knoell Germany GmbH
Konrad-Zuse-Ring 25
68163 Mannheim, Germany

Report

Impact assessment of recent changes in tools and methods for Predicted Environmental Concentration in soil calculations in the context of soil exposure and associated ecotoxicological risk assessment

Report number
116871-1

Project number
116871

Authors
Dr. Sebastian Multsch
Olga Irene Guevara Montemayor

Study completion date
16.03.2022

CropLife Europe
Andrea Alonso Ramos
9 rue Guimard
1040 Brussels
Belgium

GENERAL INFORMATION

Sponsor:	CropLife Europe Andrea Alonso Ramos 9 rue Guimard 1040 Brussels Belgium
Study monitor:	Dr. Krisztian Szegedi
Service provider:	knoell Germany GmbH Konrad-Zuse-Ring 25 68163 Mannheim Germany
Project number:	116871
Report number:	116871-1
Substance:	various
Study type, endpoint:	Soil exposure and associated ecotoxicological risk assessment
Author(s):	Dr. Sebastian Multsch Olga Irene Guevara Montemayor

TABLE OF CONTENTS

GENERAL INFORMATION 2
TABLE OF CONTENTS 3
LIST OF TABLES 4
LIST OF FIGURES 5
SUMMARY 9
1 INTRODUCTION 11
2 METHODS AND SCENARIOS 12
2.1 Soil risk assessment according to EFSA (2017) 12
2.1.1 Tiers 12
2.2 Soil risk assessment according to FOCUS (1997) 15
2.3 Model selection and automation 16
2.4 Substance data 17
2.5 Application scenarios 19
2.6 Ecotoxicological data 20
3 RESULTS AND DISCUSSION 21
3.1 Exposure assessment: $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio 21
3.2 Impact of crop interception and foliar wash-off 25
3.3 Environmental conditions of Tier-3A assessment locations 28
3.4 Risk assessment: failure rate 29
4 CONCLUSIONS 32
5 REFERENCES 34
6 APPENDIX 36

LIST OF TABLES

Table 1. Overview of general input parameters for all substances for the model FOCUS-PELMO v6.6.1 (soil) 17
Table 2. Categorization of active substances (N=56) 17
Table 3. Classification of individual active substances according to the scheme shown in Table 2 18
Table 4. Categorization of metabolites (N=65) 18
Table 5. Simulated crops (PERSAM crop name) and crop interception in percent at the respective application date. 19
Table 6. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios for individual active substance categories (with minimum and maximum in brackets) per modelled tier for all regulatory zones, median values for all categories together, and median values for each zone, irrespective of category. 21
Table 7. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios for individual metabolite substance categories (with minimum and maximum in brackets) per modelled tier for all regulatory zones, median values for all categories together, and median values for each zone, irrespective of category. 22

Table A 1. Descriptive statistical parameters of $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substance. 39
Table A 2. Descriptive statistical parameters of $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of metabolites. 40
Table A 3. Failure rates (%) of active substances and metabolites grouped by substance categories - EFSA (2017) assessment, for all categories and zones, and for all categories but separated by regulatory zone. 41
Table A 4. Failure rates (%) of active substances and metabolites grouped by substance categories - FOCUS (1997) assessment, and for all categories. 41
Table A 5. Variability of environmental conditions of 95th percentile scenario locations for Tier-3A total soil exposure assessment 55
Table A 6. Variability of environmental conditions of 95th percentile scenario locations for Tier-3A pore water exposure assessment. 56

LIST OF FIGURES

Figure 1. Scenario locations at Tier-1 for total soil (left) and pore water (right) concentration in the three regulatory zones (source: EFSA, 2019). 13
Figure 2. Top soil organic matter (source: EFSA Spatial Data)....14
Figure 3. Example input data for Tier-3A which are derived from Tier-2 simulations as defined by the 95th spatial percentile. 15
Figure 4. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of active substances separated by substance categories and FOCUS zones at Tier-1, Tier-2 and Tier-3A, respectively. 23
Figure 5. Median PECsoil,EFSA / PECsoil,FOCUS ratios of metabolites separated by substance categories and FOCUS zones at Tier-1, Tier-2 and Tier-3A, respectively. 24
Figure 6. Impact of scenario and model adjustment factor in $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances. 25
Figure 7. Relationship between crop interception and $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio at Tier-3A of active substances for each regulatory zone. 26
Figure 8. Relationship between environmental conditions at Tier-3A and $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances. 27
Figure 9. K-Means cluster analysis of the total soil $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio (*ratio*), soil bulk density (*bd*) and crop interception (*intc*) of Tier-3A scenario locations. 28
Figure 10. Variability of bulk density of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas. 29
Figure 11. Variability of organic matter of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas. 29
Figure 12. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,FOCUS}$ values for (a) active substances and (b) metabolites. 30
Figure 13. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances at (a) Tier-1, (b) Tier-2 and (c) Tier-3A. 31
Figure 14. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites at (a) Tier-1, (b) Tier-2 and (c) Tier-3A. 31

Figure A 1. Variability of $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances per regulatory zone and tier. 36
Figure A 2. LOG10-scaled variability of $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances per regulatory zone and tier. 36
Figure A 3. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of active substances per regulatory zone

and tier. 37
Figure A 4. Variability $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of metabolites per regulatory zone and tier. 37
Figure A 5. LOG10-scaled variability of $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of metabolites per regulatory zone and tier. 38
Figure A 6. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of metabolites per regulatory zone and tier. 38
Figure A 7. Failure rate (%) based on $PEC_{soil,EFSA}$ values for active substances grouped by substance categories and regulatory zone. 42
Figure A 8. Failure rate (%) based on $PEC_{soil,EFSA}$ values for of metabolites grouped by substance categories and regulatory zone. 43
Figure A 9. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances at each regulatory zone (a) North, (b) Central and (c) South. 44
Figure A 10. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances at each regulatory zone (a) North, (b) Central and (c) South - Tier-1. 44
Figure A 11. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances at each regulatory zone (a) North, (b) Central and (c) South - Tier-2. 45
Figure A 12. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances at each regulatory zone (a) North, (b) Central and (c) South - Tier-3A. 45
Figure A 13. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites at each regulatory zone (a) North, (b) Central and (c) South. 46
Figure A 14. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites at each regulatory zone (a) North, (b) Central and (c) South –Tier-1. 46
Figure A 15. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites at each regulatory zone (a) North, (b) Central and (c) South –Tier-2. 47
Figure A 16. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites at each regulatory zone (a) North, (b) Central and (c) South –Tier-3A. 47
Figure A 17. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on

$PEC_{soil,EFSA}$ values for active substances for each crop type (a) Annual crops and (b) Permanent crops. 48
Figure A 18. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances for each crop type (a) Annual crops and (b) Permanent crops – Tier-1. 48
Figure A 19. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances for each crop type (a) Annual crops and (b) Permanent crops – Tier-2. 49
Figure A 20. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances for each crop type (a) Annual crops and (b) Permanent crops – Tier-3A. 49
Figure A 21. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites for each crop type (a) Annual crops and (b) Permanent crops. 50
Figure A 22. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites for each crop type (a) Annual crops and (b) Permanent crops – Tier-1. 50
Figure A 23. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites for each crop type (a) Annual crops and (b) Permanent crops – Tier-2. 51
Figure A 24. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites for each crop type (a) Annual crops and (b) Permanent crops – Tier-3A. 51
Figure A 25. Relationship between crop interception and $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio at Tier-3A of metabolites for regulatory zones. 52
Figure A 26. Relationship between environmental conditions at Tier-3A and $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of metabolites. 52
Figure A 27. Variability of pH of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas. 53
Figure A 28. Variability of field capacity of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas. 53
Figure A 29. Variability of temperature of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas. 54
Figure A 30. Variability of precipitation of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas. 54
Figure A 31. Failure rate (%) of the risk assessment based on $PEC_{pore\ water,EFSA}$ values for active

substances at (a) Tier-1, (b) Tier-2 and (c) Tier-3A. 57
Figure A 32. Failure rate (%) based on $PEC_{pore\ water,EFSA}$ values for active substances grouped by substance categories and regulatory zone. 57
Figure A 33. Results of multivariate regression model of environmental parameters at Tier-3A 95th percentile locations and crop interception in relation to $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances in total soil. 58
Figure A 34. Results of multivariate regression model of bulk density at Tier-3A 95th percentile locations and crop interception in relation to $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances in total soil. 59

SUMMARY

In 2017, the European Food Safety Authority (EFSA) published a new guidance with four tiers for the exposure assessment of plant protection products (PPPs) in soil (EFSA, 2017). The calculation framework and underlying tools largely differ from the current modelling approach (FOCUS, 1997).

The aim of this project was to investigate the changes in predicted environmental concentrations (PECs) and potential implications for the ecotoxicological risk assessment (RA) of soil organisms using the new framework, and to compare the results with the FOCUS-based modelling approach and RA outcome. Therefore, an impact assessment was carried out using substance parameters and application patterns for 56 different active substances characterized by a broad range of environmental fate parameters and several different use patterns. Up to two metabolites per active substance for a total of 65 metabolites were simulated accordingly.

Tier-1 and Tier-2 PEC values were calculated using PERSAM (Persistence in Soil Analytical Model, v3.0.6). Tier-3A calculations were conducted using FOCUS PELMO (v6.6.1 (soil)). For each modelled compound, use pattern, and available regulatory zone (North, Central and South), exposure concentration values were calculated for two scenarios: one scenario for the concentration in total soil (PEC_{soil}) at an assessment depth of 5cm and one scenario for the concentration in pore water ($PEC_{pore\ water}$) at an assessment depth of 1 cm. For the ecotoxicological RA, the PEC_{soil} was divided by the regulatory acceptable concentration (RAC) for soil organisms based on EU agreed endpoints to calculate the failure rate (compounds with a PEC/RAC ratio ≥1).

As a general observation, it was noted that PEC_{soil} values calculated according to EFSA (2017; $PEC_{soil,EFSA}$) were - at all tiers - substantially higher than exposure values calculated according to the current FOCUS approach (FOCUS 1997; $PEC_{soil,FOCUS}$) for the same compounds. $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios were calculated for each compound to display the increase in exposure values according to the new framework. The main findings are:

- The median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of active substances are 12, 7 and 2 for Tier-1, Tier-2 and Tier-3A, respectively The median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of active substances (all Tiers combined) are 9, 7 and 6 for the Northern, Central and Southern zone, respectively.
- The median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of metabolites are 42, 22 and 2 for Tier-1, Tier-2 and Tier-3A, respectively The median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of metabolites (all Tiers combined) are 19, 13 and 11 for the Northern, Central and Southern zone, respectively.

Overall, modelled concentrations were observed to decrease with increasing tier (from Tier-1 to Tier-3A), as well as from North to South. The following factors have been identified as main drivers for the significant changes in exposure values:

- The highest $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios were observed for active substances with DT50s >100 days, irrespective of the K_{oc} value. In contrast, the lowest ratios were generally observed for active substances with DT_{50} values <50 days. These categories cover all crop types and contain GAPs targeting at higher BBCH stages. At least for active substances, a higher DT_{50} may be associated with a higher $PEC_{soil,EFSA}$ value than $PEC_{soil,FOCUS}$
- $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios are largely different between the different Tiers for each compound, and show a decreasing trend with increasing Tier.
- Further, PEC_{soil} values calculated with the new EFSA (2017) framework strongly depend on the geographic location of the scenarios automatically selected by the PERSAM model.
- Soil bulk density (derived by a European pedotransfer function from organic matter, Tiktak et al., 2002) was identified as a main driver of the concentration increase along a general gradient from North to South as demonstrated by means of linear regression and K-mean clustering.
- Foliar interception and simulated wash-off, determined by crop growth stage at time of application, were identified as other main drivers of the increase in concentrations. Crop

interception is accompanied by wash-off in case of EFSA Tier-2 and Tier-3A calculations, but is not considered in FOCUS (1997) and EFSA (2017) Tier-1 calculations. The effect was higher for uses with higher interception at the time of application, due to larger impact of simulated foliar wash-off on the amount of substance reaching the soil. The statistical analysis showed that the largest concentration increase occurs in cases with a combination of a high crop interception and low bulk density.

- Obligatory model and scenario specific correction factors contributed to an increase of PEC_{soil} values over all compounds and uses for Tier-1 and Tier-2.
- In the case of metabolites, no clear driving factor for the generally increased PEC_{soil} values could be observed, which might be related to the unbalanced allocation between categories and the net effect of range of processes that influence formation, degradation and mobility of residues. Significant variation is noted with the diversity of degradation pathways considered.

In the ecotoxicological soil RA, calculation of failure rates per compound was done by using $PEC_{soil,FOCUS}$ and $PEC_{soil,EFSA}$ values separately, in order to investigate regulatory implications due to the new modelling framework. Across all zones, elevated $PEC_{soil,EFSA}$ values consequently increased RA failure rates in the ecotoxicological Tier 1 RA. The detailed results are as follows:

- The failure rates based on $PEC_{soil,FOCUS}$ are 14% and 8% for active substances and metabolites, respectively.
- The failure rates of active substances based on $PEC_{soil,EFSA}$ are 67%, 58% and 36% for Tier-1, Tier-2 and Tier-3A, respectively.
- The failure rates of metabolites based on $PEC_{soil,EFSA}$ are 38%, 25% and 10% for Tier-1, Tier-2 and Tier-3A, respectively.

Compared to the current failure rate based on $PEC_{soil,FOCUS}$ for the given compounds and the corresponding Tier 1 RACs, this may have significant implications for PPP registrations. Currently, the only refinement option for a failing Tier 1 RA is a higher tier field study, investigating whether effects on soil organism communities occur at relevant field application rates under natural conditions. Accordingly, up to 5 times more field studies may be triggered if the new modelling framework (EFSA, 2017) would be implemented at Member State level.

Yet, it is unclear how to translate exposure values from the new modelling tiers to ecotoxicological endpoints from either lab or field. Selection procedures of geographic locations for exposure assessment results in incompatible soil properties (e.g., organic carbon content, bulk density) between e-fate and ecotoxicological data. This inconsistency hinders scientifically reasonable comparison and interpretation. At present, the new modelling framework (EFSA, 2017) should not be used for regulatory soil RA before an updated soil organism RA guidance becomes available, which specifies how these exposure values should be implemented in a tiered soil RA approach.

Ecotoxicological ‘intermediate-tier’ effect studies or modelling approaches may be a potential option to overcome such discrepancies in the future but are currently not available / accepted. A sufficiently long transition period will be required to ensure alignment between the new modelling framework and the tiered assessment for soil organisms.

1 INTRODUCTION

In 2017, the European Food Safety Authority (EFSA) published a new guidance with four tiers for the exposure assessment of plant protection products (PPPs) in soil (EFSA, 2017). Tier-1 and Tier-2 procedures can be calculated with the software tool PERSAM v3.0.6 which has been released in 2021. This software generates input for Tier-3A calculations which are performed with the PEARL and PELMO tools. In a final tier, Tier-4 addresses post-registration monitoring. The calculation framework and underlying tools have been subject to ongoing development in recent years and largely differ from the current modelling approach (FOCUS, 1997). Thus, changes in the soil exposure modelling framework can be expected to have wide implications for the ecotoxicological risk assessment (RA) of soil organisms.

For the registration of plant protection products in the European Union (EU), a RA for soil organisms exposed to PPPs is conducted as a two-tiered approach. First, laboratory derived ecotoxicity endpoints are compared to predicted environmental concentrations in soil (PEC_{soil}). If a potential risk is indicated, higher tier field studies are the only option to investigate whether effects on soil organism communities occur at relevant field application rates under natural conditions.

To investigate the changes in predicted environmental concentrations (PECs) and potential consequences for the ecotoxicological RA of soil organisms, an impact assessment was carried out. The results of the new modelling framework were compared to the current FOCUS-based modelling approach. Further, the failure rate of the ecotoxicological RA was determined based on the FOCUS and EFSA PECs ($PEC_{soil,FOCUS}$ and $PEC_{soil,EFSA}$), respectively. Therefore, the respective PEC_{soil} was divided by the regulatory acceptable concentration (RAC) for soil organisms based on EU agreed endpoints for each compound, in order to calculate the failure rate (compounds with PEC / RAC ratio ≥ 1).

A similar impact assessment was already conducted earlier by Budde (2013, knoell project No. 416301), yet based on the modelling approach as outlined in EFSA PPR Panel (2012). In the present study, the most recent versions of available tools and models (EFSA, 2017; VITO, 2019) were used.

56 different active substances (and their respective metabolites) covering a broad range of environmental fate parameters and use patterns were provided by the following six CLE member companies and were considered in the impact assessment: ADAMA (9 substances), BASF (9 substances), Bayer Crop Science (10 substances), Corteva (3 substances), FMC (12 substances) and Syngenta (13 substances).

2 METHODS AND SCENARIOS

2.1 Soil risk assessment according to EFSA (2017)

2.1.1 *Tiers*

The soil risk assessment is generally conducted in a tiered approach. Lower tiers are based on less sophisticated modelling approaches and generalized input data (i.e. scenarios) in comparison to higher tiers, but are more conservative with respect to parameterisation. Higher tier approaches account for an increased realism by using more complex models and highly detailed environmental data. Tier-1 assessment is conducted with an analytical model using predefined scenarios. Tier-2 allows a crop-specific and substance-specific assessment based on a spatially distributed version of the analytical model. In Tier-3A, the analytical model is replaced by numerical models as proposed by the FOrum for Co-ordination of pesticide fate models and their USe (FOCUS) (Pesticide Leaching Model (PELMO), Pesticide Emission Assessment at Regional and Local scales (PEARL)).

This evaluation covers Tier-1 and Tier-2 with the analytical model PERSAM and Tier-3A with the numerical model PELMO. Finally, soil concentrations were calculated with the approach described in FOCUS (1997) and compared to the calculation under the new approach (are calculated, namely the concentration in total soil and the concentration in pore water, both averaged over various depths and time windows. Until an EFSA guidance on the risk assessment for in-soil organisms becomes available, this exposure guidance proposes to use the assessment depths of 5 cm and 20 cm (the latter in case of soil incorporation) which is in line with the currently applied procedure (FOCUS, 1997).

In general, mean/median substance properties should be used for the exposure assessment and not high/low percentile values or worst-case properties. The use of mean values leads to a larger variability of PEC_{soil} values on a spatial scale, which is why the 95th spatial percentile is used as a surrogate for the 90th percentile (see Section 4.2.5 of EFSA PPR Panel (2012) for details). This approach was combined with a conservative assumption for the selection of the temporal PEC_{soil} values, for which the 97.5th temporal percentile is used. According to EFSA PPR Panel (2012), there will be only small differences between the 72.5th and 97.5th percentiles at all, so the impact of such a conservative assumption is rather small.

A further important aspect is the consideration of two types of adjustment factors. The analytical model PERSAM is used to calculate the lower tier PEC_{soil} at Tier-1 and Tier-2. Due to the fact that PERSAM does not necessarily provide more conservative values than the numerical models at Tier-3A, model adjustment factors were introduced to ensure that the lower tiers are more conservative than the more realist numerical models. The calculations of Tier-2 and Tier-3A are based on the 95th spatial percentile with reference to the total agricultural area. In contrast, in the case of Tier-1, representative locations are evaluated. To ensure that Tier-1 calculations are always more conservative than the other higher tiers, scenario adjustment factors were introduced.

<u>Tier-1</u>

Tier-1 uses a straightforward analytical model which is implemented in the PERSAM model. Six scenario sites were defined, three for each of the two exposure concentrations in total soil and pore water. Of the three scenarios, one is located in each of the regulatory zones (North, Central and South, Figure 1). Tier-1 is based on the assumption that crop interception and wash-off of the substance does not occur, i.e. crop canopy processes are not considered at all. The scenario adjustment factors are 1.4 and 1.6 for total soil and pore water concentrations, respectively. Additionally, Tier-1 assumes model adjustment factors of 3.0 and 4.0 for total soil and pore water concentrations, respectively.

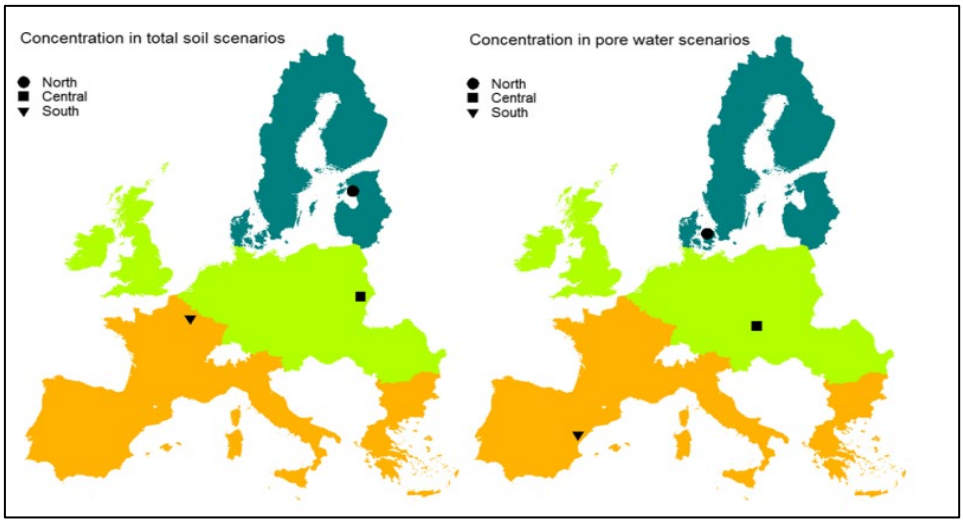


Figure 1. Scenario locations at Tier-1 for total soil (left) and pore water (right) concentration in the three regulatory zones (source: EFSA, 2019).

