The EFSA Journal (2007) 622, 1-32

Opinion on a request from EFSA related to the default Q_{10} value used to describe the temperature effect on transformation rates of pesticides in soil[1]

Scientific Opinion of the Panel on Plant Protection Products and their Residues (PPR-Panel)

(Question No EFSA-Q-2007-048)

Adopted on 12 December 2007

PANEL MEMBERS*

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SUMMARY

One factor affecting the degradation rate of chemicals (including plant protection products) is temperature. It is generally accepted that this dependency may be reasonably described by using the Arrhenius equation which gives the degradation rate coefficient as a function of the temperature and the activation energy E_a. Using this E_a value, the ratio of degradation rates between two temperatures can be calculated. The ratio between the rates at 20° and 10°C is usually written as the Q_{10} value. This value is used in environmental exposure assessment to account for the impact of different temperatures. As a default, the value of Q_{10} = 2.2 was proposed by FOCUS (1997). The Panel on Plant Protection Products and their Residues (PPR Panel) of the European Food Safety Authority (EFSA) issued an Opinion on the Q_{10} value in 2006.

EFSA asked the PPR Panel in 2007 to reconsider whether the database, on which these previous default values of Q_{10} were proposed, still reflected the scientific state of the art, or if it should be updated in view of additional data that had subsequently emerged. Accordingly the PPR Panel reviewed all the available scientific literature on the effect of temperature on the breakdown of pesticides in soils, and reached the following conclusions.

It is appropriate to use the Arrhenius equation for temperatures between 0° and 30°C. The data analysis indicated that the distribution of the median E_a values for all such compounds is lognormal, with a median of 65.4 kJ mol^{-1} and a 90-percent probability that the median value is within the range 45.8-93.3 kJ mol^{-1}. The PPR Panel has concluded that there are group-specific

[1] For citation purposes: Scientific Opinion of the Panel on Plant Protection Products and their Residues on a request from EFSA related to the default Q_{10} value used to describe the temperature effect on transformation rates of pesticides in soil. The EFSA Journal (2007) 622, 1-32

* This opinion is shared by all members of the Panel. All members of the Panel participated in (part of) the discussions on the subject referred to above.

* An interest was declared by a Panel member of participation in the FOCUS Soil Modelling Workgroup

and compound-specific differences in E_a. It is hence incorrect to assume that there is one median E_a value for all pesticides, which was the approach in the FOCUS report (1997).

The final choice of a Q_{10} value will depend upon the nature of the risk-assessment exercise, but such considerations are complex and outside the remit of this Opinion. Awaiting further review of the respective risk assessment frameworks, the standing EU practice with respect to using a Q_{10} default value in environmental exposure assessments is expected to continue. In this context, the Panel recommends that the median E_a value of 65.4 kJ mol^{-1} corresponding to a Q_{10} of 2.58 should replace the default E_a value of 54.0 kJ mol^{-1} corresponding to a Q_{10} of 2.2 (FOCUS default), which has been used until now. Compound-specific E_a values should be used instead of the default value in modelling or risk assessment when they are available and the criteria for deriving compound-specific E_a values given in the Opinion have been met.

Key words: pesticide degradation rate, temperature effect on degradation rate, soil, Q_{10}, activation energy, Arrhenius equation, modelling, extrapolation of degradation rates.

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BACKGROUND AS PROVIDED BY EFSA

An Opinion of the Scientific Panel on Plant Protection Products and their Residues (PPR Panel) relating to the default Q_{10} value used to describe the temperature effect on transformation rates of pesticides in soil was adopted by the PPR Panel on the 8th February 2006.

On 8th December 2006, the European Crop Protection Association (ECPA) sent a letter to EFSA challenging the Q_{10} value by providing additional information.

EFSA PPR decided to reconsider the issue as a substantial amount of additional information has emerged since the Opinion was adopted.

TERMS OF REFERENCE AS PROVIDED BY EFSA

The PPR Panel of EFSA was asked to provide an opinion on the default Q_{10} value taking the following into account:

The PPR panel is asked to consider whether the database, on which the proposed default of Q_{10} = 2.8 for temperature correction of DT_{50} values from soil degradation studies was based (in the EFSA Opinion adopted on 8th February 2006), still reflects the scientific state of the art, or should be updated in view of the additional data identified by ECPA and any other relevant data that have emerged since. In the light of this the PPR Panel is asked if it needs to revisit the original three questions in the adopted Opinion.

The PPR Panel has noted that the soil degradation studies are addressed in the Terms of Reference and has restricted its opinion to the soil compartment.

ACKNOWLEDGEMENTS

The European Food Safety Authority wishes to thank the members of the Working Group for the preparation of this Opinion: Damia Barcelo Culleres, Jos Boesten, Ettore Capri, Mark Montforts, Walter Steurbaut, the ad hoc experts Hans Toni Ratte, Sabine Beulke and Richard Bromilow and the EFSA staff members Mark Egsmose, Billy Amzal, Jane Richardson Christopher Lythgo, Jose Oriol Magrans, Laura Padovani and Cinzia Percivaldi.

ASSESSMENT

1. INTRODUCTION

The previous Opinion on Q_{10} (EFSA, 2006) dealt with the three following questions:

1) The PPR panel is asked to consider whether the database, on which the FOCUS default of $Q_{10} = 2.2$ for temperature correction of DT_{50} values from soil degradation studies is based (FOCUS 1997, report on Soil Persistence Models and EU Registration, 29.02.1997), still reflects the scientific state of the art or should be updated with more recent data obtained in the EU peer-review process and from other reliable sources.

2) The PPR panel is asked to give a recommendation under which circumstances it is considered appropriate to override the default Q_{10} by a compound-specific value based on measured data (paying special attention to criteria with respect to number of measurements and experimental conditions).

3) The PPR panel is asked on the range of temperatures that may be reasonably covered by the Q_{10} approach and to give opinion on procedures to be used when transformation rates need to be estimated outside this range (e.g. FOCUS groundwater modelling at very low temperatures (< 5ºC).

The FOCUS (1997) report contains the following approach to the Q_{10} value: "Models vary according to whether activation energy or a Q_{10} value is required as input. A distribution of activation energies and of Q_{10} values have been derived from extensive measurements. The average activation energy from this distribution is equivalent to a Q_{10} value of 2.2, which means that the DT_{50} at 20°C should be multiplied by 2.2 to give a best estimate of the DT_{50} at 10°C. From the distribution of Q_{10} values 90th and 95th percentiles have also been derived, which would lead to longer, worst-case DT_{50} estimates. Variations in measurements of the temperature-sensitivity of transformation rates for individual pesticides are as great as variations between pesticides, which indicates that little information would be added by measuring as opposed to estimating transformation rates at 10°C. Some debate still continues as to the suitability of these Q_{10} values for countries where average temperatures may be lower than 10°C but at present no solutions are available to the problem." The FOCUS report considered the following based on their data; "… the mean activation energy does not vary much from one compound to another which suggests that the overall variability may reflect errors in individual determinations."

From this discussion in the FOCUS Report (1997), it is understood that the distribution of activation energy values (E_a) was considered to reflect the variability around the same average E_a for every compound. The presentation of the average Q_{10} of 2.2 as a 'reasonable choice', of the 90th-percentile as a 'worst-case', and the statement that 'little information would be added by measuring transformation rates at 10°C' can therefore be understood. Given the convention to average compound properties (DT_{50}, K_{oc}) for exposure assessment purposes as proposed in FOCUS, the average value of a compound-specific Q_{10} would indeed be preferable. After all, if the distribution is representative of every compound, then experimental data will only confirm the evidence already available.

The PPR Opinion adopted on 8th February 2006 agreed with the assumption that a single default Q_{10} value for temperature correction of DT_{50} values from soil degradation studies is a reasonable choice for all compounds and recommended a value of $Q_{10} = 2.8$. Differences between one chemical class and the remaining compounds were identified, but the amount of data available was not sufficient to identify compound-specific values except for the phenylureas.

However, the scientific state of art has advanced since the previous Opinion. More data have become available from ECPA and elsewhere. It is now concluded by the PPR Panel that the database, on which the proposed default value for temperature correction of DT_{50} values from soil degradation studies was based (in the PPR Opinion adopted on 8th February 2006), should be updated in view of these developments. Therefore the Panel decided to revisit the three questions.

2. ASSESSMENT QUESTION 1

The first question refers to the quality of the dataset with respect to the scientific state-of-art. In order to evaluate the quality of the existing dataset, it is necessary first to consider the nature of the underlying theory of the Q_{10} and its purpose in exposure assessment. Then the available scientific evidence will be scrutinised and subjected to further analysis.

2.1. Introduction to activation energy

The rate of chemical reactions is temperature dependent. The Arrhenius relationship states that the reaction rate constant in homogeneous solutions and consequently the reaction half-life (assuming first-order kinetics DT_{50} = (ln 2)/k) depends on the activation energy E_a of the reaction and the temperature at which the reaction occurs. Although such conditions obviously are far away from the situation of pesticide degradation reactions taking place in the complex soil environment, the temperature dependence of the degradation rate coefficient of pesticides in soil is usually described by the Arrhenius relationship:

$$k = A \exp\left(-\frac{E_a}{RT}\right) \qquad \text{(Eqn 1)}$$

with

k = rate constant (day^{-1})

A = factor equal to the rate coefficient at infinite temperature (day^{-1})

E_a = activation energy (kJ mol^{-1})

R = gas constant (0.008314 kJ K^{-1} mol^{-1})

T = absolute temperature (K)

Datasets available in the literature consist of pairs of DT_{50}–T values. These pairs can be used to calculate E_a values from Eqn 1. The fitting procedure was as follows. Firstly, DT_{50} values were converted into k values using ln 2 / DT_{50}. Then Eqn 1 was rewritten as

$$\ln k = \ln A - \frac{E_a}{RT} \qquad \text{(Eqn 2)}$$

Subsequently linear regression was applied using ln k as the dependent variable and 1/T as the independent variable. The slope of the linear regression line multiplied by R is the E_a for the dataset.

Based on first-order kinetics, Equation 1 can be reformulated to

$$DT_{50T1} = DT_{50T2} \ \exp\left(\frac{E_a}{R}\left[\frac{1}{T_1} - \frac{1}{T_2}\right]\right) \qquad \text{(Eqn 3)}$$

where DT_{50T1} and DT_{50T2} are the half-lives at temperatures T_1 and T_2, respectively.

