$ [µg/kg] | $PEC_{sw}$ [µg/L] | 21d-TWA [µg/L] | $PEC_{sed}$ [µg/kg] | $PEC_{sw}$ [µg/L] | 21d-TWA [µg/L] | $PEC_{sed}$ [µg/kg] |
| Winter cereals 1 × 18 g a.s./ha | Step 1 | 0.453 | 0.450 | 0.376 | 0.668 | 0.664 | 1.103 | 0.294 | 0.292 | 0.003 |
| | Step 2 | | | | | | | | | |
| | N-EU Single | 0.031 | 0.031 | 0.026 | 0.046 | 0.044 | 0.076 | 0.020 | 0.020 | <0.001 |
| | S-EU Single | 0.025 | 0.025 | 0.021 | 0.037 | 0.036 | 0.061 | 0.016 | 0.016 | <0.001 |
| Spring cereals 1 × 18 g a.s./ha | Step 1 | 0.453 | 0.450 | 0.376 | 0.668 | 0.664 | 1.103 | 0.294 | 0.292 | 0.003 |
| | Step 2 | | | | | | | | | |
| | N-EU Single | 0.013 | 0.012 | 0.010 | 0.018 | 0.018 | 0.030 | 0.008 | 0.008 | <0.001 |
| | S-EU Single | 0.025 | 0.025 | 0.021 | 0.037 | 0.036 | 0.061 | 0.016 | 0.016 | <0.001 |

**Step 3**: The maximum $PEC_{sw}$ and $PEC_{sed}$ values of prothioconazole and its metabolite JAU 6476-desthio for relevant FOCUS Step 3 scenarios are given in the table below.

**Table CP 9.2.5- 7: Winter cereals: Maximum $PEC_{sw}$ and $PEC_{sed}$ values for prothioconazole and its metabolite JAU 6476-desthio at Step 3**

| Use pattern | Winter cereals, 1 × 18 g a.s./ha | | | | |
|---|---|---|---|---|---|
| | | Prothioconazole | | JAU 6476-desthio | |
| FOCUS scenario | Entry route* | $PEC_{sw}$ [µg/L] | $PEC_{sed}$ [µg/kg] | $PEC_{sw}$ [µg/L] | $PEC_{sed}$ [µg/kg] |
| D1 (Ditch) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D1 (Stream) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D2 (Ditch) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D2 (Stream) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D3 (Ditch) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D4 (Pond) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D4 (Stream) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D5 (Pond) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D5 (Stream) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D6 (Ditch) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| R1 (Pond) | R | <0.001 | <0.001 | <0.001 | <0.001 |
| R1 (Stream) | R | <0.001 | <0.001 | <0.001 | <0.001 |
| R3 (Stream) | R | <0.001 | <0.001 | <0.001 | <0.001 |
| R4 (Stream) | R | <0.001 | <0.001 | <0.001 | <0.001 |

* Entry route: letters D, and R correspond to the dominant entry path – drainage, and runoff.

**Table CP 9.2.5- 8: Spring cereals: Maximum $PEC_{sw}$ and $PEC_{sed}$ values for prothioconazole and its metabolite JAU 6476-desthio at Step 3**

| Use pattern | Spring cereals, 1 × 18 g a.s./ha | | | | |
|---|---|---|---|---|---|
| | | Prothioconazole | | JAU 6476-desthio | |
| FOCUS scenario | Entry route* | $PEC_{sw}$ [µg/L] | $PEC_{sed}$ [µg/kg] | $PEC_{sw}$ [µg/L] | $PEC_{sed}$ [µg/kg] |
| D1 (Ditch) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D1 (Stream) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D3 (Ditch) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D4 (Pond) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D4 (Stream) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D5 (Pond) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| D5 (Stream) | D | <0.001 | <0.001 | <0.001 | <0.001 |
| R4 (Stream) | R | <0.001 | <0.001 | <0.001 | <0.001 |

* Entry route: letters D, and R correspond to the dominant entry path – drainage, and runoff.

## CP 9.3 Fate and behaviour in air

For information on the fate and behaviour in air please refer to MCA Section 7, data point 7.3.

## CP 9.3.1 Route and rate of degradation in air and transport via air

For information on route and rate of degradation in air and transport via air please refer to MCA Section 7, data points 7.3.1 and 7.3.2.

Due to the low volatility and short half-life in air, no PEC calculations are required.

## CP 9.4 Estimation of concentrations for other routes of exposure

There are no other routes of exposure if the product is used according to good agricultural practice. Therefore no further estimations are considered necessary.