Tier-2

For the evaluation conducted at Tier-2, a spatially distributed version of PERSAM is used. The PEC_{soil} calculations are conducted for 1km x 1km grid cells. The 95th spatial percentile is directly obtained from the spatial cumulative frequency function. The 95th percentile locations are independently calculated for the two exposure concentrations (total soil and pore water). The spatial calculation is based on the EFSA Spatial Data (version 1.1) with a resolution of 1km x 1km. An example is shown for the parameter organic matter in Figure 2. Cropping extents of annual crops are derived from the CAPRI dataset (Leip et al., 2008) and permanent crops from CORINE Land Cover database and EUROSTAT data sets (Beulke et al., 2015).

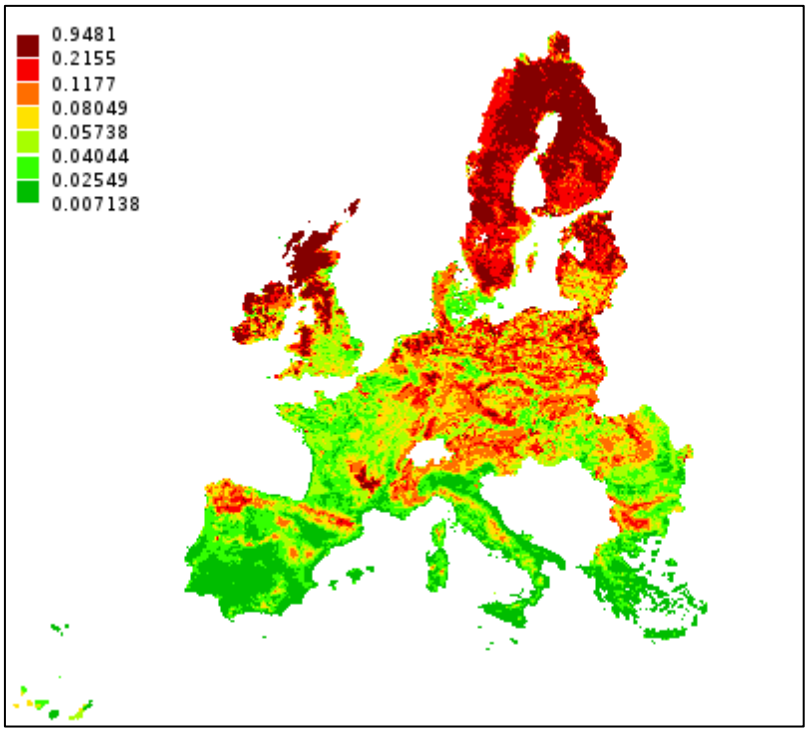
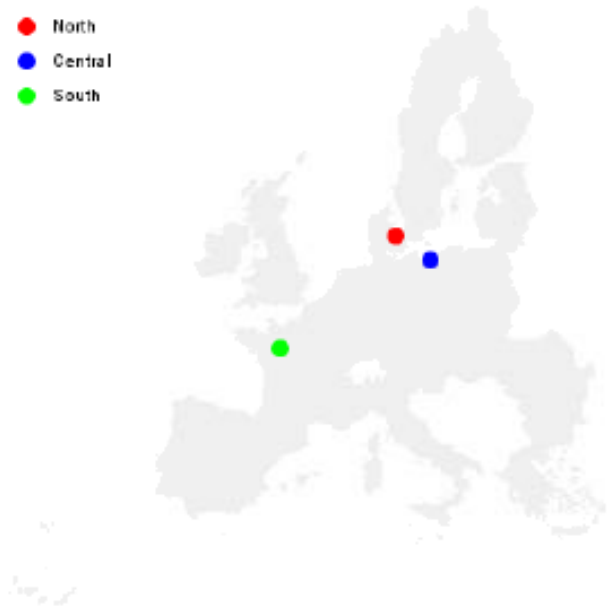


Figure 2. Top soil organic matter (source: EFSA Spatial Data).

Tier-2 considers crop interception and predefined wash-off fractions from the crop canopy as function of crop development stage, which were derived by simulations with PEARL and PELMO. Tier-2 assumes only the model adjustment factors of 3.0 and 4.0 for total soil and pore water concentrations, respectively. These factors were added to account for differences between PERSAM and the numerical models.

Tier-3A

Tier-3A uses numerical models (PEARL and PELMO), which provide more realistic modelling approaches. The assessment sites are the same as the 95th percentile locations of Tier-2. At Tier-3A, the same crop- and substance-specific scenarios as selected at Tier-2 are used. Besides the information on crop type, PEARL and PELMO require detailed data on crop development, climate and irrigation. This data is derived from the ten FOCUS groundwater scenarios (EC, 2014). The selection is based on the dominant FOCUS zone (highest crop area) within each regulatory zone. Moreover, Tier-3A considers foliar dissipation in addition to crop interception and wash-off and therefore allows for a full physically-based representation of foliar processes. Specific model parameters for foliar processes are often not available and therefore, default values were defined for the wash-off factor of 0.1 mm^{-1} and a half-life for the foliar residue on plants of 10 days (EFSA PPR Panel, 2012).



	North	Central	South
x (m)	4.413E+6	4.664E+6	3.559E+6
y (m)	3.616E+6	3.435E+6	2.798E+6
T_{arr} (° C)	9.655	10.41	12.53
ρ (kg/L)	1.378	1.420	1.480
θ (m^3/m^3)	0.3485	0.3485	0.3847
f_{om} (kg/kg)	0.02408	0.01926	0.01342
pH	6.5	6.600	6.300
Crop cover (ha/km^2)	7.520	6.830	6.800

Concentrations for z_{eco} = 5 cm (user)

Figure 3. Example input data for Tier-3A which are derived from Tier-2 simulations as defined by the 95th spatial percentile.

2.2 Soil risk assessment according to FOCUS (1997)

Maximum concentrations in the top five centimeters of the soil column ($PEC_{soil,max,FOCUS}$) were calculated for each substance after the substance-specific number of applications using Equation 1. The calculations were carried out based on the approach given in the guidance of the FOCUS workgroup on degradation kinetics (FOCUS, 2006):

$$PEC_{soil,max,FOCUS} = \sum_{i=1}^{n} \left[\left(\frac{A_i(1-f_{int,i})}{100 \times d \times bd_{soili}} \right) \times e^{-k(t_n - t_i)} \right] \qquad \textbf{Eq1}$$

with:

$PEC_{soil,max,FOCUS}$	Maximum concentration with respect to the soil load after one application period (n applications) related to a soil layer depth of 5 cm [mg kg^{-1}]
n	Number of applications [-]
A_i	Application rate at i-th application [g a. s. ha^{-1}]
$f_{int,i}$	Fraction intercepted by plant cover at i-th application [-]
d	Depth of soil layer (5 cm) [cm]
bd_{soil}	Soil bulk density (1.5 g cm^{-3}) [g cm^{-3}]
k	Degradation rate (= ln (2) / DT_{50}) [d^{-1}]
t_i	Time of i-th application [d]

t_n	Time of n-th (last) application [d]

For substances with a DT_{50} value greater than 100 days, maximum concentrations after multi-year use $PEC_{soil,accu,FOCUS}$ were calculated additionally (Eq2) and used instead of the $PEC_{soil,max,FOCUS}$ in the assessment.

$$PEC_{soil,accu,FOCUS} = \frac{PEC_{soil,ini}}{1-e^{-kt}} \times e^{-k(t_n-t_i)} + PEC_{soil,max,FOCUS} \qquad \textbf{Eq2}$$

with:	$PEC_{soil,accu,FOCUS}$	Maximum concentration in soil following accumulation [mg kg^{-1}]
	$PEC_{soil,ini}$	Initial soil concentration following last application considering a mixing depth of 20 cm for annual crops and 5 cm for permanent crops [mg kg^{-1}]
	$PEC_{soil,max,FOCUS}$	Maximum concentration with respect to the soil load after one application period (n applications) related to a soil layer depth of 5 cm [mg kg^{-1}]
	t	Interval between application seasons (365 days) [d]
	k	Degradation rate [d^{-1}]
	t_i	Time of i-th application [d]
	t_n	Time of n-th (last) application [d]

2.3 Model selection and automation

Tier-1 and Tier-2 were calculated using the most recent version of PERSAM (Persistence in Soil Analytical Model, v3.0.6). Tier-3A calculations were conducted using FOCUS PELMO (v6.6.1 (soil)). For each modelled compound, use pattern, and available regulatory zone (North, Central and South), exposure concentration values were calculated for two scenarios: one scenario for the concentration in total soil (PEC_{soil}) at an assessment depth of 5cm and one scenario for the concentration in pore water ($PEC_{pore\ water}$) at an assessment depth of 1 cm.

The model calculations can be carried out in two ways with PERSAM. The graphical user interface can be used to enter all necessary input parameters or PERSAM can be used in a batch mode. Due to the large number of model runs in this project, an automatic processing of the input and output data was necessary in order to reduce the processing time. The automations were implemented using the scripting programming language Python. The final working steps were conducted separately for each company:

- Tier-1 and Tier-2: PERSAM offers the possibility to provide the input data in the JSON (JavaScript Object Notation) format. JSON files are plain text files containing a list of PERSAM projects and related information, e.g. project information (name, output folder), project properties (tier, regions, crop) and substance information (adsorption and degradation coefficients). The JSON files were created on the basis of an EXCEL spreadsheet which hold the substances information and Good Agricultural Practices (GAPs) of each PPP. A Python script was used to create a JSON file in the format of PERSAM, which hold all Tier-1 and Tier-2 simulations for each entry in the spreadsheet. The JSON files can be directly imported to PERSAM and all projects are executed in a batch-mode.
- Tier-3A: PERSAM generates a transfer file for Tier-3A calculations. The transfer files can be directly processed from the numerical model PELMO, but some manual edits are required, e.g. the user has to revise some physicochemical parameters and must enter the correct application scheme. The degradation paths were revised as well, since errors were observed during the modelling exercise. A Python script was used to apply the required modifications in the PELMO PSM input file directly on the basis of the information given in the EXCEL spreadsheet.
- The results of Tier-1 and Tier-2 are stored in Microsoft DOCX format. A summary file of Tier-3A results can be directly created with the graphical user interface of PELMO for each model run (in the present study: PECsoil_1.plm and PECsoil_5.plm for pore water and total soil concentration, respectively). Excel summaries were created using a Python script which reads out the summaries.

An overview of the general input parameters for all substances for the model FOCUS PELMO v6.6.1 (soil) is given in the table below.

Table 1. Overview of general input parameters for all substances for the model FOCUS-PELMO v6.6.1 (soil)

Input parameter	Unit	Value	Remarks
PHYSICO-CHEMICAL PARAMETERS			
Diffusion coefficient in gas	[$cm^2\ s^{-1}$]	4.98E-02	FOCUS recommendation
DEGRADATION PARAMETERS			
Q_{10} value	[-]	2.58	EFSA opinion
Exponent of moisture correction function	[-]	0.7	FOCUS recommendation
SORPTION PARAMETERS			
pH dependency	[-]	pH independent	
CROP RELATED PARAMETERS			
TSCF (crop uptake)	[-]	0	Default value for case of no evidence for systemic behavior

2.4 Substance data

The 56 active substances provided by the six CLE member companies were classified according to their DT_{50} and K_{oc} values used in the risk assessment (Table 2). The categorization, with class value ranges based on expert judgement as given in Budde (2013), is shown in Table 2.

Table 2. Categorization of active substances (N=56)

		DT_{50}		
		0 - 50 d N=33	**51 - 100 d N=12**	**>100 d N=11**
K_{OC}	**0 - 300 mL g^{-1} N=24**	I N=16	II N=7	III N=1
	301 - 1000 mL g^{-1} N=11	IV N=6	V N=2	VI N=3
	>1000 mL g^{-1} N=21	VII N=11	VIII N=3	IX N=7

The individual classification of the active substances provided by the six CLE member companies for the impact assessment is shown in Table 3.

Table 3. Classification of individual active substances according to the scheme shown in Table 2

Substance	Class	Substance	Class	Substance	Class
ADA01	VII	BAS01	IX	BCS01	IX
ADA02	I	BAS02	VI	BCS02	VII
ADA03	IV	BAS03	IX	BCS03	II
ADA04	II	BAS04	VI	BCS04	VII
ADA05	VIII	BAS05	IX	BCS05	I
ADA06	I	BAS06	I	BCS06	IV
ADA07	I	BAS07	II	BCS07	VII
ADA08	VII	BAS08	VII	BCS08	III
ADA09	I	BAS09	IV	BCS09	I
				BCS10	VII

Substance	Class	Substance	Class	Substance	Class
CAS01	VIII	FMC01	IV	SYN01	I
CAS14	IV	FMC02	VI	SYN02	I
CAS17	I	FMC03	II	SYN03	II
		FMC04	II	SYN04	II
		FMC05	VII	SYN05	I
		FMC06	I	SYN06	IV
		FMC08	VII	SYN07	V
		FMC09	I	SYN08	V
		FMC10	I	SYN09	IX
		FMC11	I	SYN10	VII
		FMC12	I	SYN11	VIII
		FMC13	VII	SYN12	IX
				SYN13	IX

Up to two metabolites per active substance were considered for the simulations, for a total of 65 metabolites. Their categorization is shown in Table 4.

Table 4. Categorization of metabolites (N=65)

		DT_{50}		
		0 - 50 d N=49	**51 - 100 d N=8**	**>100 d N=8**
K_{OC}	**0 - 300 mL g^{-1} N=48**	I N=39	II N=7	III N=2
	301 - 1000 mL g^{-1} N=7	IV N=6	V N=0	VI N=1
	>1000 mL g^{-1} N=10	VII N=4	VIII N=1	IX N=5

In the cases where two metabolites were modelled, the pathway was implemented in PERSAM either in parallel (two primary metabolites) or in series (one primary metabolite and one secondary metabolite), depending on the route of degradation in soil. Due to the limitations in the PERSAM degradation scheme, actual formation fractions were used whenever possible, otherwise, they were derived by

multiplying the formation fractions with those of their precursors.

2.5 Application scenarios

PEC_{soil} calculations were performed using the scenarios developed by EFSA for various crops. Representative GAPs for the active substances represent real-world application patterns for the associated products (professional uses). An overview of simulated crops and use-related crop interception values is given in Table 5.

The relevant FOCUS scenario used in selecting the appropriate application date for the corresponding FOCUS crop in FOCUS PELMO v6.6.1 (soil) was chosen with reference to Table B.7 of the EFSA soil guidance (2017). The application dates are not tied to precipitation data.

The exposure assessment for spray applications in annual crops covering the entire field was carried out for cabbage, maize, oilseed rape (winter), potatoes, soybean, strawberries, sugar beets, tomatoes and winter cereals. The majority of simulations was conducted for oilseed rape and cereals with various application rates and timings. Since soybean is not present in the Northern zone, simulations for this crop were carried out only for Central and Southern zones.

In accordance with the EFSA soil guidance (EFSA, 2017), two separate soil exposure assessments were carried out for air blast applications on permanent crops grown in rows (apples, vines and olives): one for the crop row ('in-row treatment') and one for the ground between the crop rows ('between-row treatment'). To address the non-uniform distribution of pesticides in these permanent crops, the default dose rate assessment factor of 2.9 was applied to the 'in-row treatment', whereas no dose rate assessment factor was considered for the 'between-row treatment', for which uniform over-spraying was assumed. In two cases, the plant protection product is applied exclusively between the rows (Table 4, Vines). Since olives are not present in the Northern and Central zones, simulations were carried out only for the Southern zone. Similarly, vines is not present in the Northern zone, therefore, simulations were carried out for the Central and Southern zones only.

Table 5. Simulated crops (PERSAM crop name) and crop interception in percent at the respective application date.

Crop	Crop interception [%]	Number of active substances
ApplesInRow[2]	60	5
	65	
Cabbage	70	1
Grass[3]	90	1
Maize	0	2
	50	
OilseedRapeWinter	0	11
	40	
	80	
OlivesInRow[2]	70	1
Potatoes	85	1
Soybean	0	1
Strawberries	60	1
SugarBeets	0	2
	20	
Tomatoes	70	3
	80	

Crop	Crop interception [%]	Number of active substances
Vines[1]	0	1
VinesInRow[2]	60	1
WinterCereals	0	25
	20	
	80	
	90	

[1] Only between row application; no in-row.
[2] In-row and between-row application.
[3] Permanent crop covering the entire field

The EFSA soil guidance (EFSA, 2017) covers spray applications, applications of granular products, and treated small seeds. In this report, the application method considered for most annual and permanent crops was to the crop canopy, except in cases where, due to the type of pesticide or the application timing (e.g. before emergence), application method was considered directly to the soil surface. One of the analysed substances was applied as seed treatment, so the application method considered was "placing at a certain soil depth" with an incorporation depth of 4 cm.

2.6 Ecotoxicological data

The default ecotoxicological evaluation soil depth for total soil and pore water of 5 cm and 1 cm, respectively, was assumed in the calculations. Additionally, for the substance which was applied "placing at a certain soil depth", calculations were done at 20 cm.

Regulatory acceptable concentrations (RACs) in soil were supplied for each substance (active substances and metabolites) by the substance owners, together with total organic carbon (TOC), water content and soil bulk density data for the respective studies. The underlying NOEC or EC_{10} values were selected in accordance with the EU agreed endpoints for Tier 1 soil organism RA, and included a correction factor of 2 in cases of lipophilic compounds with a Log Pow >2. Where data for study conditions were not available, they were estimated at standard values of 0.06 g g^{-1} (organic carbon), 35% (water content) and 1.5 g cm^{-3} (bulk density). Additionally, pore water RACs were calculated for the active substances from the soil RACs according to Equation 3 (EFSA PPR Panel, 2012).

$$RAC_{pore\ water} = \frac{RAC_{totalsoil}}{KOC \times OC + \frac{\theta}{bd}} \qquad \textbf{Eq3}$$

with:

	$RAC_{pore\ water}$	Regulatory acceptable concentration pore water [mg L^{-1}]
	$RAC_{total\ soil}$	Regulatory acceptable concentration total soil [mg kg^{-1}]
	KOC	Adsorption coefficient [mL g^{-1}]
	OC	Organic carbon content [g g^{-1}]
	Θ	Volumetric water content [mL mL^{-1}]
	bd	Soil bulk density (1.5 g cm^{-3}) [g cm^{-3}]

3 RESULTS AND DISCUSSION

3.1 Exposure assessment: $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio

PEC_{soil} values in the top five centimeters of the soil column were calculated according to FOCUS (1997) and EFSA (2017). Resulting $PEC_{soil,EFSA}$ values were generally higher than $PEC_{soil,FOCUS}$ values with median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of active substances of 12, 7 and 2 for Tier-1, Tier-2 and Tier-3A, respectively (Table 6). A similar observation was made for metabolites as summarized in Table 7 with median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of 42, 22 and 2.0 for Tier-1, Tier-2 and Tier-3A, respectively.

To better visualize the high variance in ratios for the different substances, $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios in box plots are additionally presented for active substances and metabolites in the appendix. There, it can be seen that the ratios between EFSA and FOCUS PEC_{soil} values of active substances are in single cases greater 100 at Tier-1, but below 50 in all cases at Tier-3A (Figure A 1, Figure A 2). Metabolites contain also some large outliers with ratios >1000 at Tier-1 and Tier-2, but in all cases <1000 at Tier-3A (Figure A 4, Figure A 5). These metabolites are associated to parents with $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio >100. Moreover, most of the outlier cases for both active substances and metabolites are situations with application to apples in-row. This can be partly explained by the dose rate assessment factor of 2.9 implemented to air blast applications in the modelling according to EFSA (2017), whereas such a factor was not implemented in the modelling according to FOCUS (1997).

The overall trend of increasing PEC_{soil} values when applying the new EFSA (2017) approach is confirmed here.

Table 6. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios for individual active substance categories (with minimum and maximum in brackets) per modelled tier for all regulatory zones, median values for all categories together, and median values for each zone, irrespective of category.

Category	Tier-1 median (min – max)	Tier-2 median (min – max)	Tier-3A median (min – max)	Run count[1]
I	8.4 (5.6-149)	5.4 (3.5-62)	1.6 (1.1-28)	44
II	9.7 (5.7-92)	6.3 (4.1-37)	2.4 (1.4-19)	19
III	118 (77-203)	54 (33-80)	22 (14-34)	3
IV	35 (7.0-136)	17 (4.1-56)	5.8 (1.4-23)	17
V	20 (6.0-49)	11 (4.3-23)	4.3 (1.6-9.4)	6
VI	41 (11-150)	20 (5.1-60)	6.5 (2.6-26)	9
VII	9.0 (5.6-64)	5.8 (4.0-26)	2.0 (1.3-11)	32
VIII	13 (7.5-32)	6.8 (4.5-19)	2.8 (1.7-6.4)	9
IX	35 (8.2-68)	17 (5.1-31)	7.0 (1.9-13)	21
All categories and zones	12 (5.6-203)	7 (3.5-80)	2 (1.1-34)	160
All categories NEU	16 (8.9-203)	7.7 (4.8-80)	3.4 (1.6-34)	51
All categories CEU	12 (6.7-118)	5.7 (4.2-54)	2.4 (1.4-23)	54
All categories SEU	9.4 (5.6-77)	4.9 (3.5-35)	2.0 (1.1-16)	55

[1] Run count: number of runs performed for each active substance in the corresponding category, one per available regulatory zone

Table 7. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios for individual metabolite substance categories (with minimum and maximum in brackets) per modelled tier for all regulatory zones, median values for all categories together, and median values for each zone, irrespective of category.