Temperature dependence of degradation can also be described with the Q_{10} approach. Q_{10} is defined as the ratio of pesticide degradation rate coefficients (k_2/k_1) at a temperature T_1 that is 10°C lower than a temperature T_2. This Q_{10} approach implies the following temperature relationship between the half-lives:

$$DT_{50T1} = DT_{50T2} \ Q_{10}^{\frac{T_2 - T_1}{\Delta T}} \qquad \text{(Eqn 4)}$$

where ΔT is equal to 10^oC (i.e. 10 K).

Equation 4 can be rewritten as:

$$DT_{50T1} = DT_{50T2} \ \exp\left(\ln Q_{10}^{\frac{T_2 - T_1}{\Delta T}}\right) \qquad \text{(Eqn 5)}$$

Combining Eqns 3 and 5 leads to the following relationship between Q_{10} and E_a:

$$Q_{10} = \exp\left(\frac{\Delta T \, E_a}{R T_1 T_2}\right) \qquad \text{(Eqn 6)}$$

Eqn 6 shows that there is no unique relationship between Q_{10} and E_a: this is the consequence of the different definitions of these quantities in Eqns 3 and 4. The PPR Panel has used the Arrhenius equation to analyse the data and for all subsequent statistical analyses. Only at the end of these procedures are E_a values converted into Q_{10} values for the convenience of the reader. Thus the Panel had to make a more or less arbitrary choice for the two temperatures in Eqn 6. It was decided to set T_1 at 10^o and T_2 at 20^oC because 20^oC is the reference temperature for measuring degradation rates and because extrapolation to lower temperatures is more important than extrapolation to higher temperatures. Using these values Eqn 6 can be rewritten as:

$$Q_{10} = \exp\left(\frac{E_a}{F}\right) \qquad \text{(Eqn 7)}$$

where

$$F = \frac{R T_1 T_2}{\Delta T_2} \qquad \text{(Eqn 7b)}$$

with a value of the factor F 69.01 kJ mol^{-1} based on the above reasoning.

For example, Eqn 7 gives a Q_{10} value of 2.19 for an E_a of 54.0 kJ mol^{-1}.

In trying to assess a default Q_{10} value for pesticides, it is necessary to consider the likely variation of activation energy (E_a) both across pesticides and for individual pesticides in different soils and environments. Considering first the variation of E_a values amongst different pesticides, on theoretical grounds it is likely that there will be a spread of E_a values and that such values can be considered compound specific. For example, biotic reactions have differing E_a values, and some pesticides, at least in part, will be degraded or transformed in soil by such processes. There is no reason to suppose that the many different biotic processes operating on pesticides in soil will not also be influenced differently by changes in temperature.

Given the very limited data sets underlying the Q_{10}, in the previous Opinion the PPR Panel tried to investigate possible commonality of, or dissimilarity between, E_a values in groups of compounds related by pesticide class. This research indicated that the phenylurea herbicides (isoproturon, linuron) had E_a values substantially lower than the average for the whole data set. It should be noted that other classes of pesticides, sharing similar functionality and mode of action, may well not display similar E_a values for individual compounds if their breakdown in soil proceeds by different processes. An example of such a class would be the sulfonylurea herbicides, in which different breakdown pathways can operate for the individual compounds. Furthermore these breakdown mechanisms may be both biotic and abiotic and the importance of the latter is usually dependent on soil pH.

2.2. Data collection and cleaning

2.2.1. Data sources

The following databases were evaluated for quality:

- The database of the previous PPR Panel Opinion (EFSA 2006)
- The database of the ECPA study (Wang & Winn, 2006)
- Extra publications from a new search of the open literature
- Data available from the dossiers for plant protection products for inclusion in Annex 1 of Directive 91/414/EEC available to the EFSA PRAPeR team.

The literature search was done in external databases available to EFSA in the period from the 8th February till the 1st March 2007. The search was performed using the following search criteria:

pesticide AND soil AND temperature AND (degradation OR transformation)

The full criteria for the search are given in Appendix 7. The complete list of referenced studies selected and reviewed in this Opinion is given in Appendix 1.

2.2.2. Quality criteria for data selection

Stringent quality-control procedures were applied to each study in the database, and the criteria for rejecting studies from further consideration can be summarised as follows:

- The criteria for data elimination can be summarised as follows:
  - soil factors:
    - soils were extensively dried or stored for more than 1 day in dry conditions
    - storage of soils at room temperature for more than 30 days
    - storage of soils at 4°C for more than 3 months
    - storage of soils at -20°C for more than 13 months
    - ratio between moisture contents at the different temperatures was outside the range of 0.95 to 1.05
    - soil moisture content < 5% g g^{-1}
    - soil sample taken at different times in the field for the same study
  - test system
    - different initial concentrations
    - non-chemical analytical method
    - absence of solvent (volume) information or application of >20 ml kg^{-1} soil

- temperature > 30°C
- evaluation
  - non-SFO DT_{50} values, as they are not compatible with the Arrhenius equation.
  - the square of the correlation coefficient of the first-order (SFO)-regression (r^2) is < 0.80
  - if, by visual inspection using expert judgement, the plot of time *vs* residues of the original data seemed implausible compared to the regression line. In particular the first part until the DT_{50} is reached is relevant.
  - less than five measuring points for DT_{50} calculation.
  - DT_{50} values shorter than 1 d (because these are considered less accurate)
  - study duration and choice of the measurement points inappropriate for the DT_{50} range
  - DT_{50} values greater than twice the study duration
  - more than one E_a value per pesticide-soil combination. Selection of only one E_a value is allowed per pesticide-soil combination; the choice was based on expert judgment taking into account amongst others the moisture content (preference for Maximum Water Holding Capacity (MWHC) below 80%)
  - studies with soil samples taken at different times in the field
  - compounds with vapour pressures $>10^{-4}$ Pa were accepted only if closed systems had been applied in order to account for volatilisation

The complete database (Appendix 1) was screened accordingly and. was also checked for possibly repeated entries from different publications. The resulting dataset was then critically reviewed by the experts and checked for possible anomalies which could influence their validity and give rise to rejection. In those cases remarks are given in the comment column of Appendix 3, giving an overview of the rejected data: the comprehensive appraisal of all datasets is available on a separate EXCEL spreadsheet on the EFSA website[2]. The final database, comprising 99 datasets corresponding to 53 pesticides (Appendix 2), is the object of the statistical analysis in this Opinion.

2.3. Analysis of data

Variations of E_a across compounds and for individual compounds, as well as evidence for compound-specific E_a values, will now be considered.

2.3.1. Calculation of E_a values

Linear regression analysis according to Equation 2 was applied to all datasets in the final database (Appendix 2), using ln k as the dependent variable and $1/T$ as the independent variable. Examples are given in Figure 8 on page 27; the slope of the linear regression line multiplied by R is the E_a for the dataset. The graphs with all individual fits are provided in Appendix 5.

2.3.2. Testing of hypotheses

From this point, the final dataset given in Appendix 2 was used for all analyses and conclusions. A number of different hypotheses were investigated with this dataset.

[2] http://www.efsa.europa.eu/EFSA/ScientificOpinionPublicationReport/efsa_locale-1178620753812_ScientificOpinions.htm

First, the final dataset of E_a values was checked for lognormality (such transformations in this Opinion are all based on natural logarithms (ln)). This analysis tests the assumption that E_a values of chemicals have a definitive distribution, and that the available dataset is consistent with this distribution (here we test for normal or lognormal distributions). If a certain distribution is statistically acceptable, this gives confidence in the possible range of E_a values that can be expected to exist for those chemicals that are assumed to be represented by the distribution.

The null hypothesis was defined as follows: the distribution of E_a values in the final dataset describes the distribution of E_a values of *every* chemical. In other words, every chemical, when tested repeatedly, will show the same median E_a and distribution as the final dataset of available E_a values of all chemicals (in Section 2.1 it is argued that the opposite is more likely to be true: the logic relation defined here is that if the distribution does not represent *every* chemical then the distribution does *not* describe every chemical). In order to test this hypothesis, the final dataset is assessed in more detail in the sections below. The outcome of this testing has implications for the choice of representative compound-specific E_a values and for the choice of default E_a values.

If any of the assumptions that follow from the null hypothesis are rejected in the sections below, then the assumption that the distribution of E_a values applies to every chemical is rejected. In this case, it cannot be assumed that every chemical will have the same median E_a and the same distribution. The alternative hypothesis is that there is more than one distribution. The distribution from the final database is now seen as the distribution of compound-specific E_a values. The distribution provides an estimate of the *likelihood* that an E_a value will be applicable to a particular chemical. For example: there would be a 50% likelihood that the E_a value of a particular compound is above the median value of the final dataset (the reader is referred to the glossary for exact definitions of median and mean). If E_a values for a specific compound were to be measured there is a 50% chance that they converge to a median value which is higher than the median of half of all compounds.

2.3.3. Description of datasets

In this section, descriptive summary statistics and histograms of E_a values are displayed. The updated final dataset comprised 99 entries and, where possible, compounds were assigned to chemical families based on conventional considerations of structural features (e.g. chemical structure and dominant first transformation step) (Appendix 2). Only families with more than 10 entries were considered appropriate for investigation and comparison. Hence, this dataset does not allow full comparison of all chemical families therein with the final dataset. Finally, a distinction was made between E_a values derived from DT_{50} values at only two different temperatures in the Arrhenius fit, and those derived with more than two data points.

In summary, the subsets of data investigated are:

- Where Arrhenius fits could be done with only two points
- Where Arrhenius fits could be done with more than two points
- Chloroacetamides only
- All data except Chloroacetamides
- Phenylureas only
- All data except Phenylureas
- Triazines only
- All data except Triazines

- All data except Phenylureas, Chloroacetamides and Triazines

Normal and lognormal distributions were fitted to all data and the various subsets. It should be noted that all data were treated here as independent values. The corresponding descriptive statistics are reported in Table 1.

Table 1. Normal and lognormal distribution analysis of E_a values (kJ mol^{-1})derived from the final dataset. n = number of datapoints; # = number of compounds

			Normal distribution					Lognormal distribution				
dataset	n	#	Mean	Std	Max	Median	Min	Mean (ln E_a)	Std (ln E_a)	Median	Mean (E_a)	Median (E_a)
all data	99	53	65.3	21.1	135	61.8	19.2	4.13	0.32	4.13	65.4	62.0
Fits with two points only	42		67.5	22.4	121	62.0	19.2	4.16	0.34	4.13	67.9	64.0
Fits with more than two point	57		63.6	20.2	134	61.8	32.6	4.11	0.31	4.12	63.6	60.6
All data except Chloroacetamides	81		65.6	23.0	134	61.5	19.2	4.12	0.35	4.12	65.7	61.8
Chloroacetamides only	18	5	63.9	9.70	80.7	63.2	46.5	4.15	0.15	4.15	64.0	63.2
All data except Phenylureas	86		68.0	21.2	134	65.1	19.2	4.17	0.32	4.18	68.2	64.8
Phenylureas only	13	3	47.4	8.92	65.6	45.3	33.1	3.84	0.18	3.81	47.4	46.6
All data except Triazines	88		66.1	20.7	134	62.4	19.2	4.14	0.31	4.13	66.2	63.0
Triazines only	11	4	58.9	24.3	113	51.8	32.6	4.00	0.40	3.95	59.3	54.8
All data except Phenylureas, Chloroacetamides and Triazines	57		71.0	22.7	134	66.5	19.2	4.21	0.34	4.20	71.3	67.4

The final dataset of E_a values and the subsets were first checked for lognormality (Section 2.3.4.). Then the final dataset was checked for outliers (Section 2.3.5). From the final dataset, sub-groups of compounds were selected and these were tested against the null-hypothesis. In Section 2.3.7. several variables are subjected to significance testing. In Section 2.3.8 the variability within and between compounds is analysed. In the final Section (2.3.9) theoretical distributions of compound-specific E_a values are derived.

2.3.4. Normality *vs*. Lognormality of datasets

The final dataset of E_a values and the subsets were first checked for lognormality. Histograms of linear-scaled and log-scaled data are plotted in Figure 1.

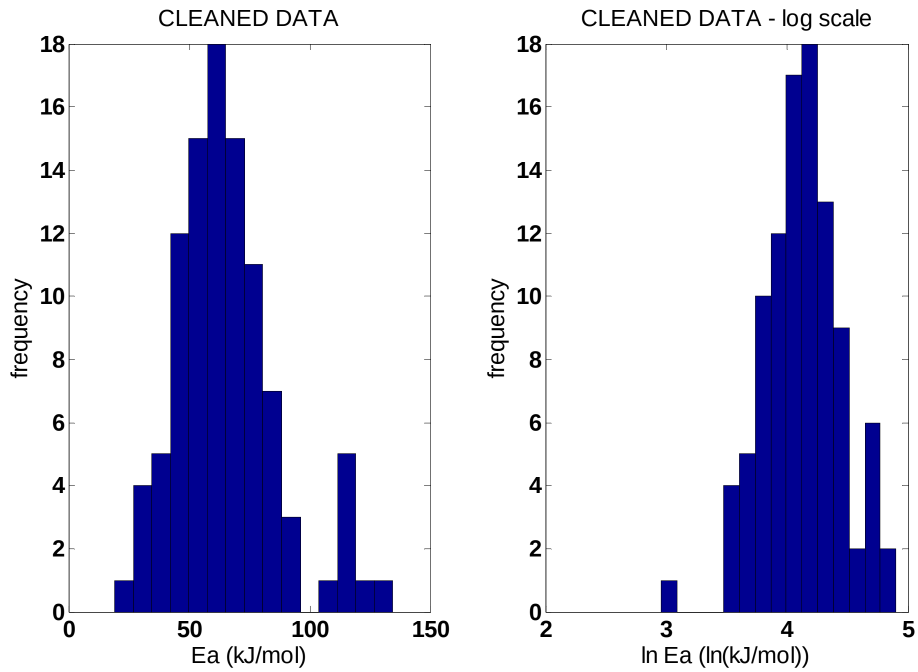


Figure 1. Histograms of the linear- and log-scaled individual values of E_a for the final dataset.

All linear- and log-scaled data were each compared to the Gaussian distribution, comparing their Cumulative Distribution Function (CDF) (Figure 2)

Cumulative Distribution Functions are generated by sorting the E_a values from the final dataset in ascending order. The cumulative frequency of each datapoint (*i.e*. the fraction of datapoints below the given value) is then plotted against the E_a value. This empirical CDF is then compared with the theoretical (Gaussian or lognormal) CDF.

Another method to compare distribution is via QQ plots (Figure 3), these being plots of the quantiles of E_a or ln E_a values in the final database (Y-axis) against the quantiles of the assumed normal distribution (X-axis). A 45-degree reference line is also plotted. If the observed and predicted sets of quantiles come from a population with the same distribution, the points should fall approximately along this reference line. The greater the departure from this reference line, the greater the evidence for the conclusion that the observed quantiles have come from a population with a different distribution (i.e. the data are not well described by the statistical distribution being tested).

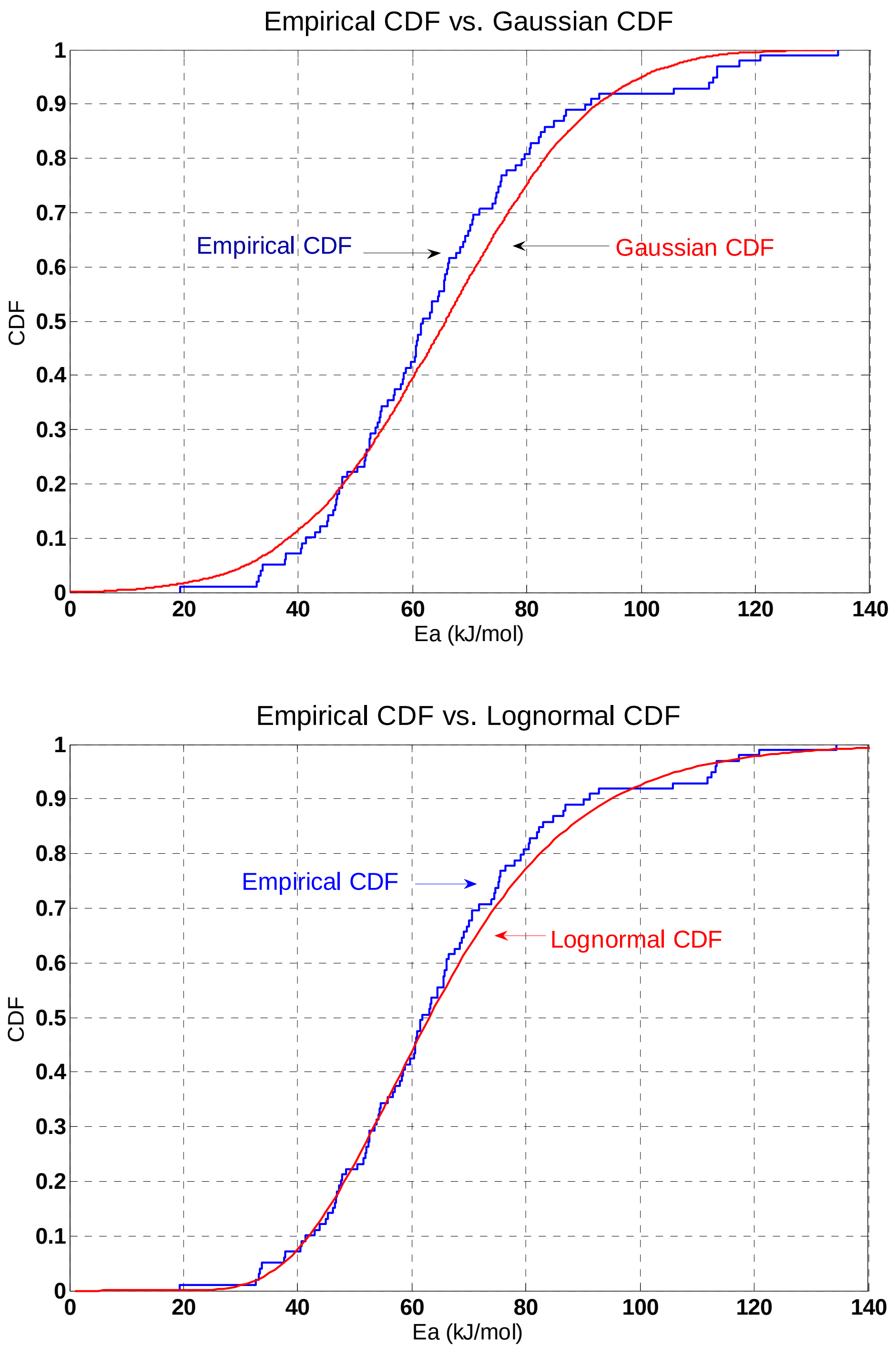


Figure 2. Cumulative Distribution Function of the linear- and log-scaled individual values of E_a for the final dataset