Category	Tier-1 median (min – max)	Tier-2 median (min – max)	Tier-3A median (min – max)	Run count[1]
I	47 (4.7-2386)	26 (3.4-965)	1.7 (0.1-41)	105
II	8.5 (0-214)	5.0 (0-89)	0.9 (0-10)	19
III	8.2 (5.1-13)	5.7 (3.6-9.1)	0.5 (0.3-0.7)	6
IV	44 (8.3-227)	26 (5.2-100)	2.6 (0.8-11)	18
V	- [2]	- [2]	- [2]	- [2]
VI	48 (38-67)	21 (18-29)	5.0 (3.9-8.2)	3
VII	22 (13-52)	11 (7.1-28)	1.7 (0.8-4.8)	12
VIII	82 (65-113)	50 (41-67)	8.5 (6.2-12)	3
IX	473 (29-6381)	219 (14-2567)	40 (2.5-598)	15
All categories and zones	42 (0-6381)	22 (0-2567)	2 (0-598)	181
All categories NEU	56 (0-6381)	29 (0-2567)	2.5 (0-598)	57
All categories CEU	36 (0-3432)	20 (0-1548)	1.9 (0-406)	61
All categories SEU	30 (0-2045)	18 (0-835)	1.5 (0-88)	63

[1] Run count: number of runs performed for each metabolite in the corresponding category, one per available regulatory zone
[2] Not calculated because no metabolite was in category V

A more detailed summary of the modelled $PEC_{soil,EFSA}$ values for the three different regulatory zones (North, Central and South) can be found in Figure 4 and Figure 5 for active substances and metabolites, respectively. A closer look at the geographical scenarios shows a decreasing trend from North to South. This trend is correlated with high proportions of organic matter in the Northern zone (average of 19%) and decreasing proportions in the Central and Southern Zones (average of 11 and 7%, respectively), and a corresponding inverse spatial trend of soil bulk density (average of 0.74 g cm^{-3}, 0.95 g cm^{-3} and 1.10 g cm^{-3} for Northern, Central and Southern zone, respectively), as shown in Table A 5.

The median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of active substances (all Tiers combined) are 9, 7 and 6 for the Northern, Central and Southern zone, respectively. The median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of metabolites (all Tiers combined) are 19, 13 and 11 for the Northern, Central and Southern zone, respectively.

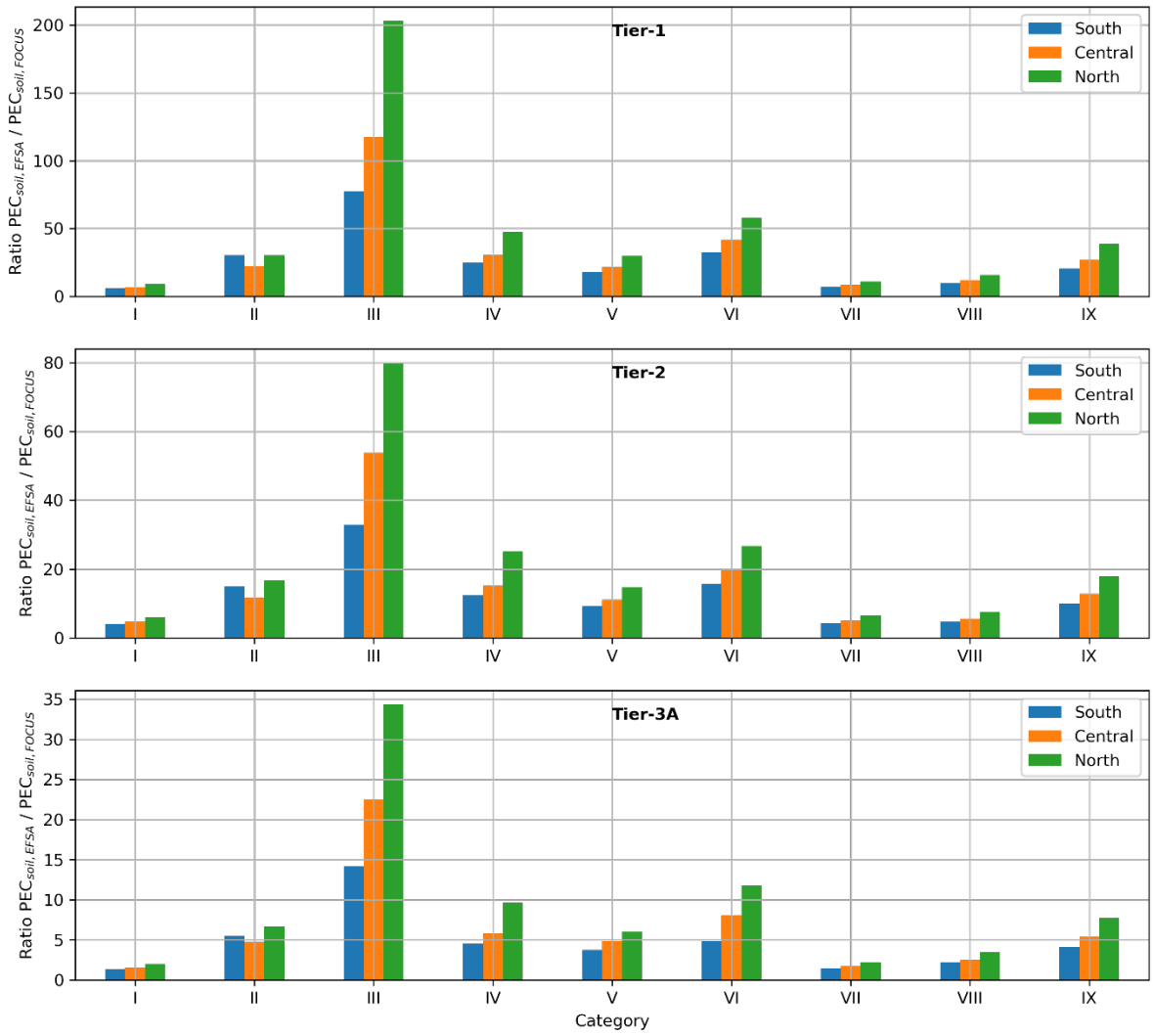


Figure 4. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of active substances separated by substance categories and FOCUS zones at Tier-1, Tier-2 and Tier-3A, respectively.

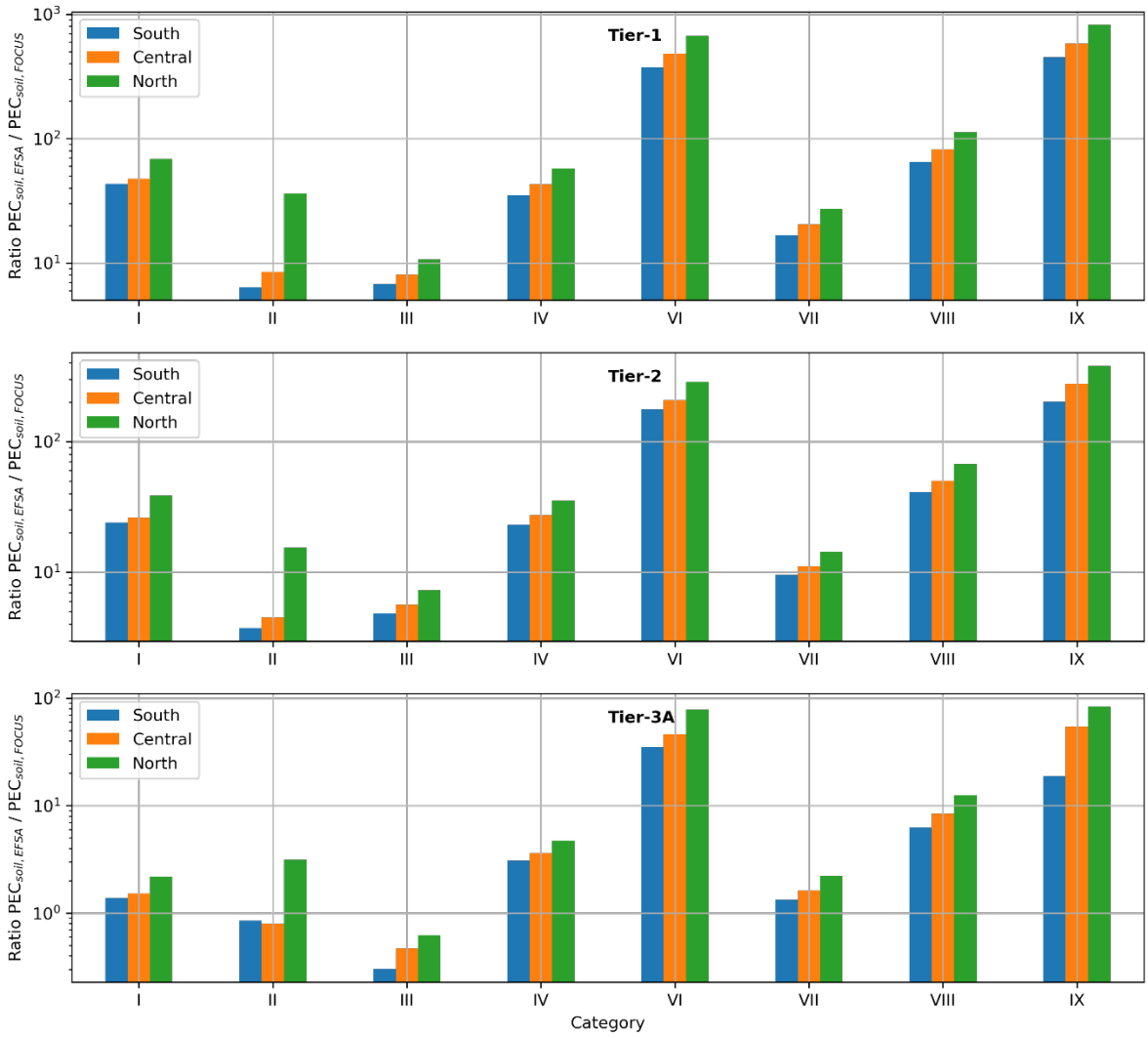


Figure 5. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of metabolites separated by substance categories and FOCUS zones at Tier-1, Tier-2 and Tier-3A, respectively.

Active substances allocated into categories III, VI, IX, which have the highest DT_{50} (>100 days), show the highest median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios. The lowest ratios occur in active substances allocated to categories I, IV and VII, which are characterized by the lowest DT_{50} (<50 days). These categories cover all crop types and include GAPs targeting at later BBCH stages. At least for active substances, a higher DT_{50} may be associated with a higher $PEC_{soil,EFSA}$ value than $PEC_{soil,FOCUS}$. However, the dataset is limited for such a conclusion. There is no clear trend in the case of metabolites, which might be related to the unbalanced allocation between substance categories and the net effect of range of processes that influence formation, degradation and mobility of residues. Significant variation is noted with the diversity of degradation pathways considered. In the FOCUS (1997) calculations, the maximum occurrences of metabolites are used, whereas in EFSA (2017) calculations, the route of degradation in soil (i.e. formation fractions in soil) are used.

Crop interception and wash-off are considered in Tier-2 (fixed values) and Tier-3A (simulated) which further reduce $PEC_{soil,EFSA}$ values in comparison to Tier-1 where such processes are not considered. Because wash-off is not considered for the calculation of $PEC_{soil,FOCUS}$, the results of $PEC_{soil,EFSA}$ are generally higher for applications at higher BBCH stages. The impact of crop interception is further addressed in detail in chapter 3.2.

A major driver for the decreasing $PEC_{soil,EFSA}$ values between Tier-1, Tier-2 and Tier-3A are the modelling and scenario adjustment factors. As described in chapter 2.1.1, scenario adjustment factors have been included at Tier-1 to ensure that that tier is more conservative than Tier-2 and Tier-3A. Modelling adjustment factors were added to account for differences between PERSAM (Tier-1, Tier-2) and the numerical models (Tier-3A, PELMO and PEARL). Thus, obligatory model and scenario specific correction factors contributed to an increase of $PEC_{soil,EFSA}$ values over all compounds and uses for Tier-1 and Tier-2 as shown in Figure 6. The actual median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances at Tier-1 is 11.7, which includes a model adjustment factor of 3.0 and a scenario adjustment factor of 1.6. Without the model adjustment factor, the median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio would have been 3 times lower (3.9) and without any adjustment factor, it would have been 2.8, which is much closer to the Tier-3A median ratio (2.4). A similar situation can be seen for Tier-2, at which the actual median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio is 6.8, but without the model adjustment factor it would have been even lower than the Tier-3A median ratio (2.3 compared to 2.4).

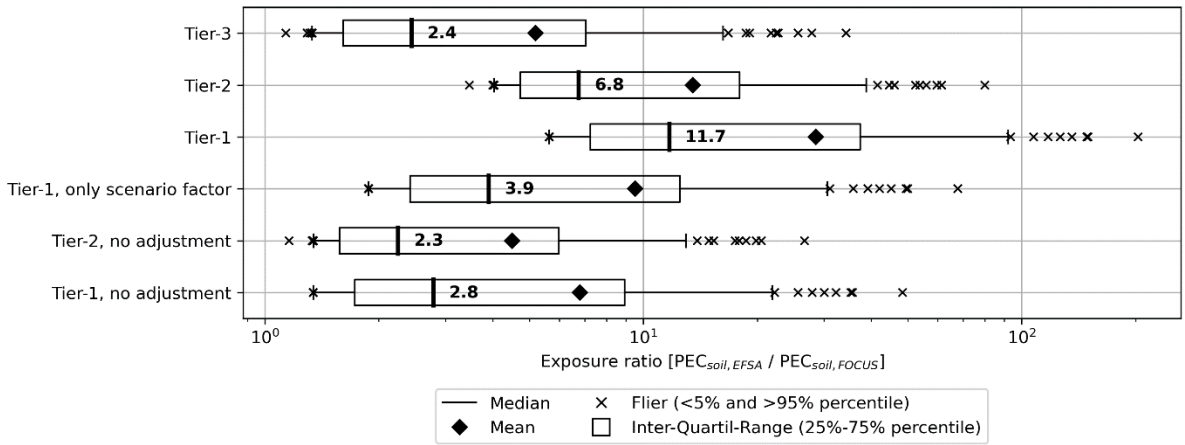


Figure 6. Impact of scenario and model adjustment factor in $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances.

3.2 Impact of crop interception and foliar wash-off

The ratio between $PEC_{soil,EFSA}$ and $PEC_{soil,FOCUS}$ increases in relation to higher crop interception. Crop interception in-turn triggers a higher wash-off in case of EFSA (2017) Tier-2 and Tier-3A calculations, but is not considered in case of FOCUS (1997) calculations. Therefore, a significant reason for high ratios between EFSA (2017) and FOCUS (1997) calculations arises due to application for some substances in periods with advanced growth stages and high crop cover and interception (active substances: Figure 7; metabolites: Figure A 25).

Thus, foliar interception and simulated wash-off, determined by crop growth stage at time of application, were identified as a further significant driver of the increase in concentrations. The effect was stronger for uses with higher interception at the time of application, due to larger impact of simulated foliar wash-off on the amount of substance reaching the soil. The active substances with the highest $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios at Tier-3A correspond to uses with high crop interception (>60%). The $PEC_{soil,EFSA}$ of these substances either occur on a day with significant rainfall (>2.5 cm day^{-1}) or can be traced back to application on a day with moderate rainfall (>1.3 cm day^{-1}), which is unrealistic.

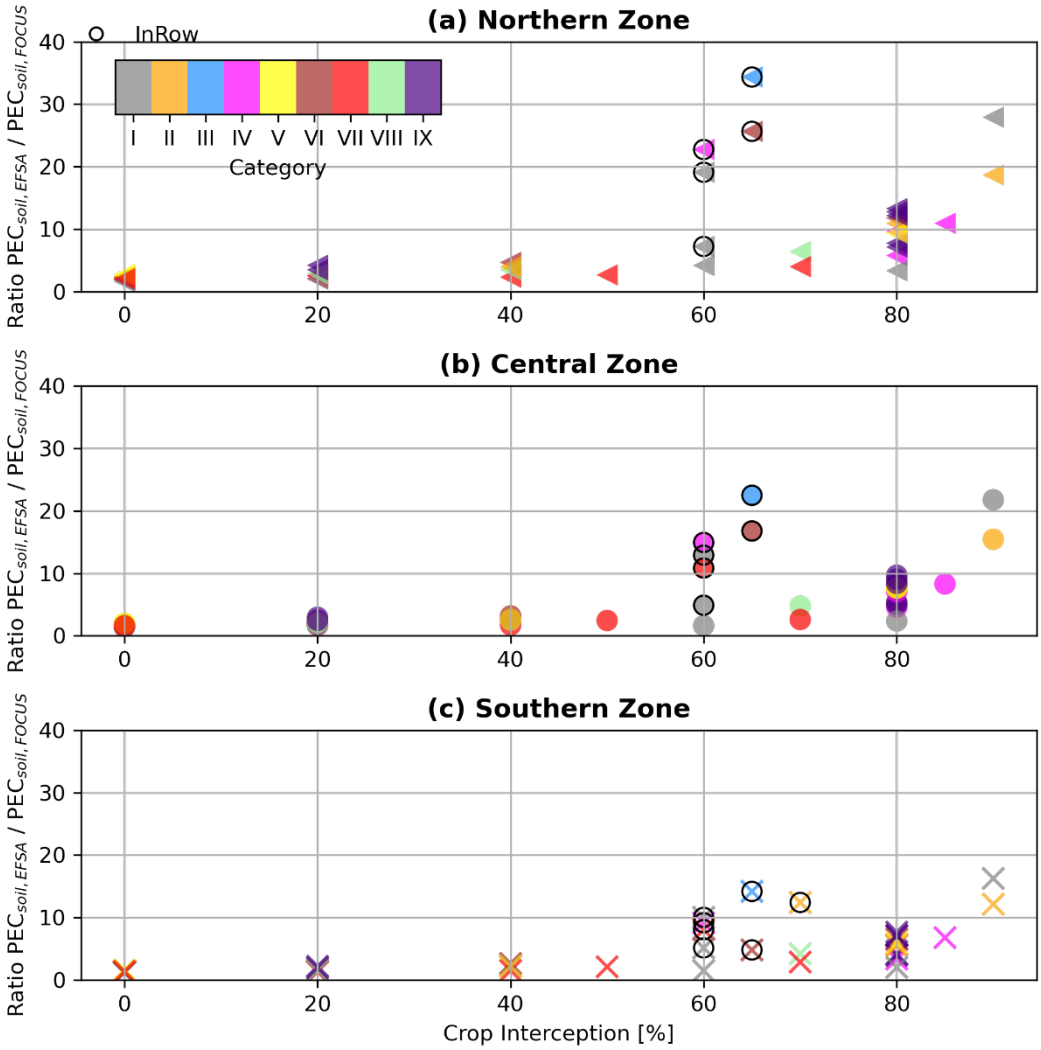


Figure 7. Relationship between crop interception and $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio at Tier-3A of active substances for each regulatory zone.

The impact of environmental parameter (organic matter, pH, precipitation, temperature) in combination with crop interception values was investigated as well, but no clear pattern could be derived by visual inspection of scatter plots (active substances: Figure 8; metabolites: Figure A 26). Therefore, further quantitative statistical analyses were applied.

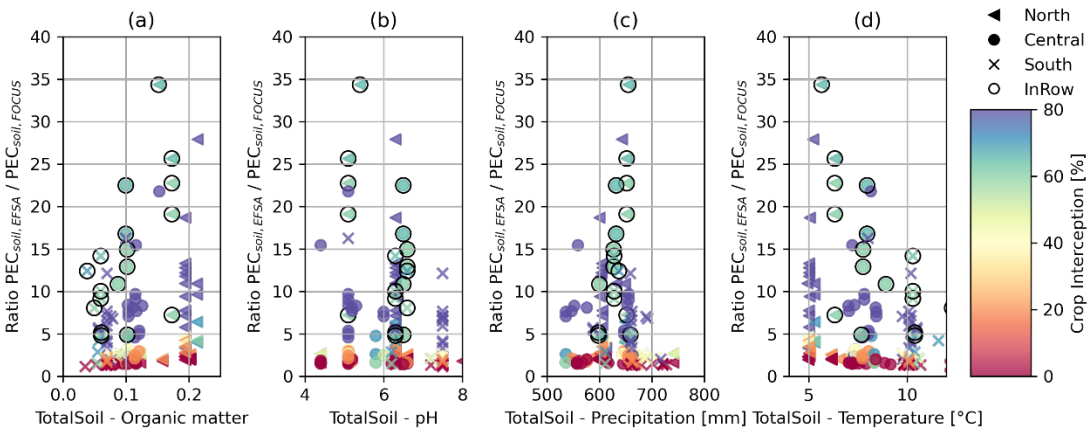


Figure 8. Relationship between environmental conditions at Tier-3A and $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances.

In order to further investigate the combined influence of the environmental parameters and the crop interception on the $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio, two statistical analyses were performed. The environmental parameters include the local Tier-3A scenario data for bulk density, organic matter, pH, field capacity, wilting point, precipitation and temperature from the EFSA Spatial Data v1.1 dataset (Hiederer, 2012). Crop Interception was used as a proxy for the application date (BBCH). The target variable was the $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio.