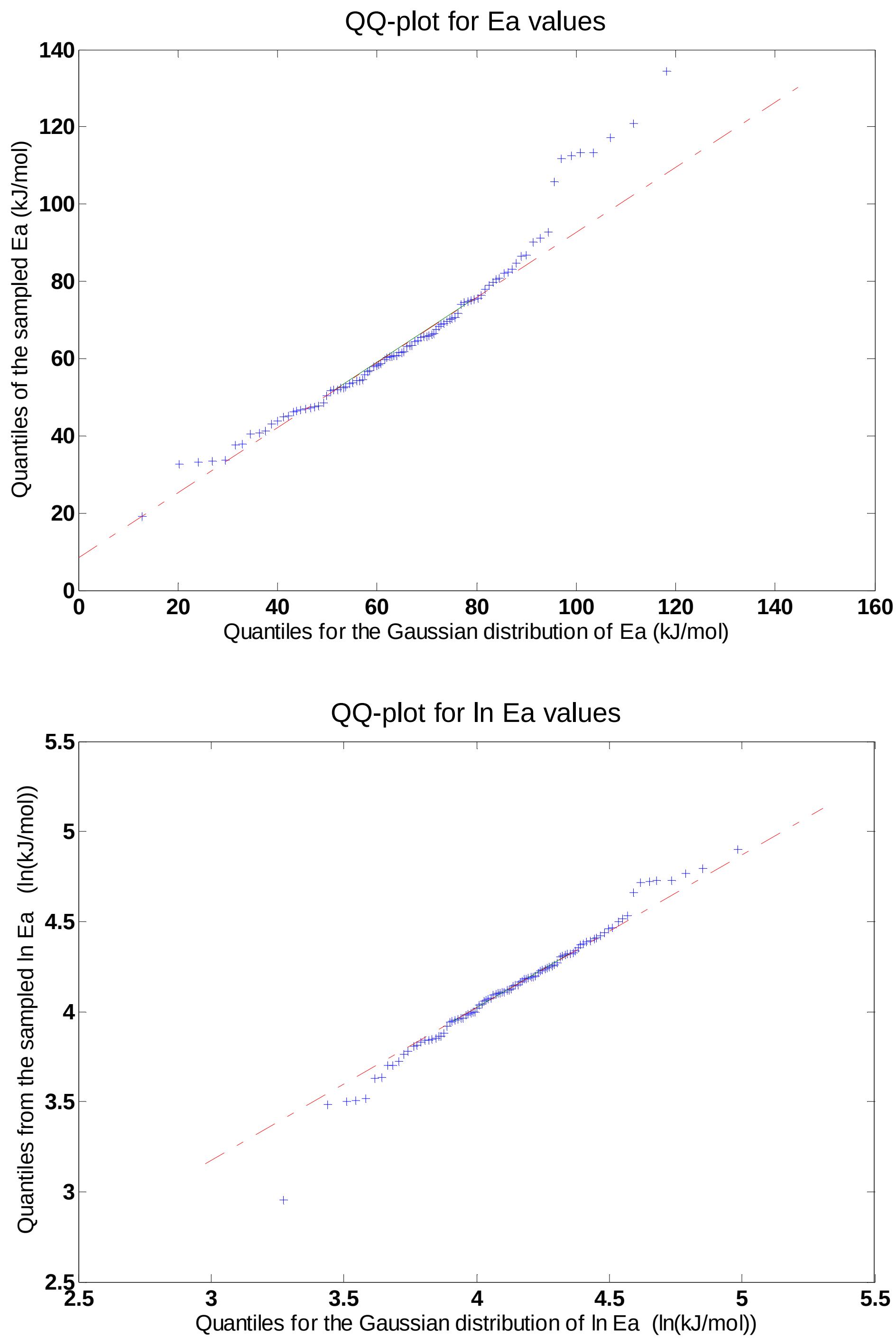


Figure 3. QQ plots of the linear- and log-scaled individual E_a values of the final dataset

For both distributions (normal and lognormal), deviation from normality mainly occur for extreme quantiles (below 5% and above 90%), especially for higher quantiles in the normal scale and for lower ones in the log-scale.

A Gaussian (normal) distribution tended to heavily underestimate higher quantiles for the data, whereas a log-normal one overestimated lower ones. The deviation from normality is considerably smaller for log-transformed data. In order to decide what type of distribution can be assumed for the data, p-values were derived using the Shapiro-Wilk's test. Normality assumptions should be rejected if the p-value for fit is <0.05 (Table 2).

Table 2. p-Values for the fit of the final dataset based on individual data, with a normal or lognormal distribution.

Dataset	n	#	p-Value (normal)	p-Value (lognormal)
All data	99	53	0.0005	0.1878
Fits with two points only	42		0.0013	0.0032
Fits with more than two point	57		0.0060	0.5301
All data except Chloroacetamides	81		0.0026	0.4937
Chloroacetamides only	18	5	0.5587	0.7758
All data except Phenylureas	86		0.0020	0.0218
Phenylureas only	13	3	0.4603	0.8371
All data except Triazines	88		0.0005	0.0683
Triazines only	11	4	0.1901	0.5952
All data except Phenylureas, Chloroacetamides and Triazines	57		0.0270	0.0223

As demonstrated in Table 2, normality for the final dataset can now be assumed only for the log scale. For the subsets the fit for the lognormal distribution appears to be better than for the normal distribution. As a consequence, from this point, all analyses were performed on the log-scale (log-normally transformed data), i.e. assuming lognormality of data.

2.3.5. Check for outliers

Given the lognormality of the data, Grubb's test for outliers was performed, using Matlab (Release 14). For a significance level of 5%, one outlier was found having ln E_a~3 (Table 1, see also the lognormal distribution of Fig. 1).

Table 3. Outlier based on Grubb's test, based on individual E_a values from the final dataset

Code	Source	Compound	Chemical family	Soil	E_a(kJ mol^{-1})	Ln(E_a)
TCWS21	WS2	ethofumesate	benzofuran	Ahlum 1	19.24	2.96

This value was disregarded as a statistical outlier (it should be noted that there are two other values for ethofumesate in the final dataset).

2.3.6. Comparison between subgroups

Each of the sub-sets of data introduced in Section 2.3.2 was then statistically compared with the complementary sub-set (phenylureas versus non-phenylureas, etc.).

The adopted approach for the subgroup comparisons was as follow. First normality and homogeneity of variance were verified for each subgroup of data. Normality was tested using the Shapiro-Wilk test whereas homogeneity of variance was determined using the Levene test. Where normality and homogeneity of variance were acceptable, a t-Test was performed to compare group means. In the other cases, the comparisons were performed using a non-parametric test (Mann-Whitney, as well as Kolmogorov-Smirnov and Cramer-Von Mises, tests similarity of distribution; results of the last two tests are not reported here but they were consistent with results obtained using the Mann-Whitney test).

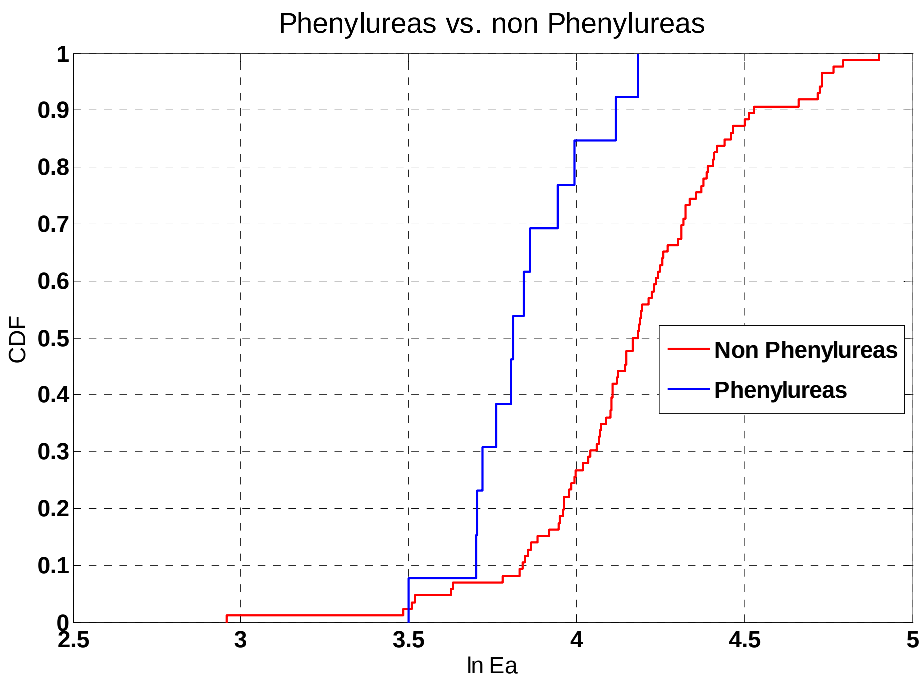


Figure 4. Comparison of the log-scaled individual E_a values (kJ mol^{-1}) for phenylureas versus non-phenylureas.

The hypothesis tested here was that Phenylureas and non-Phenylureas, and Chloroacetamides and non-Chloroacetamides, and Triazines and non-Triazines, are from the same distribution (i.e. the mean and standard deviation of the two distributions are not statistically different). All comparison tests as well as plots of empirical CDFs are presented (Appendix 4). The only case where both the group means and the standard deviation differed significantly was the comparison Phenylureas *vs*. non-Phenylureas (Figure 4).

Table 4 gives the statistical information. p-Values for similarity of the distributions are given for the non-parametric tests according to Mann-Whitney (M-W) and Kolmogorov-Smirnov (K). Assumptions of similarity assumptions should be rejected if $p<0.05$. (Table 4).

Table 4. Lognormal distribution analysis of the E_a values (kJ mol^{-1}) for the Phenylureas and non-Phenylureas in the final dataset.

	Median ln E_a	Std	p-Value (M-W)	p-Value (K)
Phenylureas	3.84	0.184	<0.001	0.004
Non-Phenylureas	4.17	0.319		

Additional plots such as histograms and QQ plots for Phenylureas and non-Phenylureas are provided in Appendix 4.

Mindful of the very limited dataset, an analysis of the current dataset showed that isoproturon (eight studies) had a low median E_a of 46.1 kJ mol^{-1} relative to the dataset median; furthermore, the E_a values for chlorotoluron (three studies) and linuron (two studies) fell within the distribution of values for isoproturon. These findings provide circumstantial evidence that this group of compounds, having closely related structures and known to undergo similar breakdown processes in soils, does indeed have similar E_a values.

The only other class of pesticides where sufficient data (>3 studies) were available to enable a similar evaluation were the Chloroacetamide and Triazine herbicides. For the Chloroacetamide, the median E_a was similar to the overall median of the remaining dataset, but the variability was much less as indicated by the low standard deviation (Table 5 and Appendix 4).

Table 5. Lognormal distribution analysis of the E_a values (kJ mol^{-1}) for the Chloroacetamide and non-Chloroacetamides in the final dataset.

	Median ln E_a	Std	p-Value (M-W)	p-Value (K)
Chloroacetamides	4.15	0.152	0.78	0.033
Non-Chloroacetamides	4.12	0.351		

For the triazines, both the median E_a and the standard deviation were similar to those of the remaining dataset (Table 6 and Appendix 4).

Table 6. Lognormal distribution analysis of the E_a values (kJ mol^{-1}) for the Triazine and non-Triazines in the final dataset.

	mean	std	T-test	Levene Test
Triazines	4.00	0.396	**0.18**	**0.43**
Non-Triazines	4.14	0.313		

For the Triazines, both the median E_a *and the standard deviation were* similar to those of the remaining dataset.

The hypothesis that Phenylureas and non-Phenylureas, and Chloroacetamides and non-Chloroacetamides, are from the same distribution is considered rejected. Hence, the hypothesis that the distribution of the final dataset is a description of the variability in E_a values for every chemical is rejected.

2.3.7. Test for significant effects of variables

The purpose of this section is to investigate possible statistically significant effects of relevant variables in the final dataset. The variables investigated were: Reference code, Compound, Name of soil and Mean temperature. The last was defined as the average of the temperatures used for the evaluation of the corresponding E_a value. The reference code is the identifier given to each publication (Appendix 1); one publication may have reported on several chemicals or the same chemical in different soils.

Based on the findings from Sections 2.3.3 and 2.3.4, the analysis was performed assuming lognormality of the data, after having removed the identified outlier. The dataset then comprised 98 different entries, corresponding to 48 different Reference Codes, 53 different compound names and 68 different soils.

The number of different soils was too high to allow any robust three-way or four-way analysis: either ANOVA's assumptions were severely not met, or the data could not provide enough evidence to use mixed-effect modelling (convergence criteria not met, non-trustable results) except for one model reported hereafter.

As an alternative first step, a 1-way ANOVA was performed for each factor separately. However such an approach is less robust (more sensitive to deviations from necessary assumptions for ANOVA) and has less power than multi-way approaches as it favours confounding-factor issues. These ANOVA were performed using SAS PROC GLM for unbalanced designs on the log-scaled data (Table 5). Both the 'Name of compound' and the 'Reference code' were highly significant, whereas the 'Soil' variable was less, but still significant. There was no statistical evidence ($p>0.05$) for any temperature effect.

Table 7. One-way ANOVAs to test the significance of the effects of variables.

Factor	p-Value (1-way ANOVA)
Compound	0.0009
Reference Code	<0.0001
Name of soil	0.0176
Mean temperature	0.15

Additionally, assuming now a random effect of the "Compound" variable, it was possible to test the effect the 'Reference code' and the 'Soil' separately from each other, but jointly with the mean temperature. This can be done using a mixed-effect model using data on the logarithmic scale with a random effect on the compound. Such an approach attempts to disentangle the name effect from other effects. Models were fitted with SAS using PROC MIXED. More details are given in Appendix 4.

Table 8. Mixed-effect modelling to test the significance of the effects of Reference code and Mean temperature variables (first test), and of Name of soil and Mean temperature (second test). Effects are considered significant for p<0.05.

First test			Second test	
Factor	p-Value		Factor	p-Value
Reference Code	0.01		Name of Soil	0.40
Mean temperature	0.86		Mean temperature	0.60

Table 6 shows that the mixed-effect model approach confirms the significance of the Reference code effect, but does not confirm the effect of the Name of soil . In conclusion, the data did not show any robust evidence of either a Temperature effect or an effect of the Name of soil.

Again, the hypothesis that the distribution is applicable to *every* chemical is considered rejected, since the distribution is strongly driven by chemical name. On the other hand, the Reference code effect remains significant when the compound effect is accounted for. Hence, the lognormal distribution of the final dataset is explained by both chemical identity and Reference code. However, confounding effects between the investigated factors are very likely as they are highly correlated (see Appendix 4 for an analysis of their association). In order to further characterise a compound/name effect, the inter- and intra-compound variability were evaluated and compared.

2.3.8. Inter- *vs.* intra-compound variability

Inter- and intra-compound variabilities were evaluated to characterise any compound-dependent effect on the distribution. This was achieved by fitting a simple linear random-effect model (using PROC MIXED in SAS), based on the log-transformed data with the outlier removed, to estimate variance (Table 9). Such a model describes the variability shown in the data as the sum (on the log-scale) of the intra- and inter-compound variances, now separated.

Table 9. Variance estimates of compound-specific E_a values, based on individual values in the final dataset and a random-effect model.

	Coefficient of Variation
Inter-compound variability	22%
Intra-compound variability	22%

The Coefficient of Variation (CV) is expressed relative to the value of the associated median. It is defined as the ratio of the standard deviation of E_a values by the mean E_a. See also Table 10 for the standard deviations (Std) and CVs of individual compounds. The considerable intra-compound variability may bias the distribution of the compound-specific E_a values in the final dataset. Such intra-compound variability confounds all unbalanced factors (e.g. Name of soil, Reference) and may therefore be biased. The random-effect model accounts for unbalanced numbers of compound replications (on normal-scaled data).

The E_a values for each replicated (n>1) compound in the final dataset, based on individual data, were calculated (Table 10). Note that the geometric mean (denoted as Geomean) gives a robust estimate of the median E_a and can be defined as:

$$\text{Geomean}(E_a) = \exp[\text{Mean}(\ln E_a)] \qquad \text{(Eqn 8)}$$

Moreover, CVs and standard deviations of ln E_a are linked according to the formula:

$$Std(\ln E_a) = \sqrt{(\ln\ (1 + CV^2))} \approx CV \qquad \text{(Eqn 9)}$$

Since numerical values of CV are markedly less than 1, CVs and Std(ln E_a) are expected to be close to each other. This is indeed the case as shown in Table 10. So the CVs are good approximations of the standard deviations (Std) in the log-transformed domain.

The intra-compound variability will be accounted for in the following analysis of the distribution of the compound-specific E_a values. The influence of variables will not be accounted for.

Table 10. E_a values (kJ mol^{-1}) for each replicated (n>1) compound in the final dataset, based on individual data.

Name	n	Mean (ln E_a)	Std (ln E_a)		Mean (E_a)	Std (E_a)		Geomean (E_a)	CV
isoproturon	8	3.83	0.15		46.8	8.03		46.1	15%
propyzamide	7	4.23	0.25		70.8	19.9		68.7	25%
alachlor	6	4.29	0.13		73.2	9.1		73.0	13%
atrazine	6	3.82	0.25		47.1	12.6		45.6	26%
metazachlor	6	4.15	0.05		63.4	3.10		63.4	5%
ethoprophos	4	4.30	0.10		74.0	7.20		73.7	10%
bentazon	3	4.18	0.62		73.8	40.0		65.4	69%
chlorotoluron	3	3.87	0.33		49.6	14.7		47.9	34%
metolachlor	3	3.95	0.11		52.3	5.98		51.9	11%
chloridazon	2	4.04	0.11		57.0	6.35		56.8	11%
ethofumesate	2	3.97	0.13		53.4	6.86		53.0	13%
linuron	2	3.83	0.16		46.4	7.24		46.1	16%
mesosulfuron-methyl	2	4.30	0.10		73.9	7.28		73.7	10%
metamitron	2	3.98	0.17		54.0	8.89		53.5	17%
metribuzin	2	4.05	0.08		57.5	4.32		57.4	8%
simazine	2	4.32	0.10		75.1	7.70		75.2	10%
triadimefon	2	4.39	0.07		80.6	5.90		80.6	7%

2.3.9. Distribution of the compound-specific E_a values

In view of the results of the analysis above, it was considered justified to perform an analysis of the final dataset based on the alternative assumption that a compound-specific E_a value exists. A distribution of compound medians and other percentiles needs to be derived. This could be achieved simply by averaging the ln E_a values for each individual compound and fitting a distribution to the means. This analysis is presented in Appendix 4. The drawback of this method is that differences in the variance and the number of E_a values between compounds are not accounted for. An alternative method was used here. The optimal distribution of the E_a compound quantiles can be derived using a random-effect model to describe the data. This was performed under the lognormal assumptions using SAS PROC MIXED (Figure 5). The use of lognormal assumptions implies that the averaging for each compound is performed on the log-scale. Conversion back to the normal E_a scale allows derivation of the distribution of inter- and intra-compound E_a medians (or geometric means).

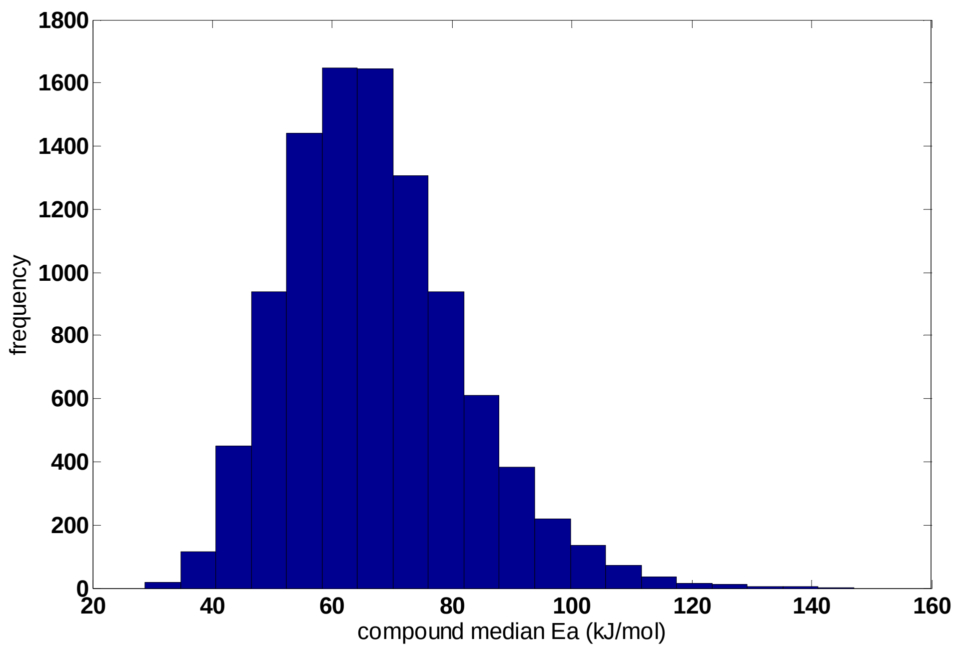


Figure 5. Theoretical distribution of the compound-specific 50-percentile E_a values based on the final dataset and fitted to a random-effect model (10,000 simulations).

The corresponding percentiles belonging to this lognormal distribution of medians are reported in Table 11.

This output can be interpreted as follows: It is assumed that the E_a values for each compound are lognormally distributed with a median and standard deviation. The median E_a value of the distribution for a new compound will be 65.35 kJ mol^{-1} or less in 50% of the cases. In 10% of the cases, the median E_a value of a new compound will be greater than 86.23 kJ mol^{-1}. The probability that a new compound will have a median E_a of 54.48 kJ mol^{-1} or less is 20%.

In order to illustrate inter-compound variability of various other quantiles (percentiles) of the E_a distributions per compound, the inter-compound theoretical distributions of the 10%-, 25%-, 75% and 90%-percentiles are plotted in Figure 6.

Table 11. Percentiles of the distribution of the compound median E_a values based on a mixed-effect model and the final dataset.