The first analysis involves a multivariate Ordinary Least Squares (OLS) regression. The function 'ols' from the Python extension statsmodels (v0.13.1, Pedregosa, 2011) was used for the calculation. The input data were standardised by removing the mean and scaling to unit variance using the Python extension scikit-learn (v1.0.1, Seabold & Perktold, 2010) function 'StandardScaler'. In the first run (Figure A 33), all parameters mentioned above were taken into account, resulting in an adjusted R-squared of 71.9%. In order to determine the major factors, the number of parameters was reduced step by step in further runs. The final regression model (Figure A 34) with only two parameters (bulk density and crop interception) achieved an adjusted R-squared of 56.4%, which suggests that the two parameters are the major influencing factors.

In the second analysis, the combined influence of the two parameters bulk density and crop interception on the $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio was investigated. For this purpose, a k-means clustering analysis was performed with the function 'KMeans' from the Python extension scikit-learn. The algorithm finds the centres of the clusters and favours groups with low variance and similar size. A total of four groups could be identified (Figure 9). Group 1 and 3 have high (factor 1-13) and very high (factor 6-35) $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio, respectively. These two groups both have a high crop interception (≥50%) and can be clearly separated by bulk density, with group 1 (high ratio) having a generally higher bulk density (0.7 - 1.2 g cm^{-3}) compared to group 3 (very high ratio) (0.4 - 1.0 g cm^{-3}).

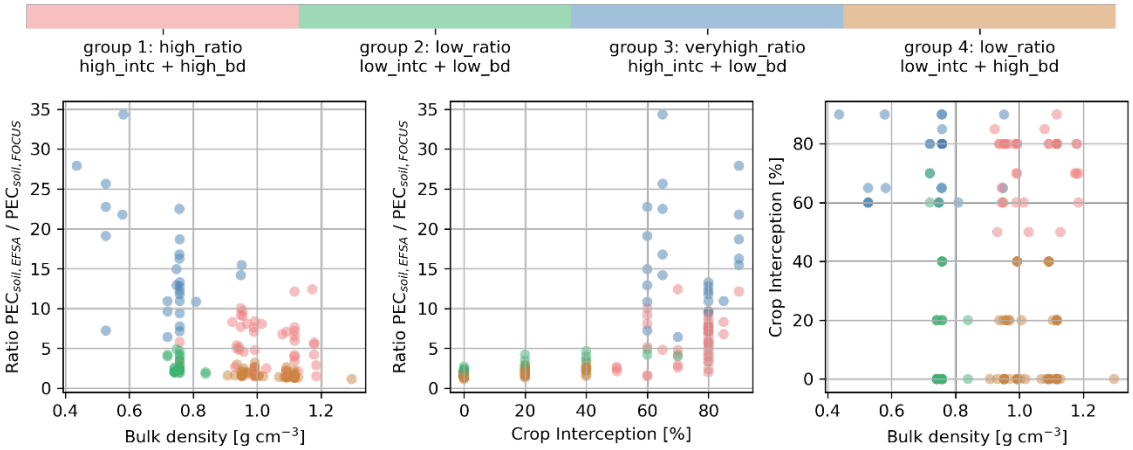


Figure 9. K-Means cluster analysis of the total soil $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio (*ratio*), soil bulk density (*bd*) and crop interception (*intc*) of Tier-3A scenario locations.

Overall, the statistical analysis showed that the two parameters crop interception (i.e. as a proxy for BBCH) and bulk density have a very high influence on the PEC_{soil} values. This explains the difference in PEC_{soil} values between FOCUS (1997) and EFSA (2017).

3.3 Environmental conditions of Tier-3A assessment locations

The environmental conditions for the Tier-3A scenarios (95th spatial percentile) were further investigated in detail to reveal spatial effects and to discuss representativeness with respect to conditions typical for agricultural land use. For this, the environmental conditions of crop specific arable areas (maize, oilseed rape, tomatoes, winter cereals) in Europe were compared to the range of Tier-3A scenario locations of total soil and pore water concentrations. Six environmental parameters were investigated, namely bulk density (Figure 10), organic matter (Figure 11), pH (Figure A 27), field capacity (Figure A 28), temperature (Figure A 29) and precipitation (Figure A 30). A tabular overview of results is given in Table A 5 and Table A 6.

A clear pattern exists for the parameters organic matter and bulk density (calculated via a pedotransfer function based on organic matter according toTiktak et al., 2002). The locations for the assessment of total soil concentration have bulk density values far below the median of European agricultural areas of the four crops. The bulk density values of the areas for the evaluation of the pore water concentration are higher than the European median. Median values of bulk density range between 0.76 - 1.12 g cm^{-3} and 1.38 - 1.50 g cm^{-3} for total soil and pore water concentration, respectively. An inverse relationship can be observed for organic matter with a similar pattern as compared to bulk density. Median temperature and pH values of total soil scenario locations are generally lower in comparison to the European median, but only in a small extent. Pore water sites have generally higher median temperature and pH values, also in a small extent.

In conclusion, the selection procedures of geographic locations for exposure assessment might result in incompatible soil properties (e.g., organic carbon content, bulk density) between e-fate and ecotoxicological data. It is unclear how to apply exposure values from the new modelling tiers in the current risk assessment framework, i.e. higher tier risk assessment. Selection procedures of geographic locations for exposure assessment results in incompatible soil properties (e.g., organic carbon content, bulk density) between e-fate and ecotoxicological data (i.e. from higher tier studies). This inconsistency hinders scientifically reasonable comparison and interpretation. Worst case assumptions coming from the new exposure assessment add to the already implemented worst case character of the existing effect and risk assessment which could finally lead to an overly conservative risk evaluation. Ecotoxicological

'intermediate-tier' effect studies or effect modelling approaches may be a potential option to overcome such discrepancies in the future but are currently not available / accepted. A sufficiently long transition period will be required to ensure alignment between the new modelling framework and the tiered assessment for soil organisms.

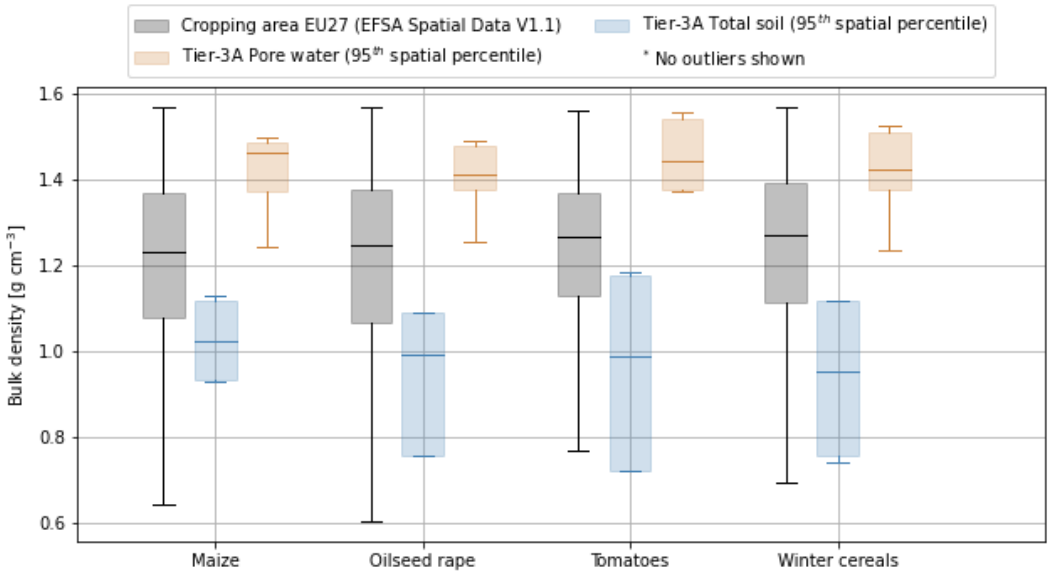


Figure 10. Variability of bulk density of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas.

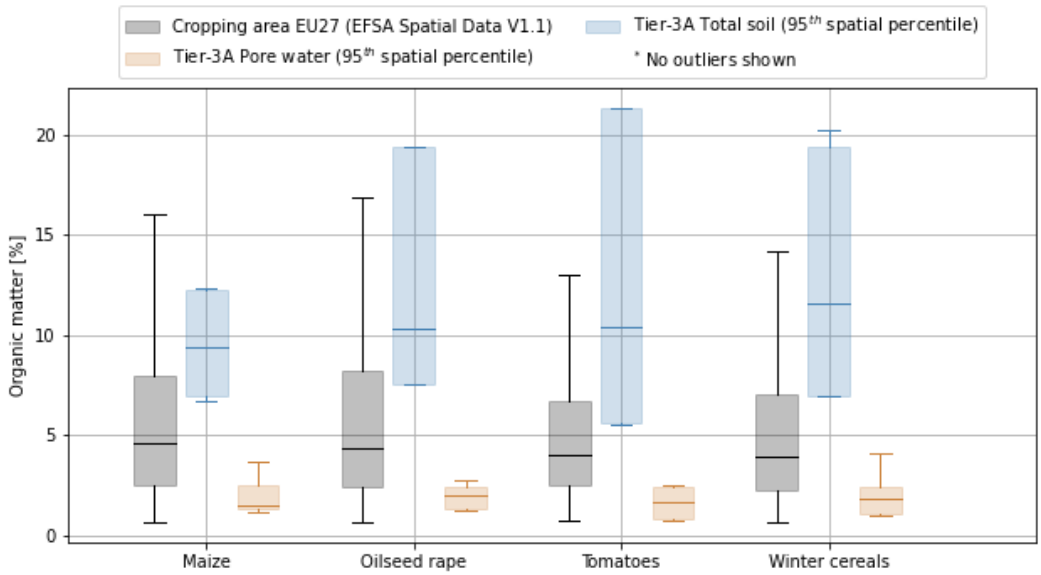


Figure 11. Variability of organic matter of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas.

3.4 Risk assessment: failure rate

The RA for soil organisms was performed using PEC_{soil} values from FOCUS (1997) and EFSA (2017) calculations. Failure rates were calculated by dividing the respective PEC_{soil} value by the ecotoxicological Tier-1 RAC value. In case the resulting PEC / RAC ratio values were <1, the RA is

passed, otherwise it failed (ratio ≥1) and further refinement is required.

The comparison of PECsoil,FOCUS-based RA ratios with PECsoil,EFSA-based RA ratios showed a substantial increase when using the new modelling framework. The failure rates of the soil RA based on FOCUS (1997) modelling are 14% for active substances and 8% for metabolites, respectively (Figure 12). When considering the EFSA (2017) modelling framework, the failure rates of active substances are 67%, 58% and 36% for Tier-1, Tier-2 and Tier-3A (Figure 13), respectively, and the failure rates of metabolites are 38%, 25% and 10% for Tier-1, Tier-2 and Tier-3A (Figure 14), respectively.

The observations are similar for all substance categories and regulatory zones. No distinct pattern could be identified between increased failure rates with the EFSA (2017) modelling framework and substance categories, nor between increased failure rates and regulatory zones (Table A 3, Figure A 7, Figure A 8). For active substances, the Northern zone shows a slightly higher overall failure rate (60%) when compared to the Central and Southern zones (52% and 50%, respectively, Figure A 9). The failure rate of active substances is higher for the crop type "permanent crops", which includes apples, grass, olives and vines, when compared to the crop type "annual crops", which includes cabbage, maize, oilseed rape (winter), potatoes, soybean, strawberries, sugar beets, tomatoes and winter cereals. This may, at least in part, trace back to significant proportion of these permanent crop uses being carried out at later growth stages where there is higher interception and consequently are more vulnerable to wash-off. However, such a distinction is not present in metabolites (Figure A 17, Figure A 21).

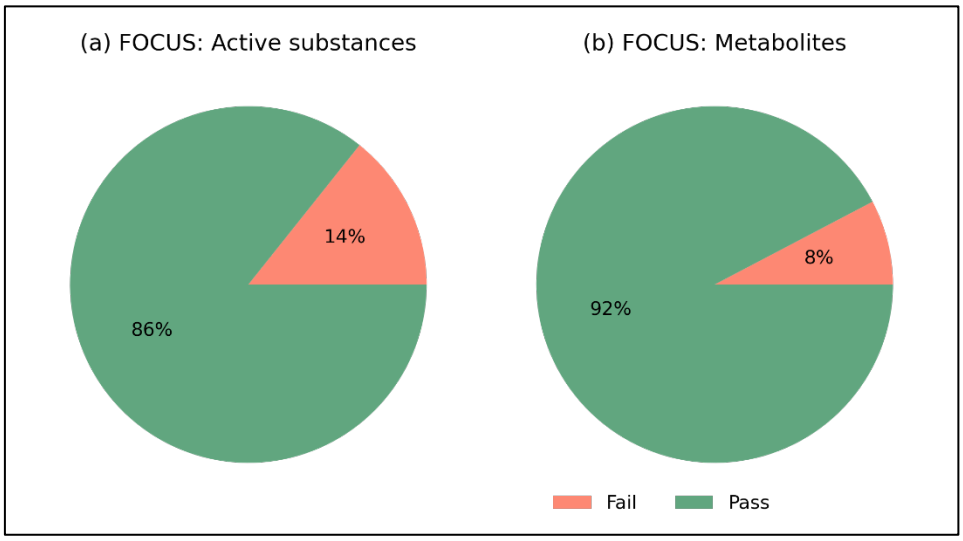


Figure 12. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,FOCUS}$ values for (a) active substances and (b) metabolites.

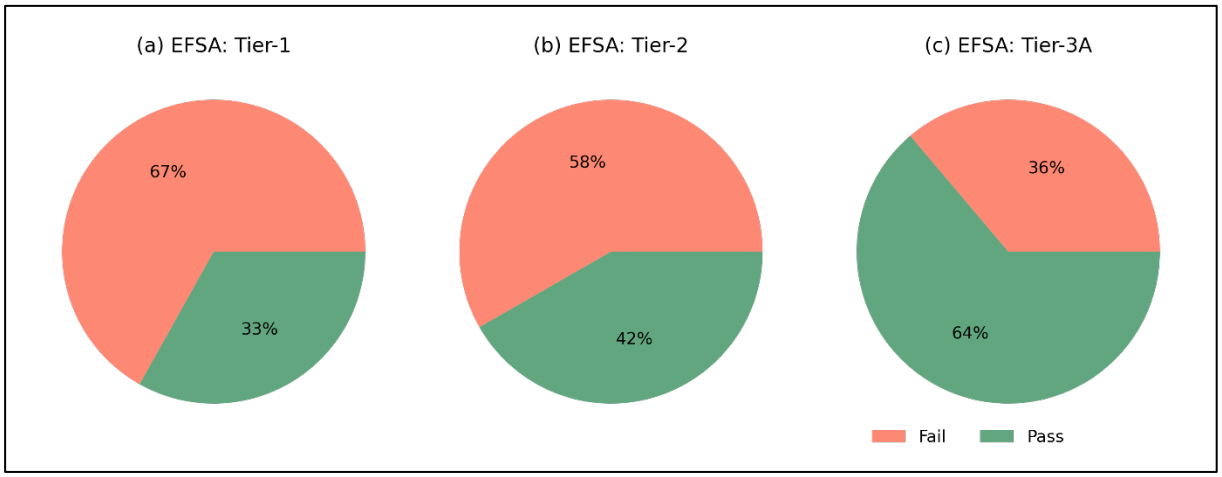


Figure 13. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances at (a) Tier-1, (b) Tier-2 and (c) Tier-3A.

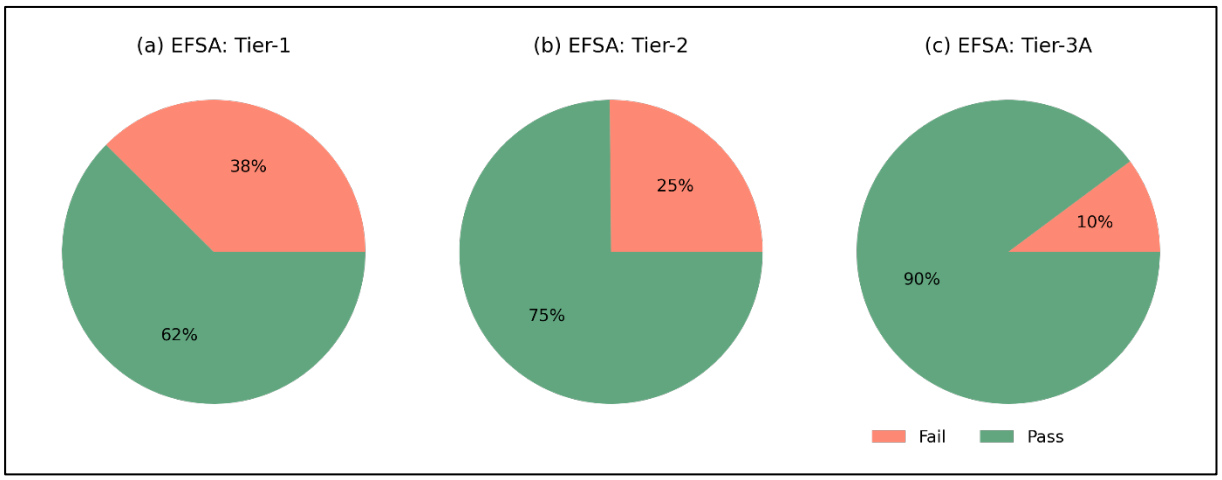


Figure 14. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites at (a) Tier-1, (b) Tier-2 and (c) Tier-3A.

In case of failure, either a refinement of the RAC (by ecotoxicological higher tier studies) or PEC (by higher tier exposure modelling) is required. Across all zones, elevated $PEC_{soil,EFSA}$ values (based on total concentrations) increased RA failure rates by more than 52% (at Tier-1). Thus, compared to the current failure rate of 14% based on $PEC_{soil,FOCUS}$, up to 5 times more refinements (e.g. soil organism field studies) will be triggered if new modelling is implemented at Member State level, and if Tier-1 is used for the soil organism RA. If considering the refined EFSA Tier-3A exposure values for the soil risk assessment, still 22% more active substances fail the risk assessment, and around 2.5 times more refinements, e.g. higher tier ecotoxicological studies, would be required for regulatory purposes.

Additionally, the failure rates of $PEC_{pore\ water}$ values for active substances as calculated according to EFSA soil guidance (2017) are shown in Figure A 31 and Figure A 32. However, it was beyond the scope of this report to analyse them in detail.

4 CONCLUSIONS

An impact assessment was applied to 56 active substances and their respective metabolites to investigate the extent to which PEC_{soil} values modelled according to FOCUS (1997) differ when modelled according to EFSA (2017). The main drivers for the changes could be determined for the given dataset. Further, the impact of the new modelling framework on the associated ecotoxicological risk assessment of soil organisms was illustrated.

It was observed that PEC_{soil} values calculated according to EFSA (2017; $PEC_{soil,EFSA}$) were - at all tiers - substantially higher than exposure values calculated according to the current FOCUS approach (FOCUS 1997; $PEC_{soil,FOCUS}$) for the same compounds. $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios were calculated for each compound to quantify the increase in exposure values according to the new framework. The main findings are:

- The median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of active substances are 12, 7 and 2 for Tier-1, Tier-2 and Tier-3A, respectively The median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of active substances (all Tiers combined) are 9, 7 and 6 for the Northern, Central and Southern zone, respectively.
- The median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of metabolites are 42, 22 and 2 for Tier-1, Tier-2 and Tier-3A, respectively The median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of metabolites (all Tiers combined) are 19, 13 and 11 for the Northern, Central and Southern zone, respectively.

Overall, modelled concentrations were observed to decrease with increasing tier (from Tier-1 to Tier-3A), as well as from North to South. The following factors have been identified as main drivers for the significant changes in exposure values:

- Categories III, VI, IX have the highest median ratios with the highest DT_{50} (>100 days) in case of active substances. The lowest ratios occur in case of categories I, IV and VII, which have the lowest DT_{50} (<50 days) in case of active substances. These categories cover a range of crop types and included GAPs targeting use at higher BBCH stages. At least for active substances, a higher DT_{50} may be associated with a higher $PEC_{soil,EFSA}$ value than $PEC_{soil,FOCUS}$.
- $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios differ significantly between the different Tiers for each compound, and show a decreasing trend with increasing Tier.
- Further, PEC_{soil} values calculated with the new EFSA (2017) framework strongly depend on the geographic location of the scenarios automatically selected by the PERSAM model.
- Soil bulk density (derived by a European pedotransfer function from organic matter, Tiktak et al., 2002) was identified as a main driver of the concentration increase along a gradient from North to South as proved by means of linear regression and k-mean clustering.
- Foliar interception and simulated wash-off, determined by crop growth stage at time of application, were identified as other main drivers of the increase in concentrations. Crop interception triggers higher wash-off in case of EFSA Tier-2 and Tier-3A calculations, but is not considered in FOCUS (1997) and EFSA (2017) Tier-1 calculations. The effect was higher for uses with higher interception at the time of application, due to larger impact of simulated foliar wash-off on the amount of substance reaching the soil. The statistical analysis showed that the largest concentration increase occurs in cases with a combination of a high crop interception and low bulk density.
- Obligatory model and scenario specific correction factors contributed to an increase of PEC_{soil} values over all compounds and uses for Tier-1 and Tier-2.
- In the case of metabolites, no clear driving factor for the generally increased PEC_{soil} values could be observed, which might be related to the unbalanced allocation between substance categories and the net effect of range of processes that influence formation, degradation and mobility of residues. Significant variation is noted with the diversity of degradation pathways considered. In the FOCUS (1997) calculations, the maximum occurrences of metabolites are used, whereas in EFSA (2017) calculations, the route of degradation in soil (i.e. formation fractions in soil) are used.