Percentile	E_a (kJ mol^{-1})
0.05	45.79
0.1	49.53
0.15	52.23
0.2	54.48
0.25	56.48
0.3	58.34
0.35	60.13
0.4	61.87
0.45	63.60
0.5	65.35
Table continued	
Percentile	**E_a (kJ mol^{-1})**
0.55	67.15
0.6	69.03
0.65	71.03
0.7	73.20
0.75	75.62
0.8	78.40
0.85	81.78
0.9	86.23
0.95	93.29

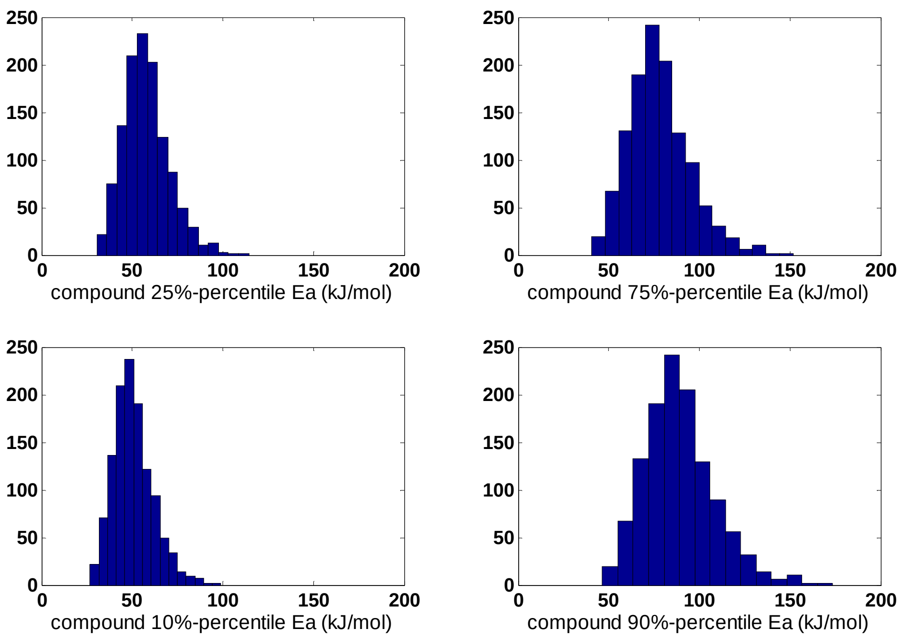


Figure 6. Theoretical distributions of the compound-specific 10-, 25-, 75- and 90-percentile E_a values based on the final dataset and fitted to a random-effect model (1200 simulations).

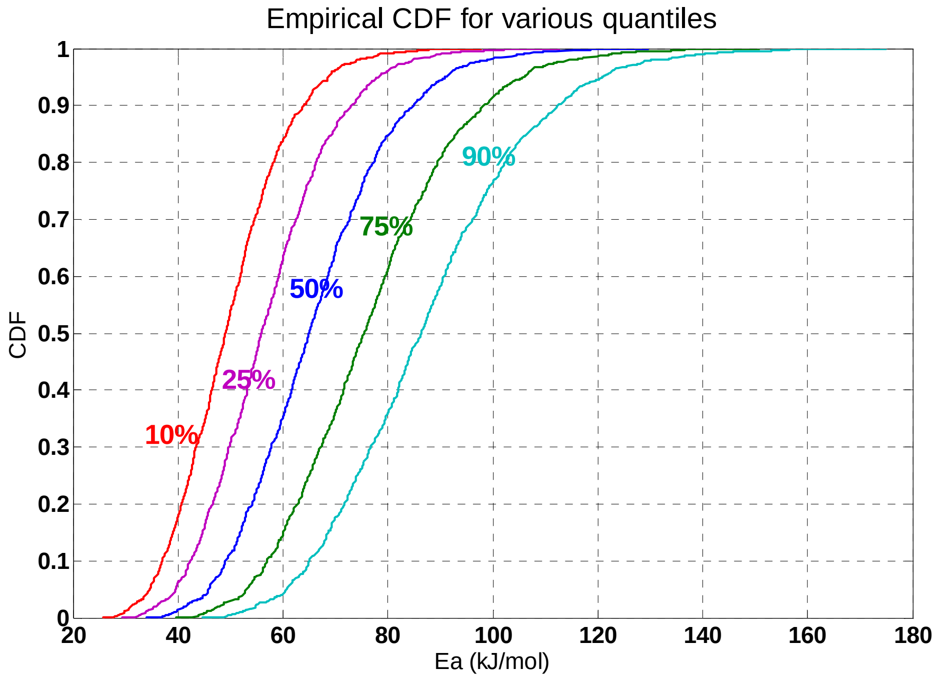


Figure 7. Cumulative Distribution Functions of the compound-specific 10-, 25-, 50,- 75- and 90-percentile E_a values based on the final dataset and fitted to a random-effect model (10,000 simulations for the 50-percentile and 1200 simulations each for the other percentiles).

Figures 6 and 7 provide information on the distribution of the compound E_a values taken from the lower and higher ends (i.e. 10- and 90-percentiles) of their own distributions. Depending on the purpose of the modelling, these distributions can be of help in choosing the most relevant value from a known dataset of compound-specific values.

2.4. Assessment and Recommendations for Question 1

The PPR Panel is of the opinion that the database, on which the proposed default of $Q_{10} = 2.8$ for temperature correction of DT_{50} values from soil degradation studies was based (in the EFSA Opinion adopted on 8th February 2006), no longer reflects the scientific state of the art. More data have become available.

The assessment presented in Section 2.3 leads to several conclusions. First of all, in the final dataset, normality of data can only be assumed for log-transformed data. One outlier was detected at the 5% level for the log-transformed data, and this was then discarded. The effects of Reference code and Compound on the distribution of E_a values were significant. The effects of Reference, Compound and Name of Soil were strongly associated. The analysis further showed that the chemicals did not fall within the same overall distribution, leading to the subsequent conclusion that there is more than one distribution. Thus it can neither be assumed that every chemical will have the same median E_a value nor the same distribution of E_a values.

Table 12. Theoretical estimates of compound-specific E_a values (kJ mol^{-1}) at three percentiles based on the final dataset and fitted to a random-effect model (derived from Figure 7).

Percentile curves from Figure 7	E_a value corresponding to CDF fraction		
	0.10	0.50	0.90
10%	35	50	65
25%	45	55	70
50%	50	65	85
75%	55	75	100
90%	65	85	110

The E_a values of the compounds in our final data-set are lognormally distributed. Examples of E_a values estimated for selected percentiles of different distributions are given in Table 10, which shows that a measured E_a value will usually be between 35 and 110 kJ mol^{-1}.

The data analysis indicated that based on a lognormal distribution of the E_a values for a given chemical there is a 90-percent probability that the median value is within the range 45.8-93.3 kJ mol^{-1}.

3. ASSESSMENT QUESTION 2 (COMPOUND-SPECIFIC Q_{10} VALUES)

3.1. Introduction

The PPR panel is asked to give a recommendation under which circumstances it is considered appropriate to override the default Q_{10} by a compound-specific value based on measured data (paying special attention to criteria with respect to number of measurements and experimental conditions).

Statistical comparison with the final dataset is not required to demonstrate the need or the acceptability of a specific E_a value for a new compound. It is not logical to require statistically significant deviations from the default E_a value, the reason being that the median and distribution of (average) E_a values of all chemicals is irrelevant to the median and distribution of E_a values within one chemical, as concluded in the previous section.

The statistical analysis of the whole database (98 accepted studies) indicates that the compound name is a significant factor influencing the E_a value. However, the difficulty in trying to identify or assign compound-specific E_a values is that the data set of 99 studies for 53 compounds is too limited for conclusive statistical analysis of this type. This has implications for the number of data sets required to set a compound-specific E_a value.

3.2. Criteria for compound-specific E_a values

The PPR Panel recommends a requirement for at least four reliable studies performed in accordance with the test conditions as specified in Section 2.2.2. The soils used in these four studies should be different, preferably reflect likely use patterns and show reasonable differences in pH, percentage of organic material, and clay content.

The tests should be performed with at least three temperatures within the range of 0° to 30°C. The selection of the temperature range should be considered particularly carefully for the more persistent compounds, to minimise the chance that the test will result in unacceptable degradation rate estimates within the maximum time window for the test.

The geometric mean of all these studies is the compound-specific E_a value (note that the geometric mean is a more robust estimate of the true median than the sample median where the number of studies is limited, whereas these values are theoretically identical for a lognormal distribution). The coefficient of variation of the geometric mean value should not exceed 10%. This value is approximately equivalent to the average CV of 22% for intra-compound variability (Table 9). Note that the CV of the geometric mean E_a is derived from the sample CV (Table 10) by dividing by the square root of the number of studies.

4. ASSESSMENT QUESTION 3 (EXTRAPOLATION OF Q_{10} TO OTHER TEMPERATURES)

4.1. Introduction

The analyses presented so far assume that the Arrhenius equation describes the relationship between rate constant and temperature well over the temperature range between 0° and 30°C. However, the Panel was asked to determine whether this assumption is defensible.

The data-collection phase led the Panel to the conclusion that sizable errors in estimated accepted DT_{50} values cannot be excluded. Thus even if the Arrhenius equation did describe the relationship between the rate constant and temperature perfectly, there would be datasets that would show poor Arrhenius fits. The Panel tested the null hypothesis that the Arrhenius equation describes the relationship between rate constant and temperature well over the temperature range between 0° and 30°C. The alternative hypothesis was then that a more complex relationship than the Arrhenius equation would be necessary for a good description of the relationship.

4.2. Statistical procedures and results

The null hypothesis was tested using two different methods. The first method was as follows. After logarithmic transformation, the Arrhenius equation has the following form:

$$\ln k_L = a_L + \frac{b_L}{T} \qquad \text{(Eqn 10)}$$

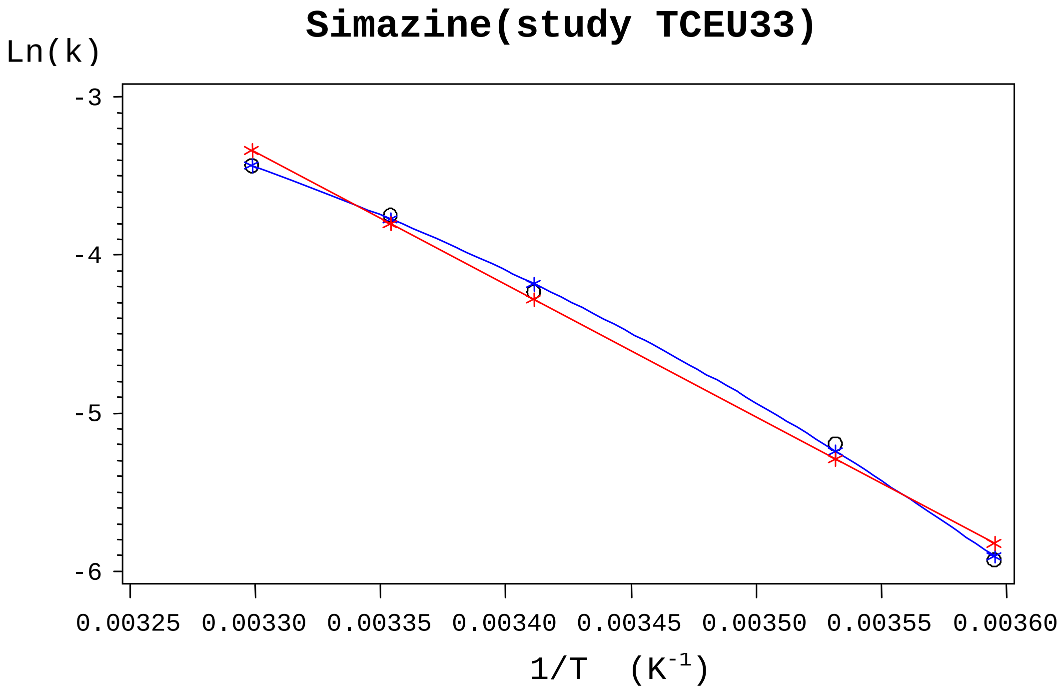
where k_L is the rate constant (d^{-1}) based on this linear fit, T is the absolute temperature (K), and a_L ($\ln[d^{-1}]$) and b_L (K) are regression coefficients ($b_L = E_a/R$).

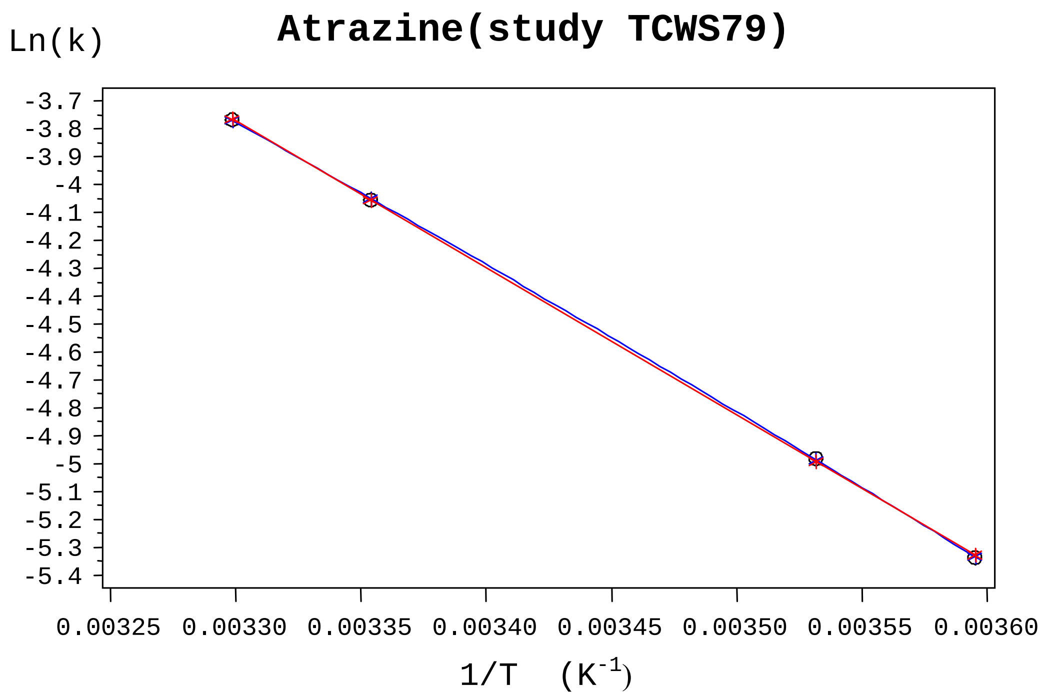
For the test, the following alternative quadratic equation was considered:

$$\ln k_Q = a_Q + \frac{b_Q}{T} + \frac{c_Q}{T^2} \qquad \text{(Eqn 11)}$$

where k_Q is the rate constant (d^{-1}) based on this quadratic fit, and where a_Q ($\ln[d^{-1}]$), b_Q (K),and c_Q (K^2) are regression coefficients. Eqn 11 is considered the most straightforward alternative to the Arrhenius equation, as it corresponds to the second-order approximation of the true value of ln k.

Eqn 11 can be applied only to data sets with more than two data points. Of the 98 studies, 56 had three or more data points and these were used in the analysis. All data sets were fitted to both Eqn 10 and Eqn 11. Figure 8 shows a number of the fits of the datasets with at least four datapoints as an illustration.





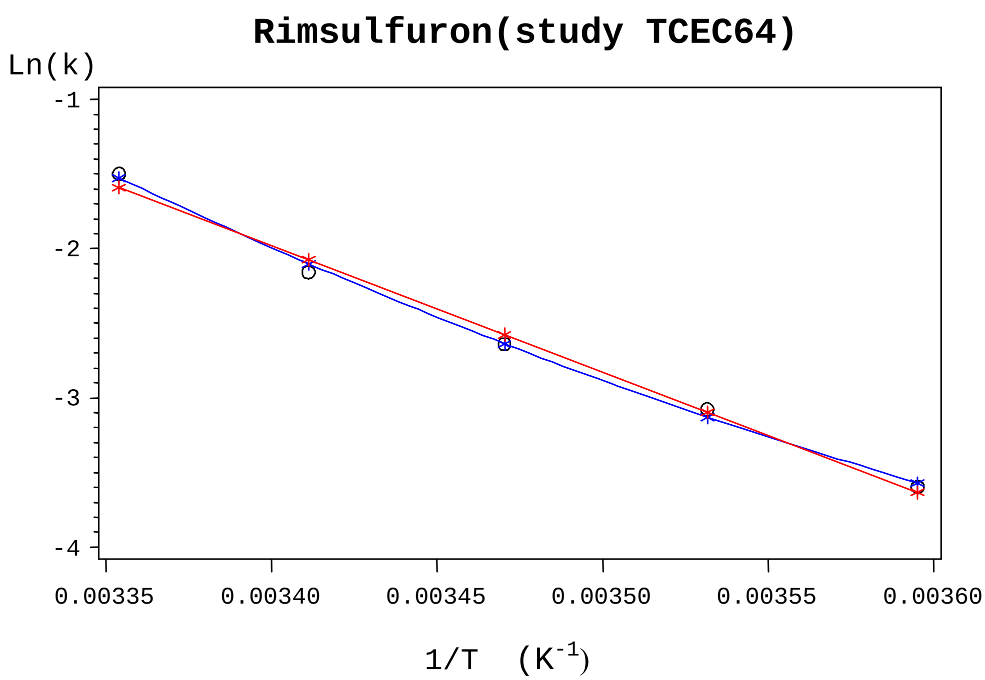


Figure 8. A selection of the fits of the data (black; ○) to both Eqn 10 (red; *) and Eqn 11 (blue; *). Vertical axes represent the natural logarithm of the degradation rate constant and horizontal axes the inverse of the absolute temperature.

Thereafter the difference between the ln k values at 5°, 10°, 20° and 30°C was calculated for the two fits for each dataset. This difference was defined as:

$$\Delta = \ln k_L - \ln k_Q = \ln \frac{k_L}{k_Q} \qquad \text{(Eqn 12)}$$

Subsequently the ratios of the two rate constants were calculated from

$$\frac{k_L}{k_Q} = \exp(\Delta) \qquad \text{(Eqn 13)}$$

These ratios were calculated for all 56 data sets. Summary statistics of these ratios show that the ratio is very close to 1 between 10° and 20°C (Table 13). In this range, k_L is slightly lower than k_Q. The situation is reversed outside that range, and the difference was on average 17% at 5°C and 26% at 30°C. The standard deviation of the differences was 42% at 5°C and 61% at 30°C which indicates that the variability in these ratios was considerable at these temperatures. It should further be noted that the ratios at 5° and 30°C in Table 13 are only to a small extent based on measurements at these temperatures because most datasets with at least three points do not contain measurements at 5° and 30°C (so most of these ratios are based on extrapolation).

Table 13. Statistics of the k_L/k_Q ratio at different temperatures as calculated for the 56 data sets with more than two data points.

Temperature (°C)	Mean	Std. Dev.	Minimum	Maximum
5	1.17	0.42	0.37	2.76
10	1.00	0.12	0.68	1.56
20	0.97	0.11	0.67	1.27
30	1.26	0.61	0.45	4.34

Now we consider the second method. Instead of considering fits individually and independently, this method analyses all data together, using a random-effect model. The model is also based on Eqn 11 and it assumes that for each data set the regression coefficients a_Q, b_Q and c_Q can be computed, but they are linked to each other in the sense that all a_Q values can be considered as drawn from a normal distribution (or lognormal or any other) and the same applies to b_Q and c_Q and all variances parameters.

Using this approach, the c_Q parameter was investigated. The quadratic equation collapses to the linear Arrhenius equation for $c_Q = 0$. It is therefore interesting to investigate this parameter more closely. The WinBUGS[3] software package was used for this purpose. This package uses Bayesian inference. Bayesian statistics allow more flexible inference on parameters in the sense that the analysis is not restricted to the evaluation of a single-value estimate of c_Q and the test of $c_Q = 0$. Instead, the whole distribution of possible c_Q values (and all other parameters) can be evaluated[4]. Thus it is possible to assess the probability that c_Q lies in any given range of

[3] WinBUGS User Manual, version 1.4.2, The BUGS project http://www.mrc-bsu.cam.ac.uk/bugs

[4] Bayesian Data Analysis, Second Edition. Gelman, Andrew, Carlin, John B., Stern, Hal S., and Rubin, Donald B. Chapman & Hall, July 2003

values (such distributions of model parameters are called 'posterior distributions'). WinBUGS allows simulation-based evaluation of such distributions.