Risk assessment for terrestrial organisms was performed using PEC_{soil} values from FOCUS (1997) and EFSA (1997) calculations, respectively. The comparison showed a substantial change in overall pass/fail ratios. Across all zones, elevated PEC_{soil} values (based on total concentrations) increased RA failure rates by up to 67% using the new approach according to EFSA (2017). Compared to the current failure rate of 14% (FOCUS, 1997 approach), up to 5 times more field studies will be triggered if new modelling is implemented at Member State level. Time needed for performing such studies should be considered in the implementation plan of the new assessment scheme. The detailed results are as follows:

- The failure rates of FOCUS calculations are 14% and 8% for active substances and metabolites, respectively.
- The failure rates of active substances of EFSA (2017) calculations are 67%, 58% and 36% for Tier-1, Tier-2 and Tier-3A, respectively.
- The failure rates of metabolites of EFSA calculations are 38%, 25% and 10% for Tier-1, Tier-2 and Tier-3A, respectively.

Yet, it is unclear how to translate exposure values from the new modelling tiers to ecotoxicological endpoints from either lab or field. Selection procedures for geographic locations for exposure assessment present risks of inconsistent soil properties (e.g., organic carbon content, bulk density) between simulated exposure scenarios and ecotoxicological data (i.e. from higher tier studies). This inconsistency hinders scientifically appropriate and meaningful comparison and interpretation. Worst case assumptions coming from the new exposure assessment, add to the already implemented worst case character of the existing effect and risk assessment which could finally lead to an overly conservative risk evaluation. It is suggested that the new modelling framework should not be used before the availability of an updated soil organism RA guidance which specifies how these exposure values should be implemented in a tiered RA approach. The conservativeness of the overall risk assessment framework should be evaluated and validated before being implemented. Ecotoxicological 'intermediate-tier' effect studies or modelling approaches may provide a potential option to overcome such discrepancies in the future but are currently not available / accepted. It is apparent that any transition period for implementation should factor in all of these uncertainties and should be long enough to ensure alignment and coherence between the new modelling framework and the tiered risk assessment for soil organisms.

5 REFERENCES

Beulke S., De Wilde T., Balderacchi M., Garreyn F., Van Beinum W. and Trevisan M. (2015): Scenario selection and scenario parameterisation for permanent crops and row crops on ridges in support of predicting environmental concentrations of plant protection products and their transformation products in soil. EFSA supporting publication 2015:EN-813, 170 pp.

Budde, E. (2013): Impact Assessment of PECsoil Calculations with the EFSA soil scenarios. Report No. 416301-1. knoell Germany GmbH.

EC, European Commission (2014): Assessing potential for movement of active substances and their metabolites to ground water in the EU. Report of the FOCUS Ground Water Work Group, EC Document Reference SANCO/ 13144/2010 version 3, 613 pp.

EFSA (2007): Scientific opinion of the Panel on Plant Protection Products and their Residues on a request from EFSA related to the default Q10 value used to describe the temperature effect on transformation rates of pesticides in soil. The EFSA Journal (2007) 622, 1-32. doi: https://doi.org/10.2903/j.efsa.2008.622.

EFSA (2012): Tier-1 and Tier-2A Scenario Parameterisation and Example Calculations. EFSA Journal 2012;10(1):2433. doi: https://doi.org/10.2903/j.efsa.2012.2433.

EFSA (2017): EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal, 15(10). doi: 10.2903/j.efsa.2017.4982.

EFSA PPR Panel (EFSA Panel on Plant Protection Products and their Residues) (2012): Scientific opinion on the science behind the guidance for scenario selection and scenario parameterisation for predicting environmental concentrations of plant protection products in soil. EFSA Journal 2012;10(2):2562, 76 pp. doi: https://doi.org/10.2903/j.efsa.2012.2562.

FOCUS (1997): “Soil persistence models and EU registration” The final report of the work of the Soil Modelling Work group of FOCUS; 7617/VI/96_29Feb1997, 77 pp.

FOCUS (2006): “Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration” Report of the FOCUS Work Group on Degradation Kinetics, EC Document Reference Sanco/10058/2005 version 2.0, 434pp.

FOCUS (2011): Generic guidance for Tier 1 FOCUS Ground Water Assessments, v2.0, 63 pp.

Hiederer, R. (2012): EFSA Spatial Data Version 1.1 Data Properties and Processing. Publications Office of the European Union EUR 25546, ISBN 978-92-79-27004-8, doi:10.2788/54453.

Leip, A., G. Marchi, R. Koeble, M. Kempen, W. Britz, and C. Li (2008): Linking an economic model for European agriculture with a mechanistic model to estimate nitrogen and carbon losses from arable soils in Europe. Biogeosciences (5):73-94. doi: https://doi.org/10.5194/bg-5-73-2008.

Pedregosa, Fabian, et al. "Scikit-learn: Machine learning in Python." Journal of Machine Learning Research 12 (2011) 2825-2830.

Seabold, Skipper, and Josef Perktold. "Statsmodels: Econometric and statistical modeling with python." Proceedings of the 9th Python in Science Conference. Vol. 57. 2010.

Tiktak, A., D.S. de Nie, A.M.A. van der Linden and R. Kruijne (2002): Modelling the leaching and drainage of pesticides in the Netherlands: the GeoPEARL model. Agronomie (22):373-387. doi: https://doi.org/10.1051/agro:2002022.

VITO NV (2019): Update of PERSAM software models for predicting environmental concentrations in soil in permanent crops and annual crops: User manual PERSAM 3.0.5. EFSA supporting publication 2019: EN-1756. 96 pp. doi:10.2903/sp.efsa.2019.EN-1756.

6 APPENDIX

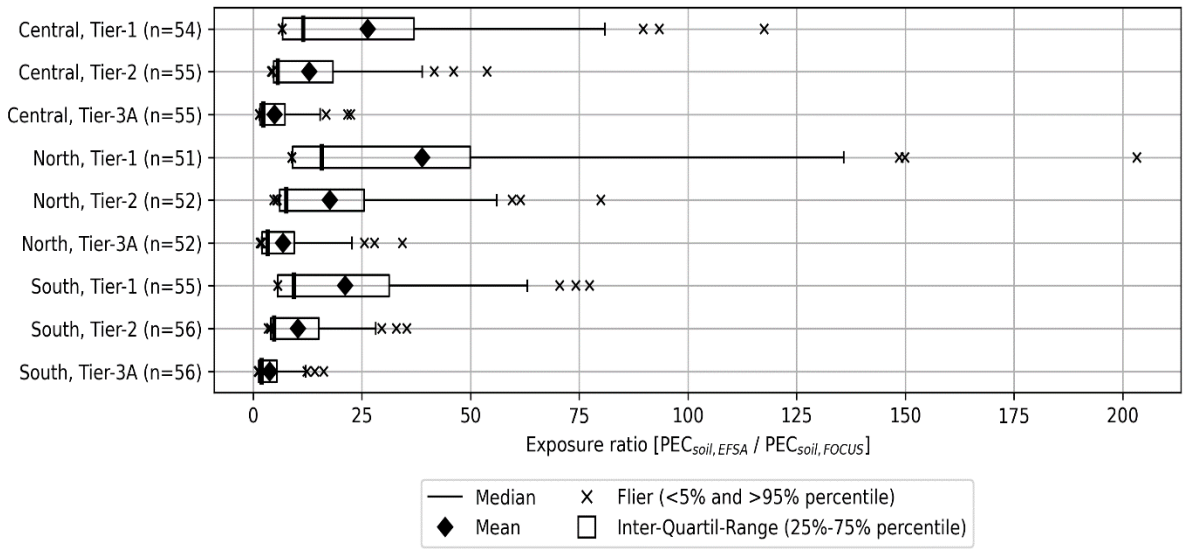


Figure A 1. Variability of PEC$_{soil,EFSA}$ / PEC$_{soil,FOCUS}$ ratio of active substances per regulatory zone and tier.

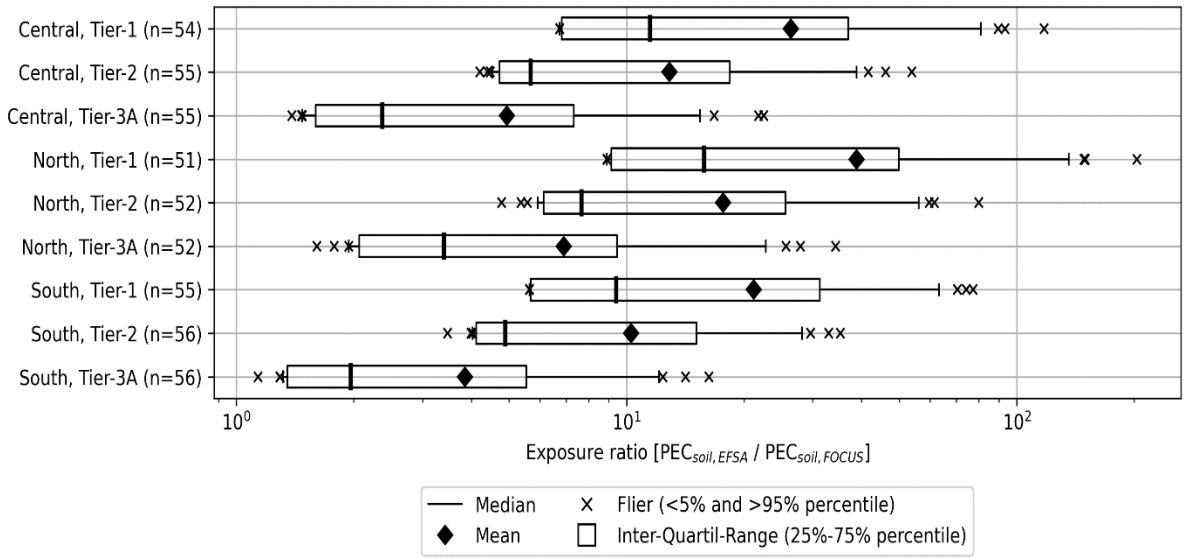


Figure A 2. LOG10-scaled variability of PEC$_{soil,EFSA}$ / PEC$_{soil,FOCUS}$ ratio of active substances per regulatory zone and tier.

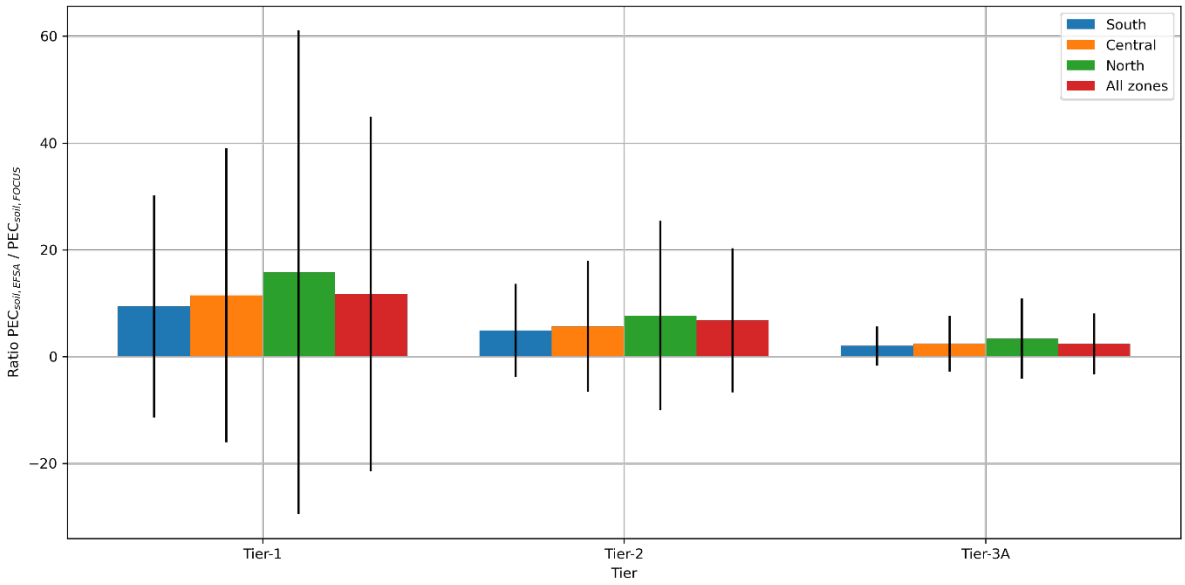


Figure A 3. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of active substances per regulatory zone and tier.

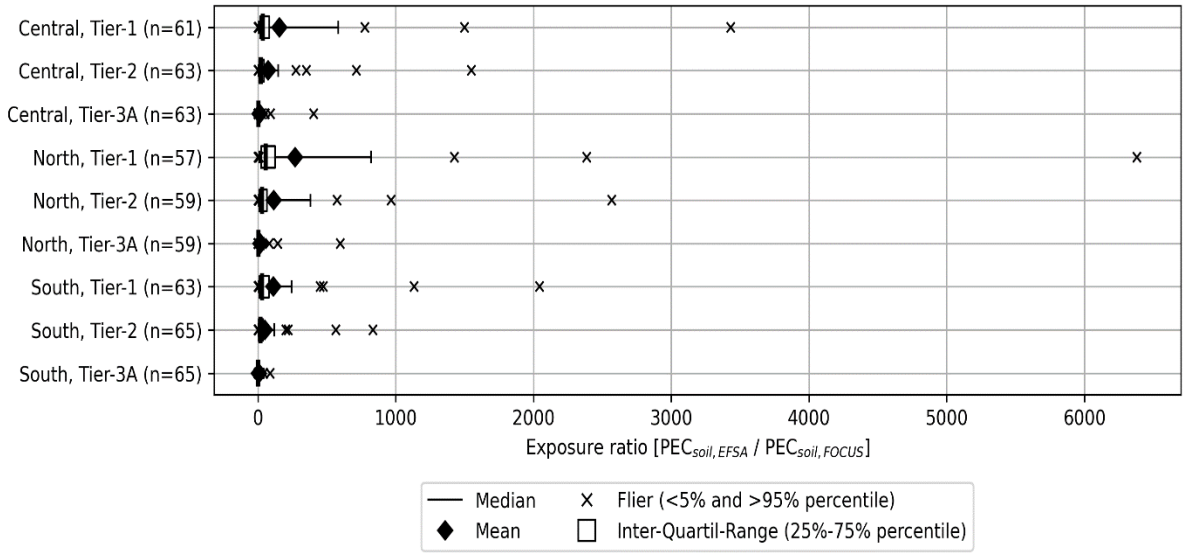


Figure A 4. Variability $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of metabolites per regulatory zone and tier.

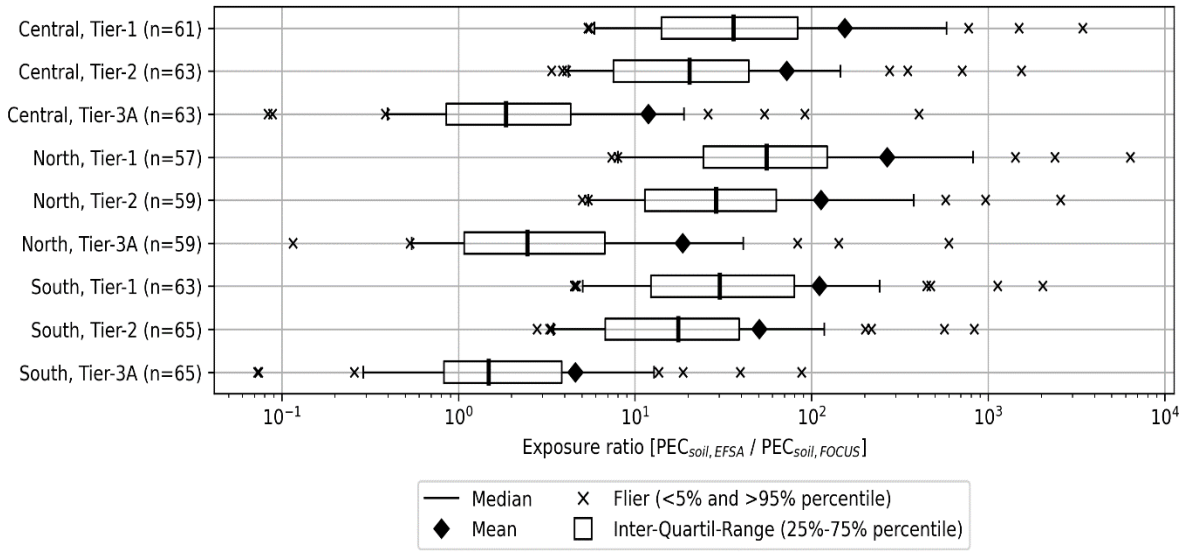


Figure A 5. LOG10-scaled variability of $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of metabolites per regulatory zone and tier.

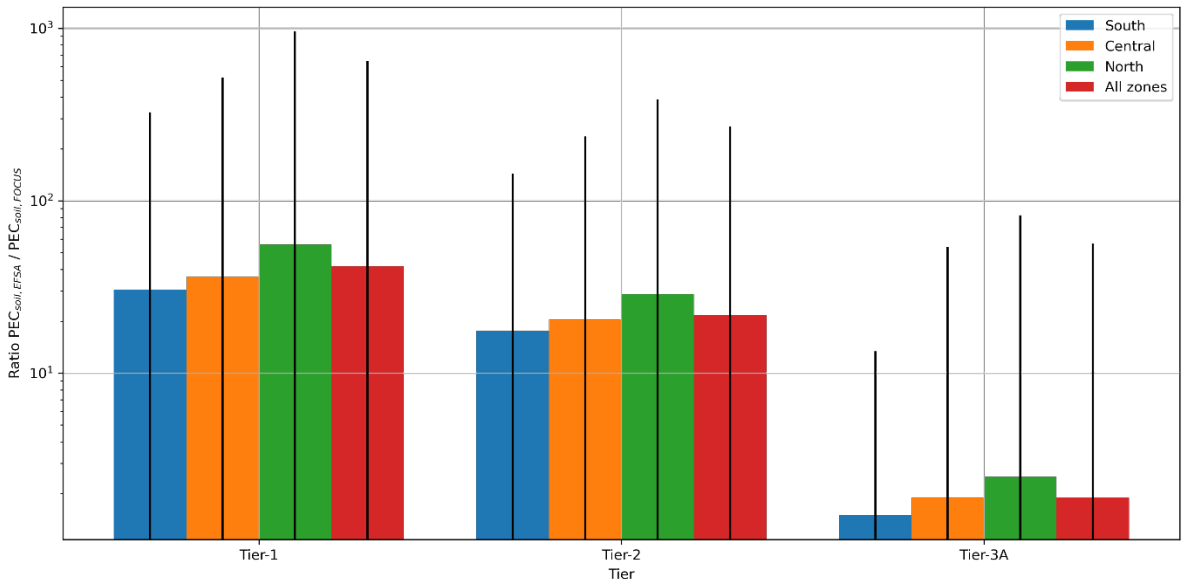


Figure A 6. Median $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratios of metabolites per regulatory zone and tier.

Table A 1. Descriptive statistical parameters of $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substance.

Tier	Category	min	5%	25%	median	75%	95%	max	run count[1]
Tier-1	I	5.6	5.6	6.7	8.4	29.6	105.5	148.6	44
	II	5.7	5.7	7	9.7	44.1	76.1	92.1	19
	III	77.4	81.4	97.5	117.5	160.4	194.7	203.3	3
	IV	7	7.1	11.7	35.4	47.4	91.9	135.8	17
	V	6	6.4	8.2	19.8	34.4	45.8	49.1	6
	VI	10.8	12.1	19.4	41.5	63.1	125.8	149.9	9
	VII	5.6	5.6	6.8	9	12.3	37	64.4	32
	VIII	7.5	8.2	9.6	12.7	19.5	29.1	32.5	9
	IX	8.2	9.2	16.9	35.4	45.7	64.5	68	21
Tier-2	I	3.5	4	4.3	5.4	11.2	45.7	61.5	47
	II	4.1	4.2	4.7	6.3	17	29.5	37.3	19
	III	32.9	35	43.4	53.8	66.9	77.4	80	3
	IV	4.1	4.4	7	16.6	25.1	42.3	56	17
	V	4.3	4.5	5.7	10.6	16.4	21.3	22.7	6
	VI	5.1	5.4	8.3	19.6	29.6	52.4	59.6	9
	VII	4	4	4.7	5.8	6.9	15.3	26	32
	VIII	4.5	4.6	5.1	6.8	10.8	16.5	18.7	9
	IX	5.1	5.8	9.5	16.6	20.2	29.8	31.5	21
Tier-3A	I	1.1	1.3	1.5	1.6	2.2	18.2	27.9	47
	II	1.4	1.4	1.8	2.4	9.2	15.8	18.7	19
	III	14.2	15	18.3	22.5	28.4	33.2	34.4	3
	IV	1.4	1.5	2.5	5.8	9.2	16.5	22.7	17
	V	1.6	1.7	2.2	4.3	7.2	9	9.4	6
	VI	2.6	2.8	4.7	6.5	11.8	22.1	25.7	9
	VII	1.3	1.3	1.6	2	2.3	5.8	10.8	32
	VIII	1.7	1.8	2.2	2.8	4.2	5.7	6.4	9
	IX	1.9	2.2	3.9	7	8.4	12.8	13.3	21

[1] run count: number of runs performed for each active substance in the corresponding category, one per available regulatory zone

Table A 2. Descriptive statistical parameters of $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of metabolites.

Tier	Category	min	5%	25%	median	75%	95%	max	run count[1]
Tier-1	I	4.7	6.7	19	47.5	92.6	300.7	2386.2	105
	II	0	0	5	8.5	31.6	140.1	213.9	19
	III	5.1	5.3	6.6	8.2	9.7	12.6	13.4	6
	IV	8.3	9.8	14.6	44.2	80.7	174.5	227.3	18
	V	- [2]	- [2]	- [2]	- [2]	- [2]	- [2]	- [2]	- [2]
	VI	37.6	38.6	42.9	48.2	57.7	65.4	67.3	3
	VII	12.9	14.1	17.7	22	30.7	44.7	51.8	12
	VIII	65.3	66.9	73.6	81.9	97.2	109.5	112.6	3
	IX	28.8	35.7	126.8	473.3	1123.3	4316.3	6381	15
Tier-2	I	3.4	4.3	11.5	26.1	46.2	132	965.1	111
	II	0	0	3.3	5	16.1	67.3	88.6	19
	III	3.6	3.8	4.5	5.7	6.8	8.6	9.1	6
	IV	5.2	6.1	8.4	25.7	47.9	81	100.4	18
	V	- [2]	- [2]	- [2]	- [2]	- [2]	- [2]	- [2]	- [2]
	VI	17.6	17.9	19.2	20.7	24.7	28	28.8	3
	VII	7.1	7.3	8.3	11	19.2	26.3	27.7	12
	VIII	41.1	42	45.6	50.2	58.8	65.7	67.4	3
	IX	14.3	17.3	53.2	218.8	477.2	1853.9	2566.8	15
Tier-3A	I	0.1	0.3	0.9	1.7	3.9	12	41.1	111
	II	0	0	0.7	0.9	3.2	7.4	10.4	19
	III	0.3	0.3	0.4	0.5	0.5	0.7	0.7	6
	IV	0.8	0.8	1.2	2.6	4.5	9.1	11.5	18
	V	- [2]	- [2]	- [2]	- [2]	- [2]	- [2]	- [2]	- [2]
	VI	3.9	4	4.4	5	6.6	7.9	8.2	3
	VII	0.8	0.9	1.1	1.7	2.8	4.4	4.8	12
	VIII	6.2	6.5	7.4	8.5	10.5	12.1	12.5	3
	IX	2.5	3.2	15.8	39.6	89.9	463.4	598.2	15

[1] run count: number of runs performed for each metabolite in the corresponding category, one per available regulatory zone
[2] Not calculated because no metabolite was in category V

Table A 3. Failure rates (%) of active substances and metabolites grouped by substance categories - EFSA (2017) assessment, for all categories and zones, and for all categories but separated by regulatory zone.

Category	Active substances			Metabolites		
	Tier-1	Tier-2	Tier-3A	Tier-1	Tier-2	Tier-3A
I	59	49	34	38	26	8
II	63	53	37	53	16	0
III	100	100	33	0	0	0
IV	59	53	29	17	17	17
V	50	50	0	- [1]	- [1]	- [1]
VI	100	100	100	0	0	0
VII	56	50	25	50	50	25
VIII	100	100	56	100	100	100
IX	81	62	38	40	20	7
All categories and zones	67	58	36	38	25	10
All categories NEU	71	63	46	44	27	14
All categories CEU	67	56	33	38	25	10
All categories SEU	64	55	30	32	23	8

[1] Not calculated because no metabolite was in category V

Table A 4. Failure rates (%) of active substances and metabolites grouped by substance categories - FOCUS (1997) assessment, and for all categories.

Category	Active substances	Metabolites
I	25	5
II	14	0
III	0	0
IV	0	17
V	0	- [1]
VI	33	0
VII	9	25
VIII	0	100
IX	14	0
All categories	14	8

[1] Not calculated because no metabolite was in category V

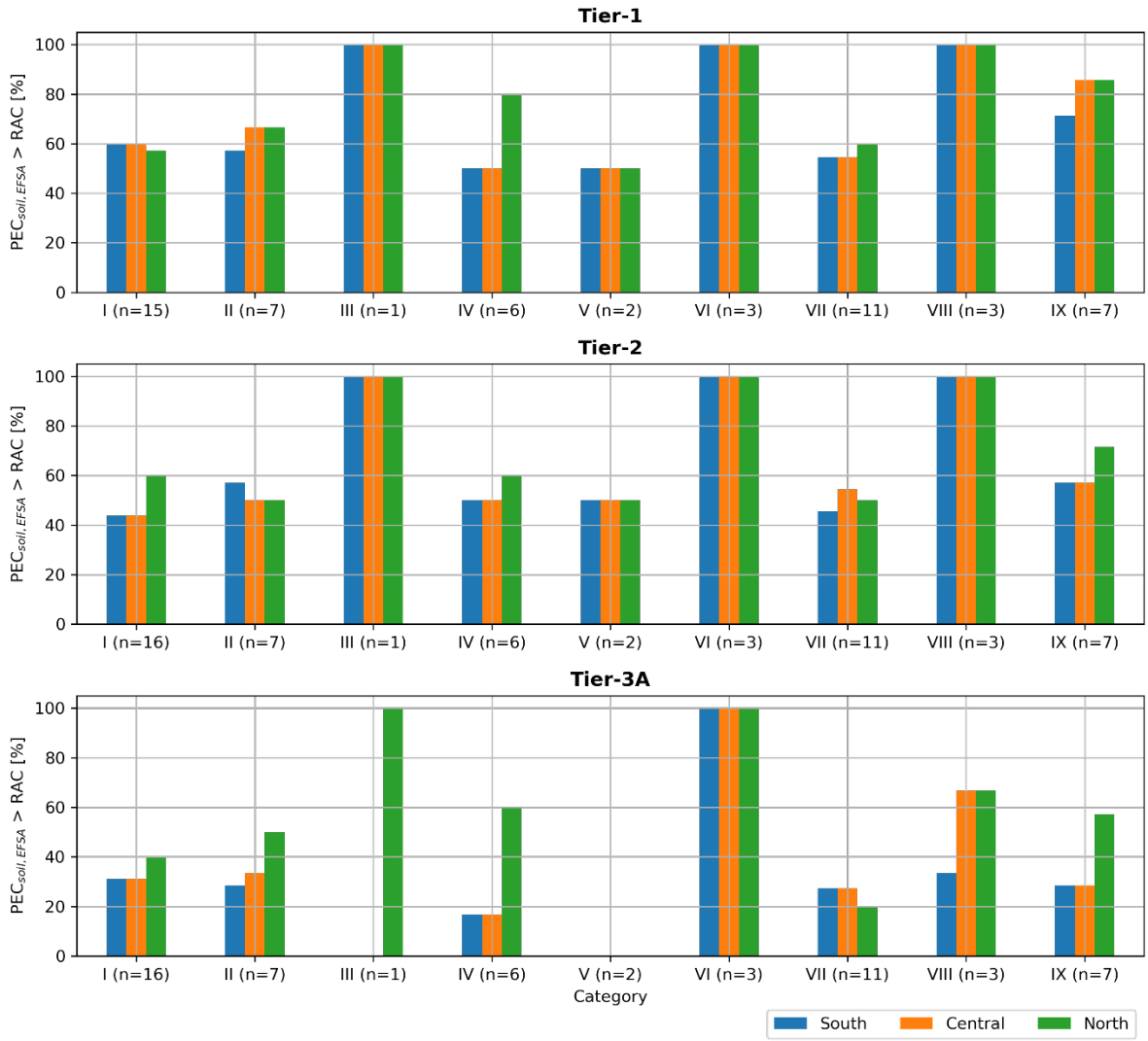


Figure A 7. Failure rate (%) based on $PEC_{soil,EFSA}$ values for active substances grouped by substance categories and regulatory zone.

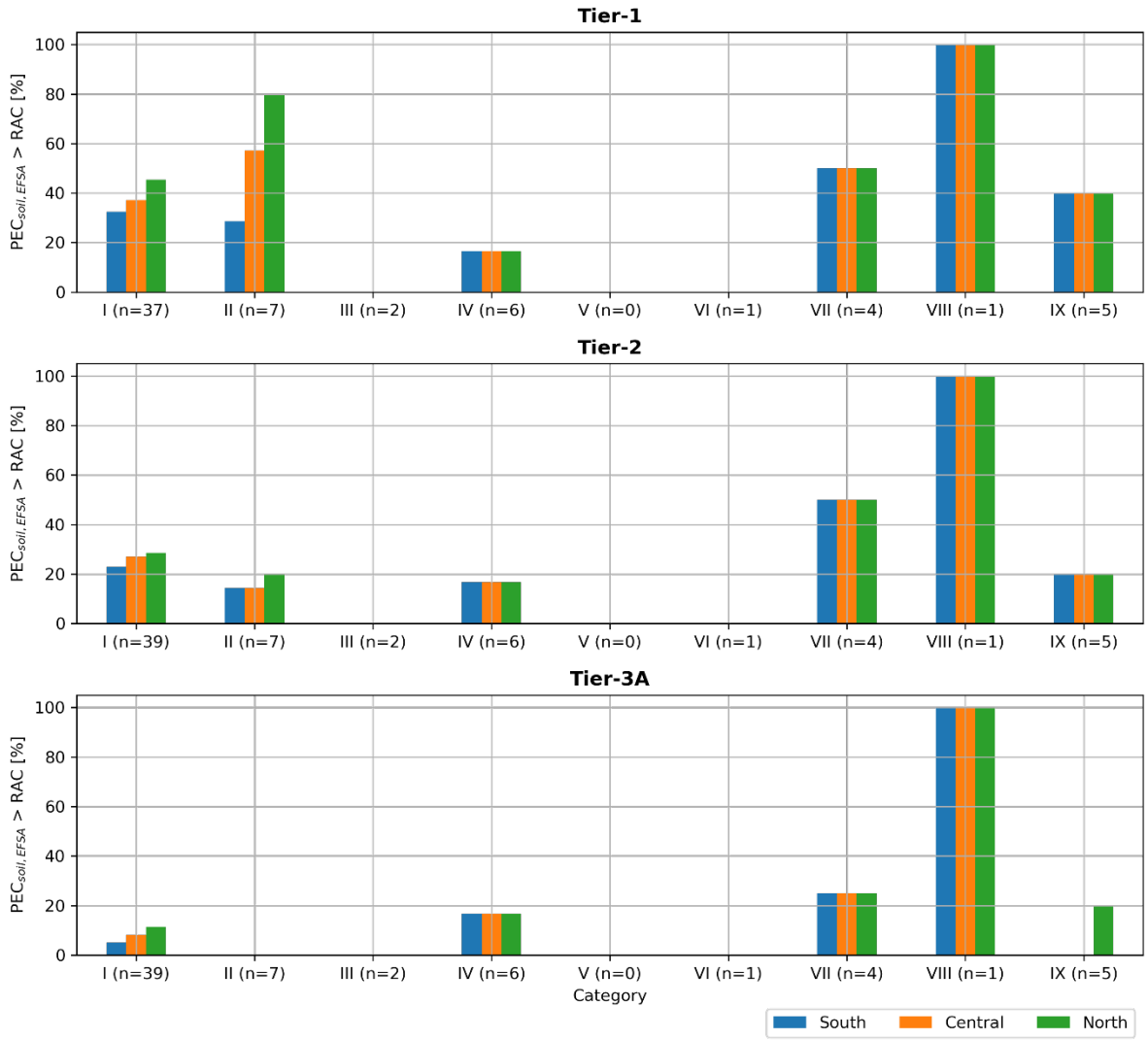


Figure A 8. Failure rate (%) based on $PEC_{soil,EFSA}$ values for of metabolites grouped by substance categories and regulatory zone.

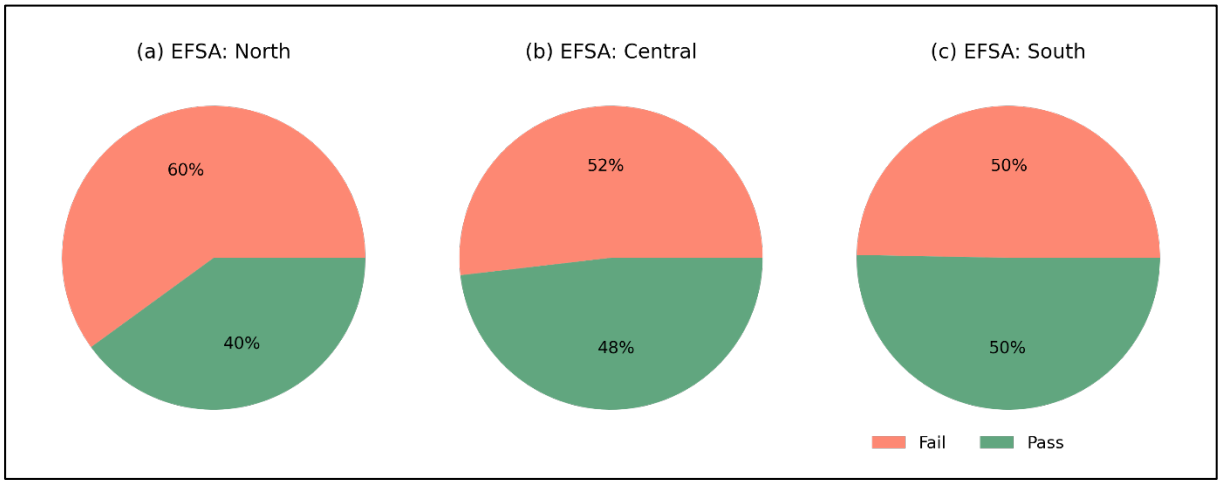


Figure A 9. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances at each regulatory zone (a) North, (b) Central and (c) South.

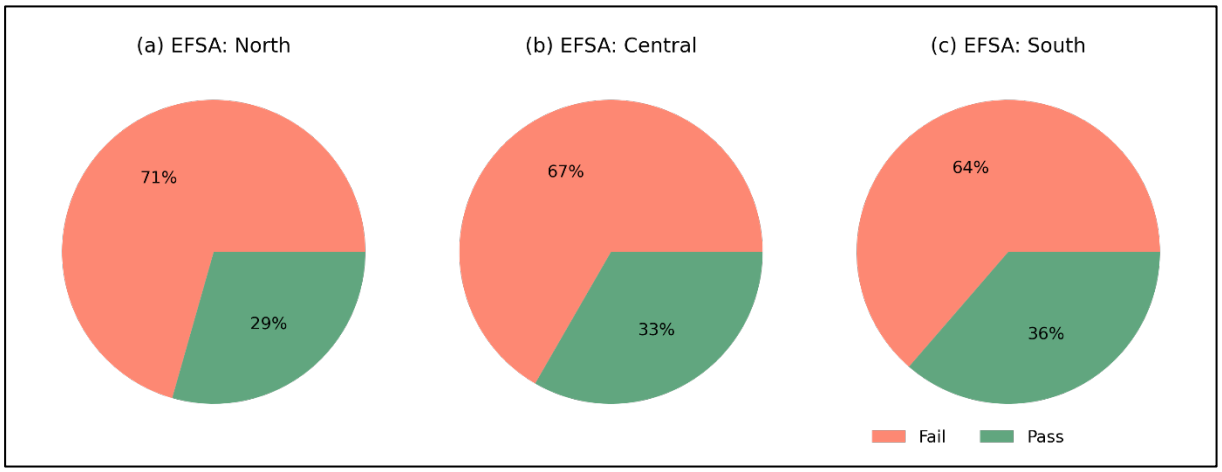


Figure A 10. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances at each regulatory zone (a) North, (b) Central and (c) South - Tier-1.

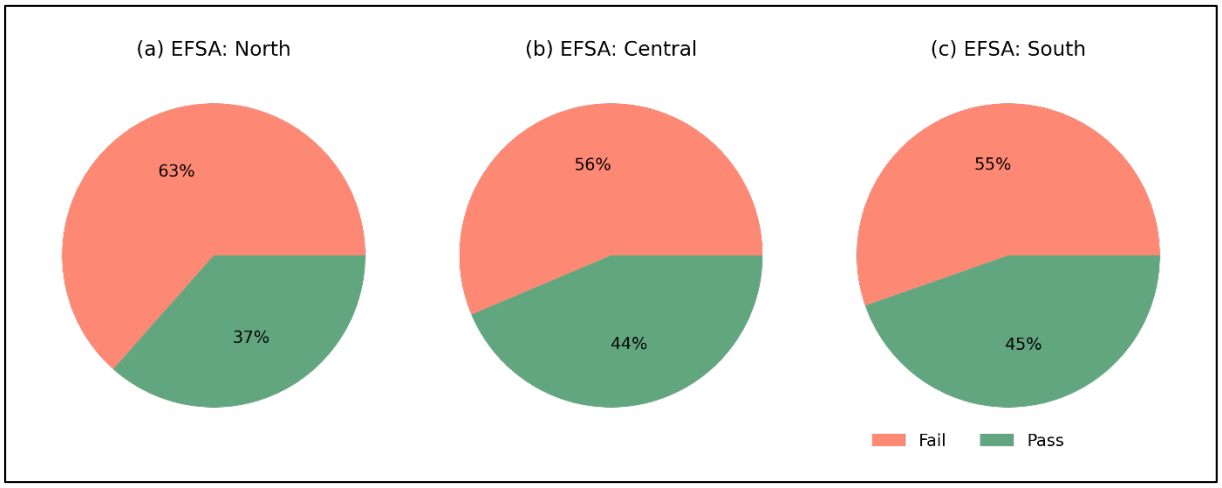


Figure A 11. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances at each regulatory zone (a) North, (b) Central and (c) South - Tier-2.

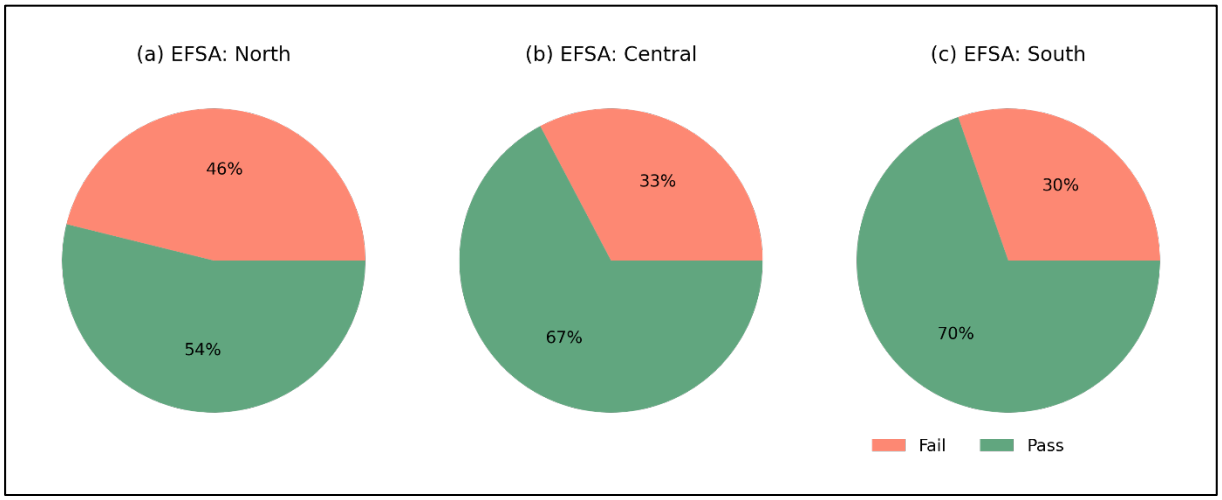


Figure A 12. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances at each regulatory zone (a) North, (b) Central and (c) South - Tier-3A.

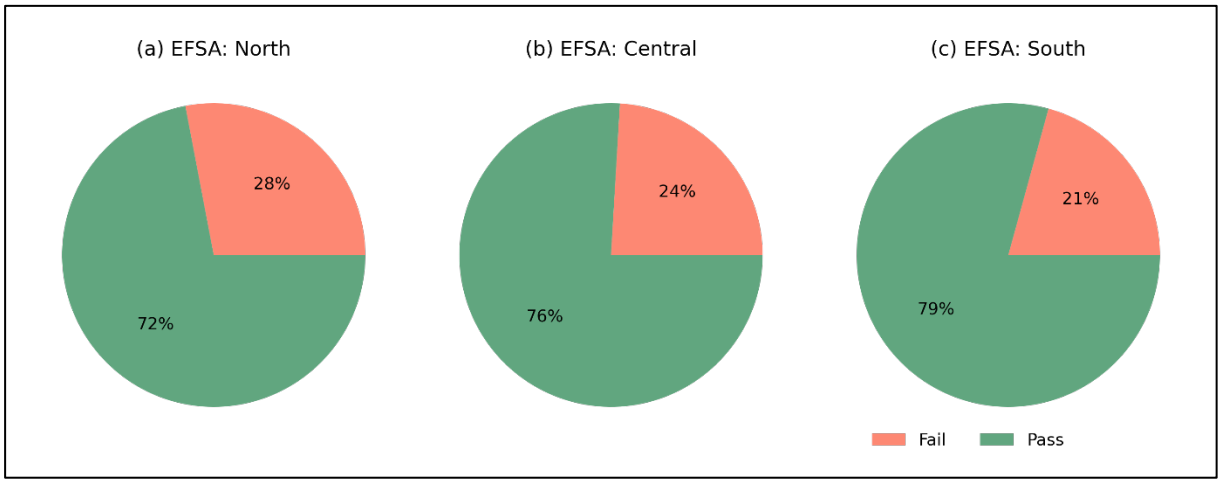


Figure A 13. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites at each regulatory zone (a) North, (b) Central and (c) South.

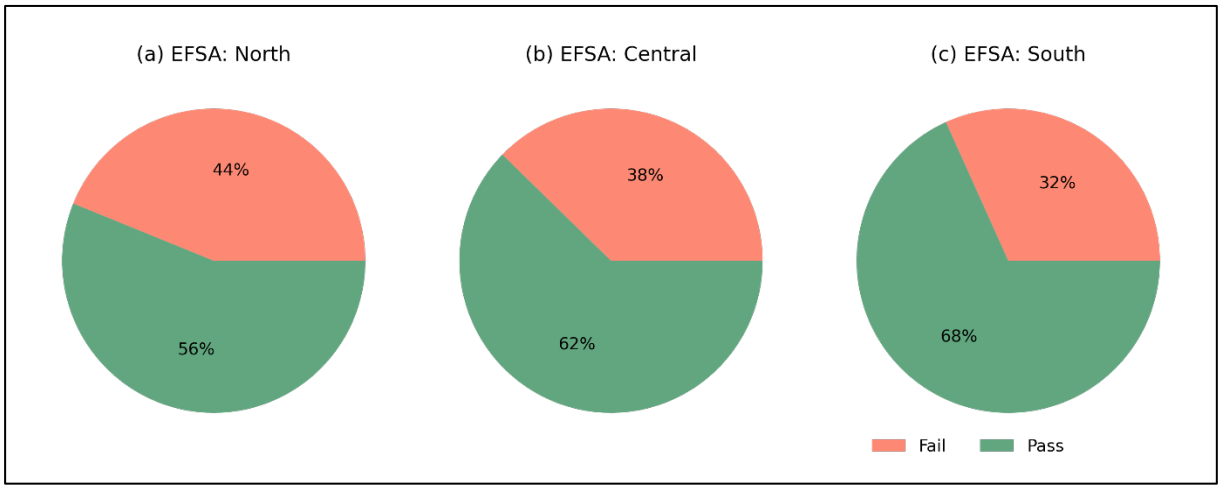


Figure A 14. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites at each regulatory zone (a) North, (b) Central and (c) South – Tier-1.

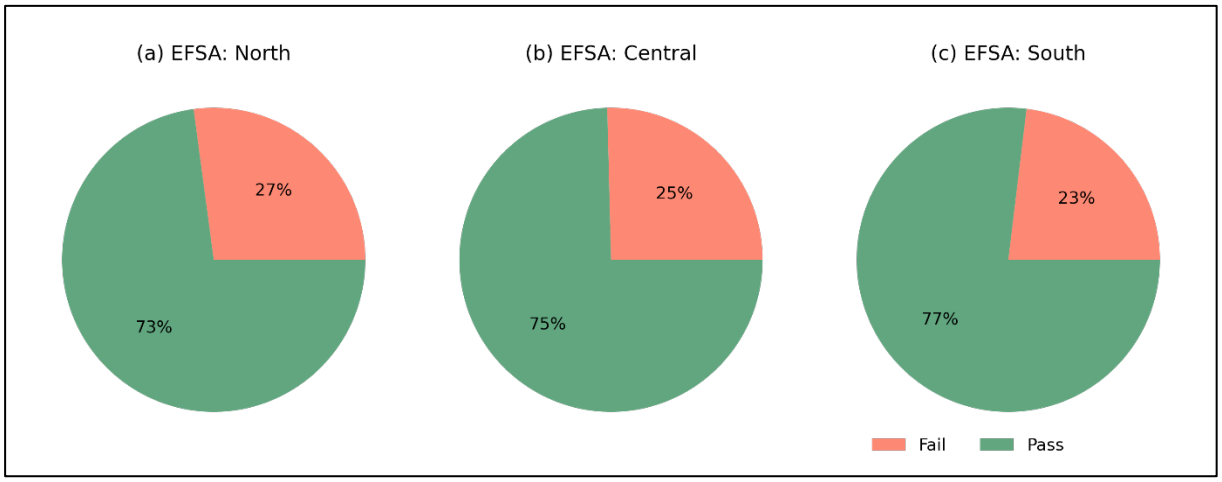


Figure A 15. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites at each regulatory zone (a) North, (b) Central and (c) South – Tier-2.

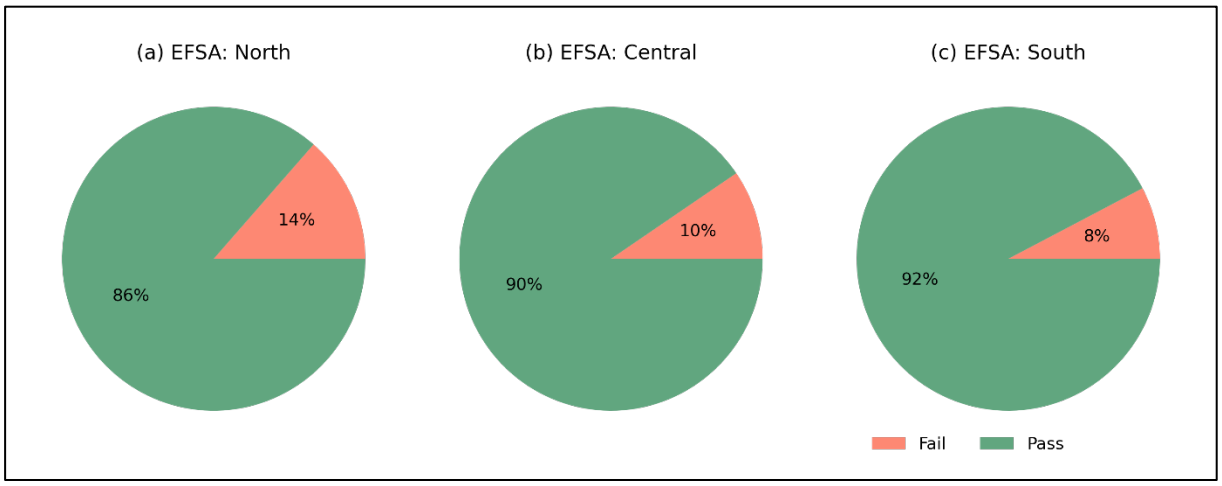


Figure A 16. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites at each regulatory zone (a) North, (b) Central and (c) South – Tier-3A.

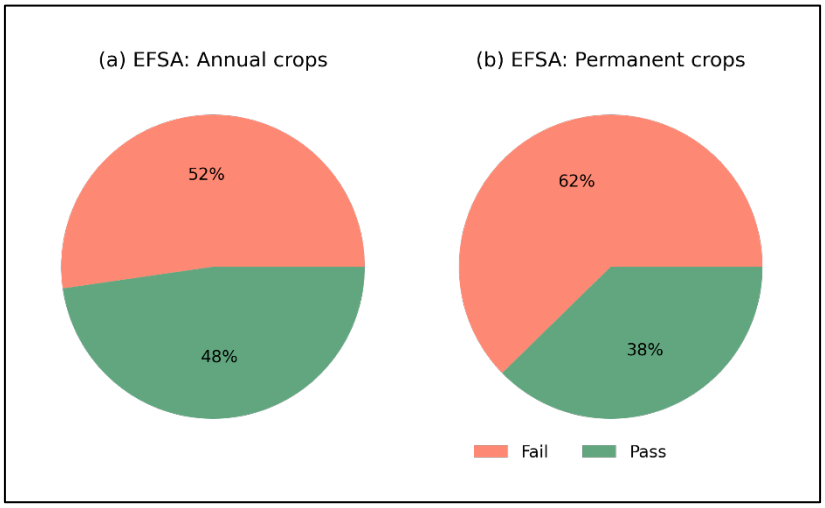


Figure A 17. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances for each crop type (a) Annual crops and (b) Permanent crops.

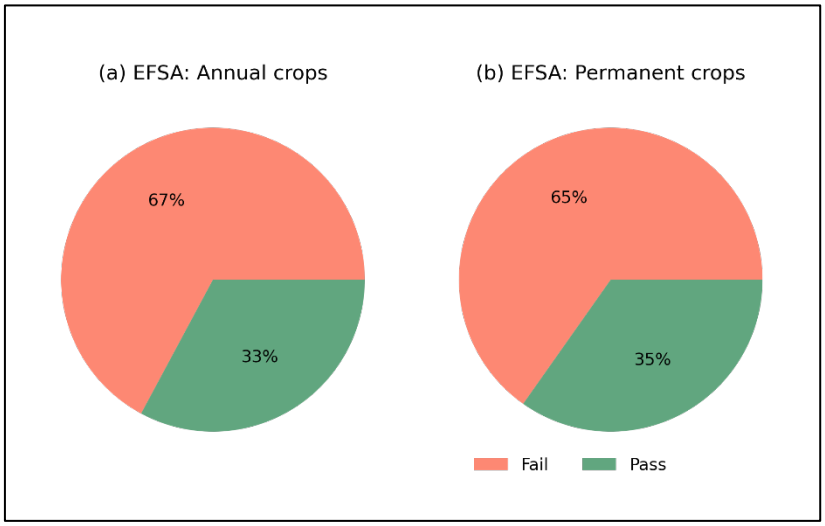


Figure A 18. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances for each crop type (a) Annual crops and (b) Permanent crops – Tier-1.

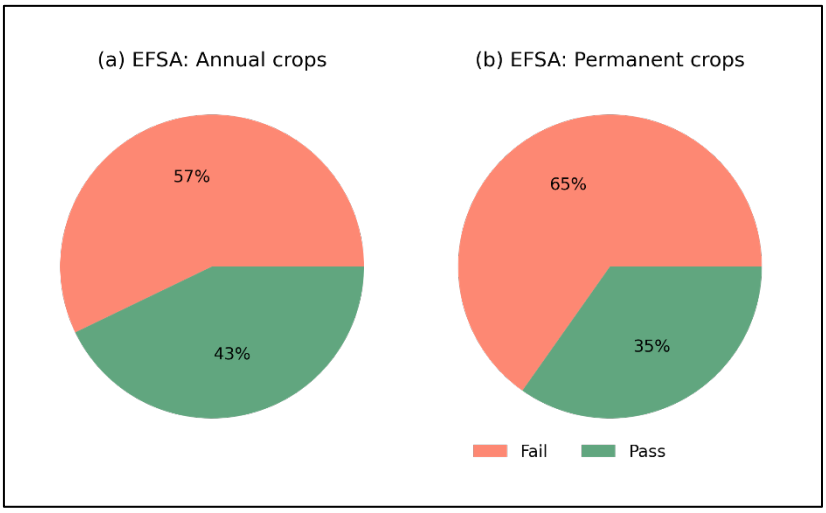


Figure A 19. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances for each crop type (a) Annual crops and (b) Permanent crops – Tier-2.

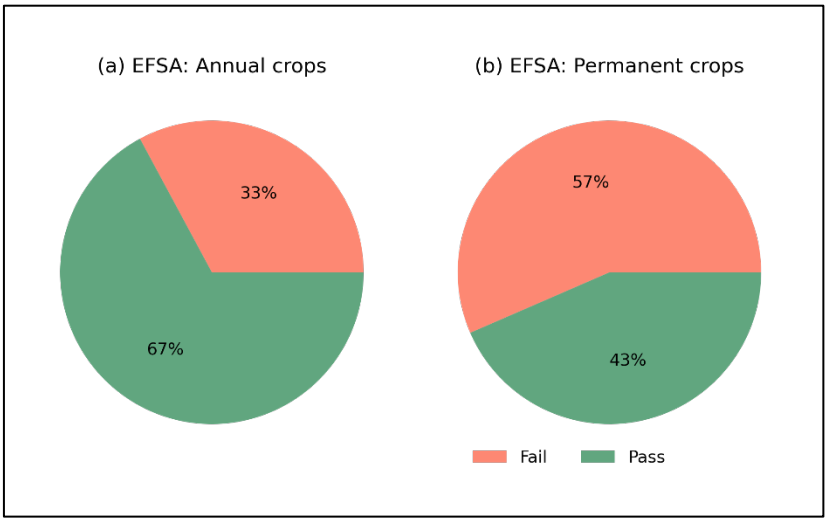


Figure A 20. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for active substances for each crop type (a) Annual crops and (b) Permanent crops – Tier-3A.

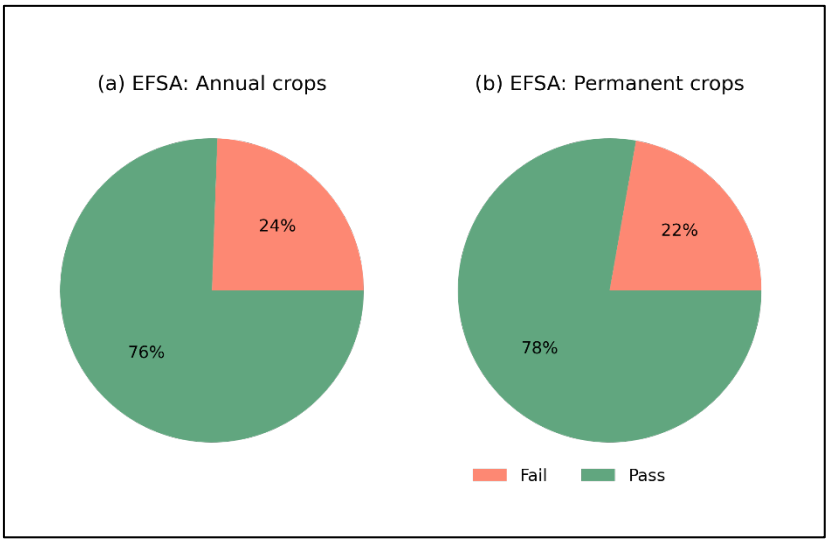


Figure A 21. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites for each crop type (a) Annual crops and (b) Permanent crops.

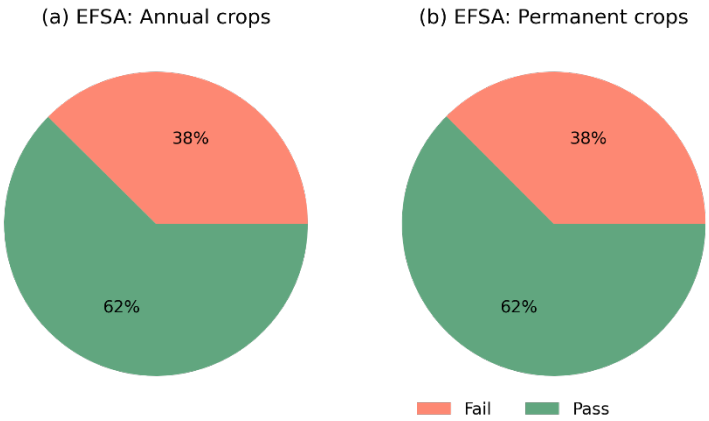


Figure A 22. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites for each crop type (a) Annual crops and (b) Permanent crops – Tier-1.

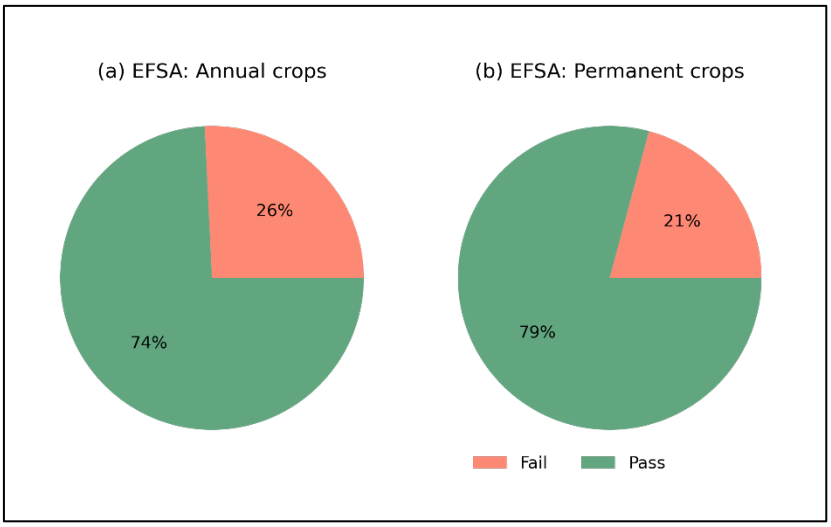


Figure A 23. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites for each crop type (a) Annual crops and (b) Permanent crops – Tier-2.

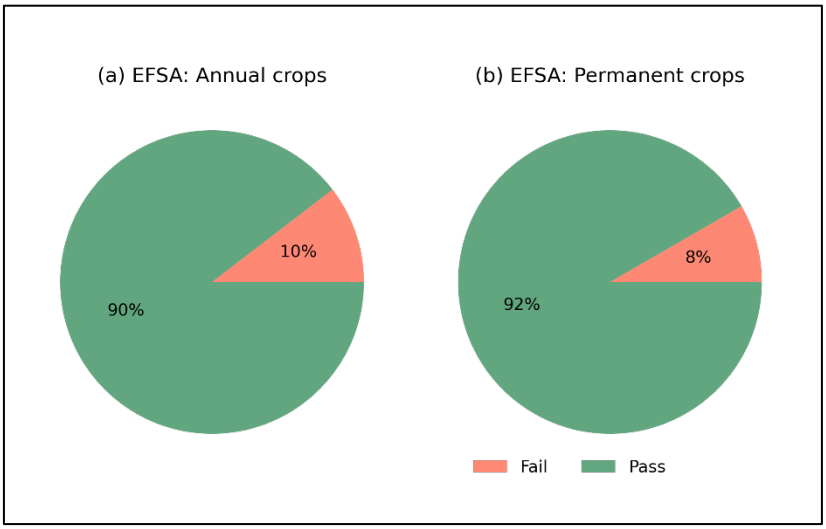


Figure A 24. Failure rate (%) of the ecotoxicological Tier 1 soil risk assessment based on $PEC_{soil,EFSA}$ values for metabolites for each crop type (a) Annual crops and (b) Permanent crops – Tier-3A.

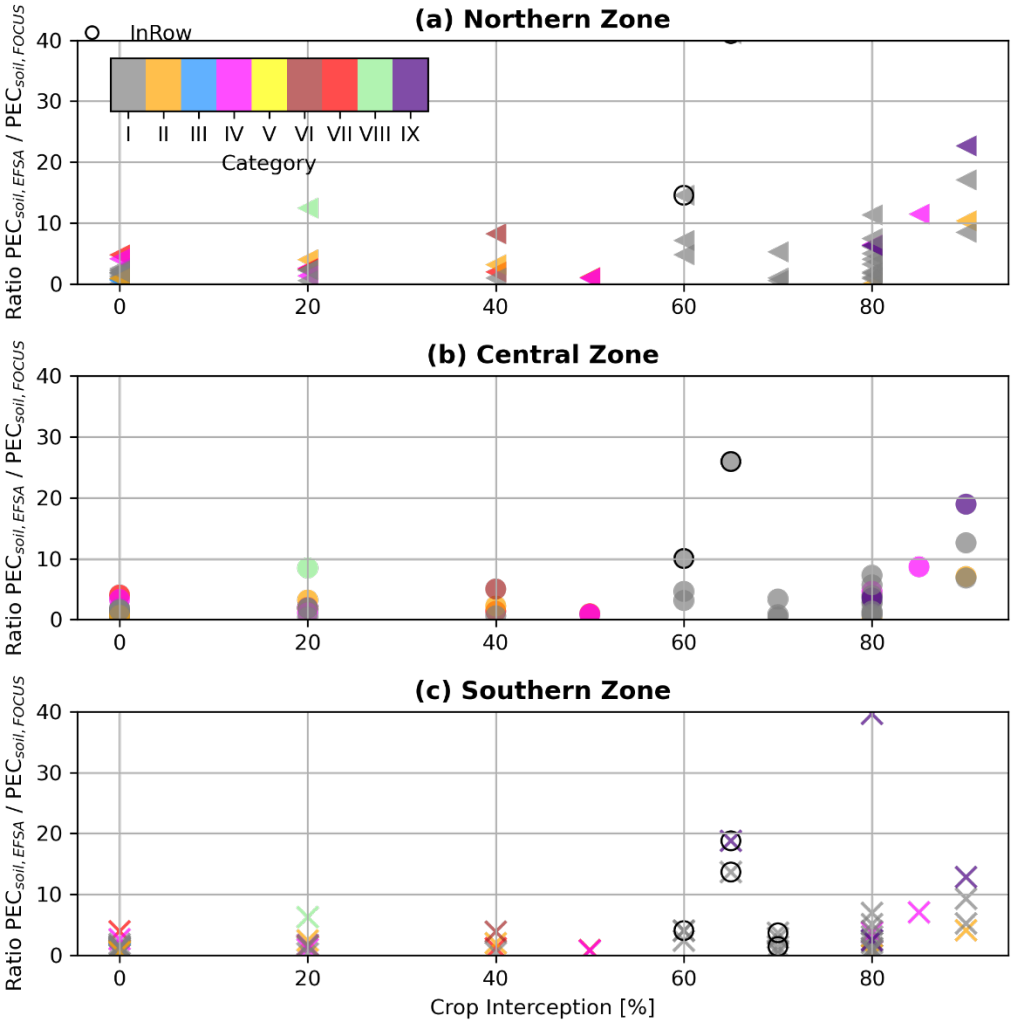


Figure A 25. Relationship between crop interception and $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio at Tier-3A of metabolites for regulatory zones.

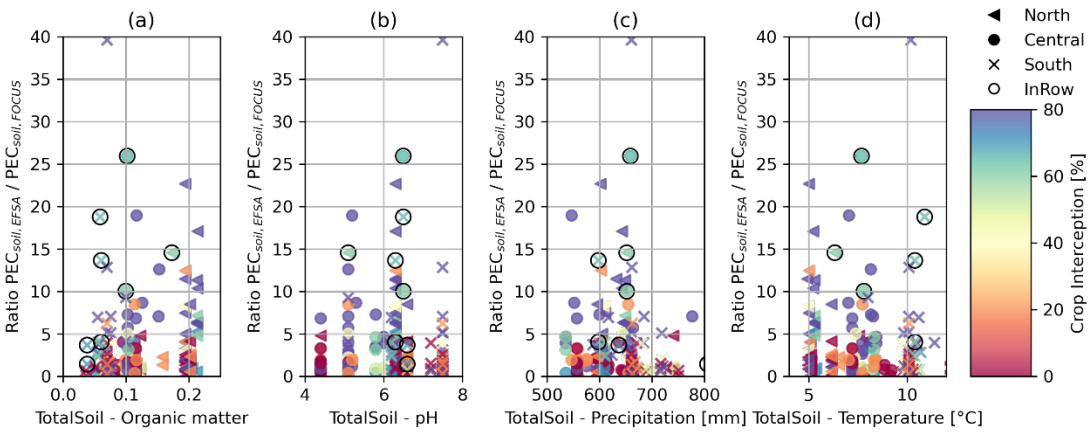


Figure A 26. Relationship between environmental conditions at Tier-3A and $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of metabolites.

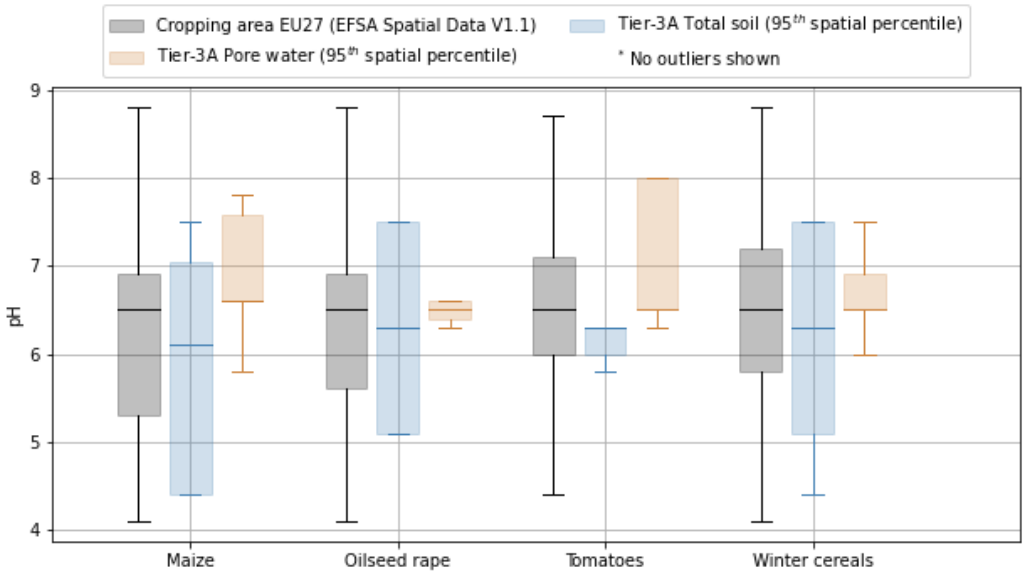


Figure A 27. Variability of pH of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas.

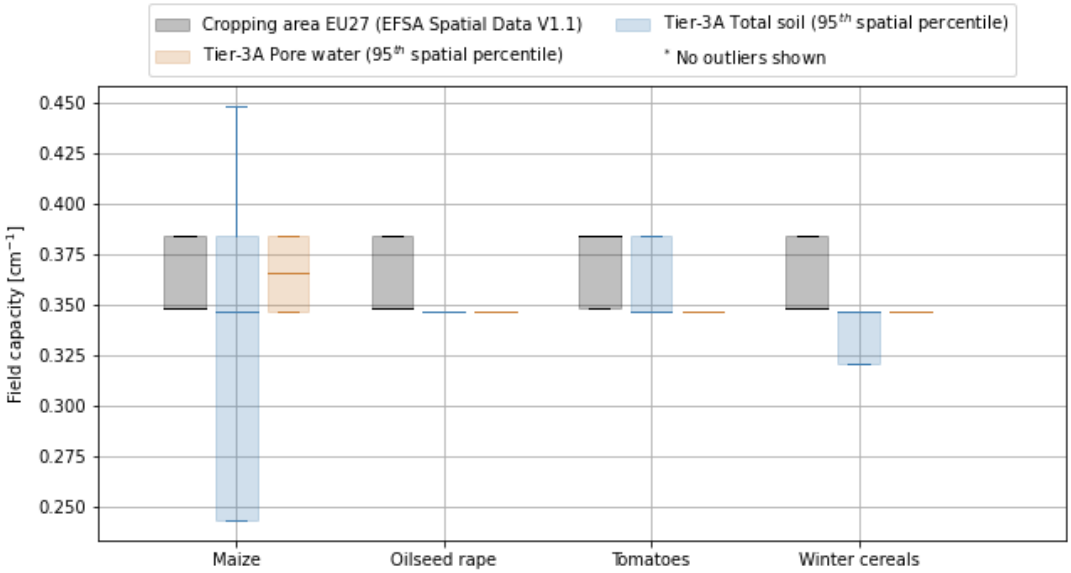


Figure A 28. Variability of field capacity of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas.

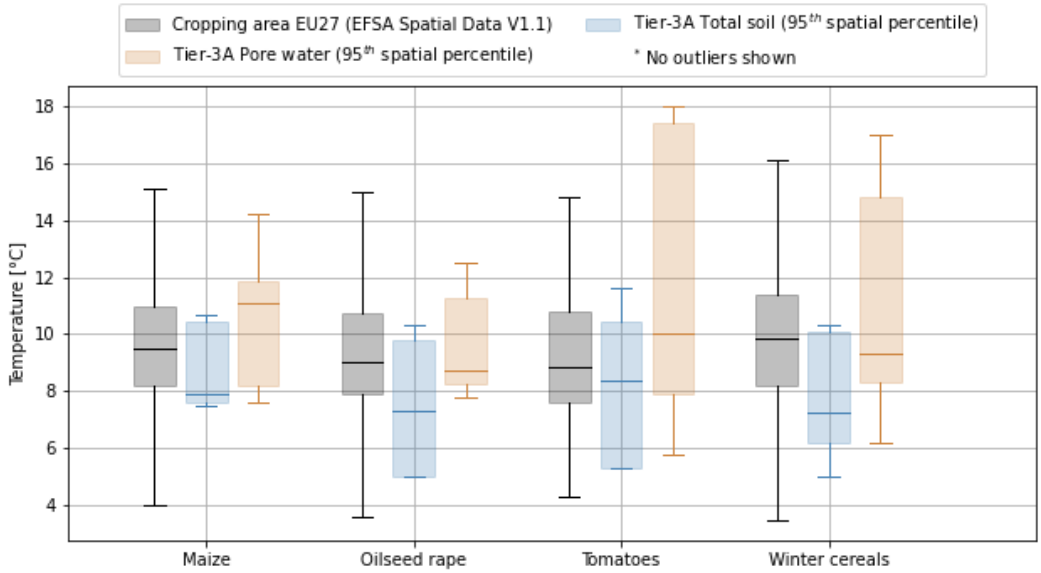


Figure A 29. Variability of temperature of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas.

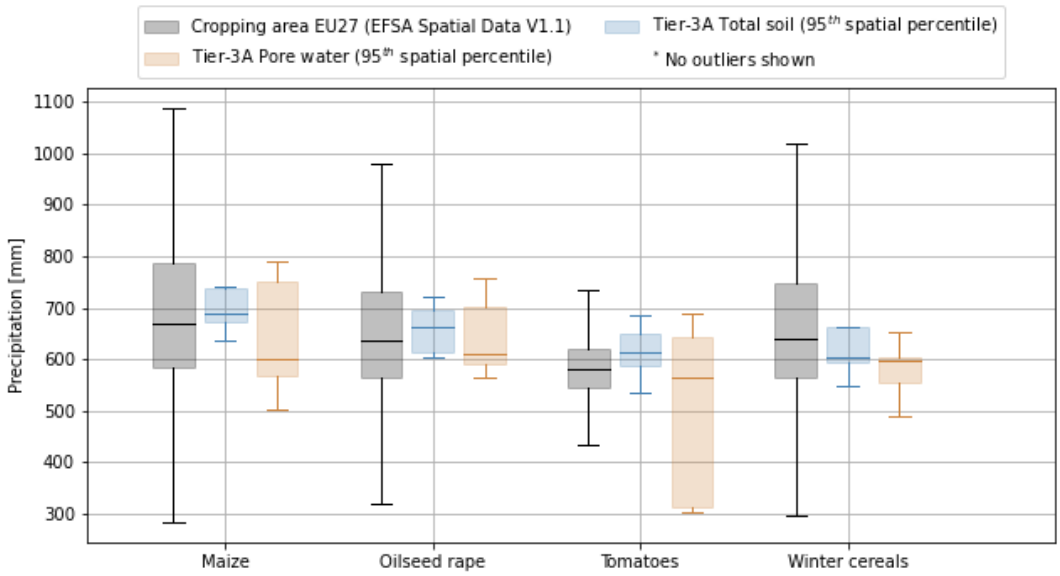


Figure A 30. Variability of precipitation of 95th percentile scenario locations for Tier-3A exposure assessment in comparison to European cropping areas.

Table A 5. Variability of environmental conditions of 95th percentile scenario locations for Tier-3A total soil exposure assessment.

Zone	Minimum	5th Perc.	25th Perc.	Median	75th Perc.	95th Perc.	Maximum	Mean	Standard deviation
	Bulk density [g cm^{-3}]								
North	0.44	0.53	0.74	0.76	0.76	0.89	0.94	0.74	0.09
Central	0.58	0.75	0.95	0.96	0.99	1.02	1.07	0.95	0.09
South	0.76	0.94	1.09	1.12	1.12	1.19	1.30	1.10	0.08
	Field capacity [cm cm^{-1}]								
North	0.24	0.30	0.35	0.35	0.35	0.35	0.38	0.34	0.02
Central	0.24	0.24	0.24	0.35	0.35	0.38	0.45	0.31	0.06
South	0.35	0.35	0.35	0.35	0.35	0.38	0.38	0.36	0.02
	Organic matter [%]								
North	12.00	13.75	19.40	19.40	20.20	21.30	21.40	19.13	2.13
Central	8.17	8.74	10.30	10.40	11.60	12.10	15.30	10.85	1.18
South	3.54	4.97	6.09	7.00	7.00	7.59	9.98	6.73	1.09
	pH								
North	4.40	4.75	6.30	6.30	6.40	6.60	8.00	6.21	0.57
Central	4.40	4.40	5.10	5.10	5.95	6.60	6.60	5.35	0.73
South	5.10	6.20	6.60	7.50	7.50	7.50	7.50	7.12	0.60
	Precipitation [mm]								
North	542	595	596	606	647	705	741	621	36
Central	536	536	557	607	655	668	891	611	63
South	588	598	661	662	692	826	926	679	60
	Temperature [°C]								
North	4.94	4.97	5.02	5.23	6.16	7.38	7.57	5.59	0.73
Central	7.02	7.05	7.22	7.73	8.27	8.86	9.22	7.75	0.57
South	7.96	9.78	10.10	10.10	10.40	12.20	14.90	10.37	0.97

Table A 6. Variability of environmental conditions of 95th percentile scenario locations for Tier-3A pore water exposure assessment.

Zone	Minimum	5th Perc.	25th Perc.	Median	75th Perc.	95th Perc.	Maximum	Mean	Standard deviation
	Bulk density [g cm^{-3}]								
North	1.04	1.22	1.37	1.38	1.38	1.38	1.38	1.34	0.07
Central	0.79	1.23	1.41	1.43	1.43	1.45	1.47	1.38	0.11
South	1.20	1.36	1.46	1.50	1.52	1.54	1.56	1.48	0.06
	Field capacity [cm cm^{-1}]								
North	0.24	0.24	0.35	0.35	0.35	0.35	0.38	0.33	0.04
Central	0.24	0.24	0.35	0.35	0.35	0.38	0.45	0.34	0.04
South	0.24	0.24	0.35	0.35	0.38	0.38	0.38	0.35	0.05
	Organic matter [%]								
North	2.41	2.41	2.41	2.41	2.46	4.41	8.32	2.71	0.81
Central	1.41	1.52	1.74	1.87	1.98	3.93	9.27	2.22	1.24
South	0.76	0.86	1.03	1.08	1.34	2.17	2.75	1.26	0.44
	pH								
North	4.40	5.40	6.50	6.50	6.50	6.50	6.60	6.36	0.40
Central	4.10	6.17	6.50	6.50	6.60	7.80	7.80	6.54	0.49
South	5.30	6.30	6.60	6.90	6.90	8.00	8.00	6.96	0.57
	Precipitation [mm]								
North	580	585	597	602	637	654	675	612	25
Central	491	537	571	601	611	647	772	596	44
South	301	308	529	555	712	758	879	589	135
	Temperature [°C]								
North	5.14	5.67	7.78	8.22	8.28	8.31	8.37	7.69	0.99
Central	7.70	8.42	8.94	9.35	9.78	10.83	11.20	9.42	0.70
South	10.10	11.10	13.20	14.90	15.80	17.70	18.00	14.41	2.07

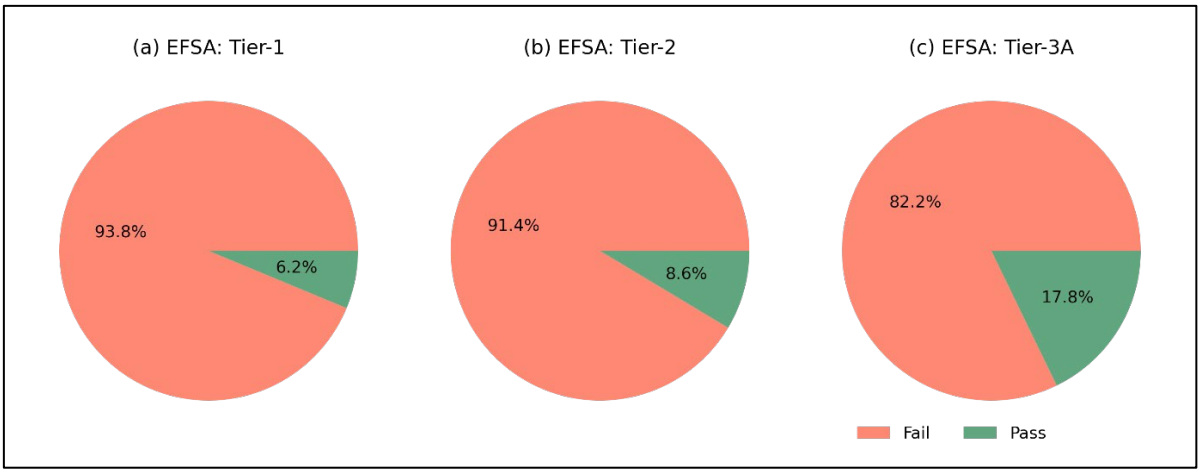


Figure A 31. Failure rate (%) of the risk assessment based on $PEC_{pore\ water,EFSA}$ values for active substances at (a) Tier-1, (b) Tier-2 and (c) Tier-3A.

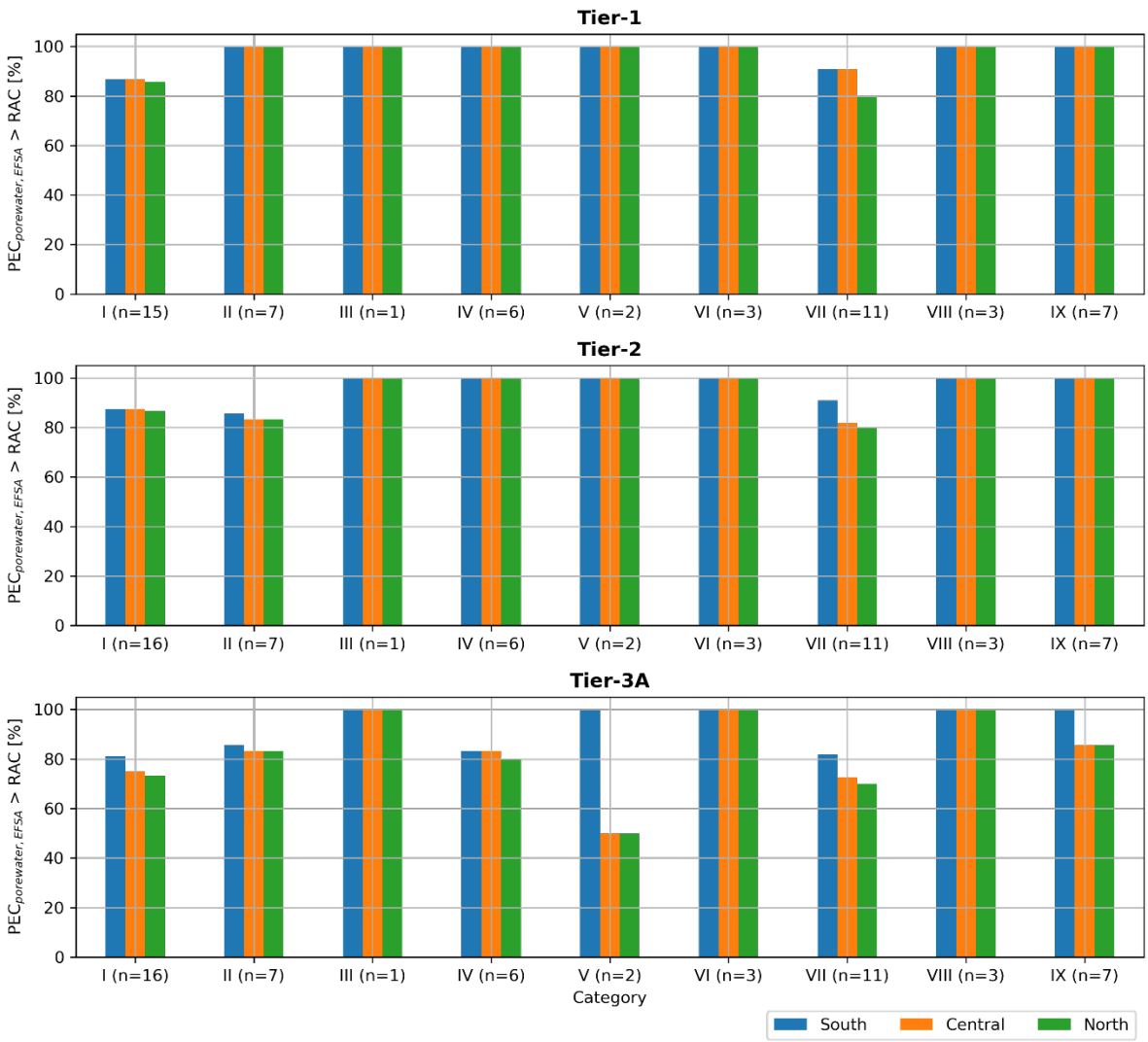


Figure A 32. Failure rate (%) based on $PEC_{pore\ water,EFSA}$ values for active substances grouped by substance categories and regulatory zone.

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                  ratio   R-squared:                       0.733
Model:                            OLS   Adj. R-squared:                  0.719
Method:                 Least Squares   F-statistic:                     52.88
Date:                Thu, 03 Feb 2022   Prob (F-statistic):           2.19e-40
Time:                        11:30:55   Log-Likelihood:                -408.17
No. Observations:                 163   AIC:                             834.3
Df Residuals:                     154   BIC:                             862.2
Df Model:                           8
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      5.1937      0.239     21.775      0.000       4.722       5.665
bd_scaled     -6.9061      0.550    -12.568      0.000      -7.992      -5.821
om_scaled     -4.3806      0.855     -5.123      0.000      -6.070      -2.691
ph_scaled      0.5458      0.373      1.463      0.146      -0.191       1.283
fc_scaled     -0.9167      0.593     -1.546      0.124      -2.088       0.255
wp_scaled      0.4103      0.615      0.668      0.505      -0.804       1.624
prec_scaled    0.2580      0.289      0.893      0.373      -0.313       0.829
temp_scaled    0.4391      0.796      0.551      0.582      -1.134       2.012
intc_scaled    2.7125      0.251     10.811      0.000       2.217       3.208
==============================================================================
Omnibus:                       49.926   Durbin-Watson:                   1.287
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              382.876
Skew:                           0.831   Prob(JB):                     7.24e-84
Kurtosis:                      10.322   Cond. No.                         8.64
```

Figure A 33. Results of multivariate regression model of environmental parameters at Tier-3A 95th percentile locations and crop interception in relation to $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances in total soil.

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                  ratio   R-squared:                       0.569
Model:                            OLS   Adj. R-squared:                  0.564
Method:                 Least Squares   F-statistic:                     105.6
Date:                Thu, 03 Feb 2022   Prob (F-statistic):           5.79e-30
Time:                        11:30:55   Log-Likelihood:                -447.25
No. Observations:                 163   AIC:                             900.5
Df Residuals:                     160   BIC:                             909.8
Df Model:                           2
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept      5.1937      0.297     17.464      0.000       4.606       5.781
bd_scaled     -2.4538      0.301     -8.156      0.000      -3.048      -1.860
intc_scaled    3.2059      0.301     10.656      0.000       2.612       3.800
==============================================================================
Omnibus:                       78.860   Durbin-Watson:                   1.112
Prob(Omnibus):                  0.000   Jarque-Bera (JB):              401.733
Skew:                           1.737   Prob(JB):                     5.82e-88
Kurtosis:                       9.862   Cond. No.                         1.16
```

Figure A 34. Results of multivariate regression model of bulk density at Tier-3A 95th percentile locations and crop interception in relation to $PEC_{soil,EFSA}$ / $PEC_{soil,FOCUS}$ ratio of active substances in total soil.