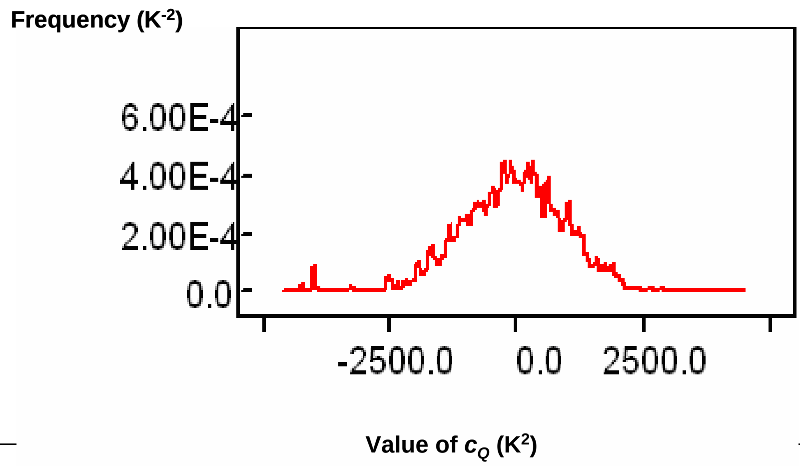


Figure 9. Frequency distribution of c_Q values for the 56 datasets with more than two data points.

From the resulting distribution of c_Q (Figure 9), the mean c_Q was found to be -94 K^2 and the median was -54 K^2. The standard deviation of c_Q was found to be 1079 K^2. These results indicate that c_Q does not differ significantly from zero. The results in Table 13 indicate that 'on average' the quadratic equation is linear (quadratic estimates of ln *k* lower than linear estimates of ln *k* at high and low temperatures, but quadratic estimates equal linear estimates at intermediate temperatures). So Table 13 indicates that 'on average' c_Q is close to zero. The random-effect model (Figure 9) showed qualitatively the same result.

Thus the PPR Panel concludes that the Arrhenius equation can be accepted as the descriptor for the relationship between rate constant and temperature for temperatures ranging between 0^o and 30^oC.

4.3. Conclusion

Considering all available data, the PPR Panel concludes that it is defensible to use the Arrhenius equation for describing the relationship between the degradation rate constant and soil temperature for temperatures between 0^o and 30^oC.

5. Discussion and Conclusions

In order to allow extrapolation of degradation rates of plant protection products to temperatures other than those used in experimental studies, the Panel was asked in a previous Opinion (2006) to (1) reconsider the use of an adapted default value of E_a and consequently Q_{10} as a key factor in the Arrhenius equation, (2) to give an opinion on possible compound-specific factors and (3) to give the range of temperatures that can be used by the proposed Q_{10} approach.

However, the scientific state-of-art has advanced since the previous Opinion. It is now concluded by the PPR Panel that the database, on which the proposed default value for temperature correction of DT_{50} values from soil degradation studies was based (in the PPR Opinion adopted on 8th February 2006), should be updated in view of the additional data identified by ECPA and other relevant data that have emerged since.

For **Question 1**, the data analysis indicated that the distribution of the median E_a values for specific chemicals is lognormal, with a median value of 65.4 kJ mol^{-1} and a 90-percent probability that the median value is within 45.8-93.3 kJ mol^{-1}. The estimated E_a values and corresponding Q_{10} values for selected percentiles are given in Table 14.

From the FOCUS report (1997), a default average E_a value of 54.0 kJ mol^{-1} was derived corresponding to a Q_{10} of 2.2. The proposed default average value of 68.9 kJ mol^{-1} of the previous PPR Opinion (EFSA, 2006) corresponded to a Q_{10} of 2.8. Statistical analysis of the updated database in this Opinion has indicated that it is incorrect to assume that there is a single E_a value for all pesticides which was the approach in the FOCUS report (1997).

Table 14. Percentiles of the distribution based on compound-specific median E_a values (kJ mol^{-1}) (based on Figure 5) and corresponding Q_{10} values (based on Eqn 7)

Percentile	Median E_a	Q_{10}
5	45.8	1.94
10	49.5	2.05
15	52.2	2.13
20	54.5	2.20
25	56.5	2.27
30	58.3	2.33
35	60.1	2.39
40	61.9	2.45
45	63.6	2.51
50	65.4	2.58

Table 14 continued		
Percentile	Median E_a	Q_{10}
55	67.2	2.65
60	69.0	2.72
65	71.0	2.80
70	73.2	2.89
75	75.6	2.99
80	78.4	3.11
85	81.8	3.27
90	86.2	3.49
95	93.3	3.86

The final choice of a Q_{10} value will depend upon the nature of the risk-assessment exercise, but such considerations are complex and outside the remit of this Opinion. Awaiting further review of the respective risk assessment frameworks, the standing EU practice with respect to using a Q_{10} default value in environmental exposure assessments is expected to continue. In this context the Panel recommends that the median E_a value of 65.4 kJ mol^{-1} corresponding to a Q_{10}

of 2.58 should replace the default E_a value of 54.0 kJ mol^{-1} corresponding to a Q_{10} of 2.2 (FOCUS default), which has been used until now.

For **Question 2**, compound-specific E_a values should be used instead of the default value in modelling or risk assessment when they are available and the criteria for deriving compound-specific E_a values as given in Section 3.2. have been met.

For **Question 3**, it is considered defensible to use the Arrhenius equation for describing the relationship between the degradation rate constant and soil temperature for temperatures between 0^o and 30^oC.

This Opinion replaces the PPR Panel Opinion adopted on the 8th February 2006.

GLOSSARY / ABBREVIATIONS

Term	**Explanation**
Q_{10}	Q_{10} is defined as the ratio of pesticide degradation rate coefficients (k_2/k_1) at a temperature T_1 that is 10°C lower than a temperature T_2 (see Section 2.1)
ECPA	European Crop Protection Association
SFO	Simple first-order kinetics.
$E_{\mathbf{a}}$	Activation energy (see Section 2.1.)
$K_{\mathbf{oc}}$	Sorption coefficient to soil organic carbon
CV	Coefficient of Variation
Std	Standard Deviation
CDF	Cumulative Distribution Function
QQ-plots	Plots of the quantiles of the variable against the quantiles of another variable. If the observed and predicted sets of quantiles come from a population with the same distribution, the points should fall approximately along a 45-degree reference line.
Average	See Mean
Mean	The mean of a statistical distribution with a discrete random variable is the mathematical average of all the terms. To calculate the mean, add up all the terms, and then divide by the number of terms in the distribution.
Median	Median is used here only for distributions, not for sets of discrete data. See also geomean. The median of a distribution of a continuous random variable is the central point such that 50% of the values are above and 50% are below it.
Geomean (or geometric mean)	The mean of ln-transformed terms.

European Food Safety Authority

The EFSA Journal (2007) 622, 1-122

APPENDICES

Opinion on a request from EFSA related to the default Q_{10} value used to describe the temperature effect on transformation rates of pesticides in soil

Scientific Opinion of the Panel on Plant Protection Products and their Residues (PPR-Panel)

(Question No EFSA-Q-2007-048)

Adopted on 12 December 2007

TABLE OF CONTENTS

Appendix 1

References of experimental studies. Sources by reference code

Ref Code	FOCUS	Author(s)	Year	Source
JB2	y	Walker A	1987	Weed Research 27: 143-152
JB3	y	Pestemer W, Auspurg B	1987	Weed Research 27: 275-286
JB4	n	Berger B, Heitefuss R	1990	Z. PflKrankh. PflSchutz Sonderh. XII: 399-407
JB5	y	Blair AM, Martin TD, Walker A, Welch SJ	1990	Crop Protection 9: 289-294
JB6	y	Mudd PJ, Hance RJ, Wright SJL	1983	Weed Research 23: 239-246
JB7	n	Smelt JH, Leistra M, Dekker A, Schut CJ	1981	Soil Science 131: 242-248
JB8	n	Scorza Junior RP, Smelt JH, Boesten JJTI, Hendriks RFA, van der Zee SEATM	2004	J. Environ. Qual. 33: 1473-1486
JB9	n	Boesten JJTI, van der Pas LJT	2000	Agricultural Water Management 44: 21-42
JB10	y	Usoroh NJ, Hance RJ	1974	Weed Research 14: 19-21
EU1	y	Walker A	1974	J. Environ. Quality 3:396-401
EU2	y	Walker A, Bond W	1978c	Proceedings 1978 British Crop Protection Conference-Weeds, 565-572
EU3	y	Walker A	1978a	Weed Research 18:305-313
EU4	y	Walker A, Brown PA	1985	Bull. Environ. Contam. Toxicol. 34:143-149
EU5	n	Moon Y-H, Walker A	1991	Brighton Crop Protection Conference-Weeds, 499-506,
EU6	n	Walker A, Moon Y-H, Welch SJ	1992	Pesticide Sci. 35:109-116
EU7	n	Walker A	1978b	Pesticide Sci. 9:326-332
EU8	n	Walker A, Brown PA	1983b	Bull. Environ. Contam. Toxicol. 30:365-372
EU9	y	Walker A, Zimdahl RL	1981	Weed Research, 21:255-265
EU10	y	Walker A	1976a	Pesticide Sci. 7:41-49
EU11	y	Walker A	1976b	Pesticide Sci. 7:59-64
EU12	y	Walker A, Bond W	1977	Pesticide Sci. 8:359-365

Ref Code	FOCUS	Author(s)	Year	Source
EU13	y	Smith AE, Walker A	1989	Can. J. Soil Sci. 69:587-595
EU14	y	Walker A, Hance AJ, Allen JG, Briggs GG, Yuh-Lin Chen, Gaynor JD, Hogue EJ, Malquori A, Moody K, Moyer JR, Pestemer W, Rahman A, Smith AE, Streibig JC, Torstensson NTL, Widyanto LS, Zandvoort R	1983	Weed Research 23:373-383
EU15	y	Walker A, Smith AE	1979	Pesticide Sci. 10:151-157
EU16	n	Koch Singles S, Dean GM, Kirkpatrick DM, Mayo BC, Langford-Pollard AD, Barefoot AC, Bramble FQ Jr	1999	Pesticide Sci. 55: 288-300
EU17	n	James TK, Holland PT, Rahman A, Lu YR	1999	Weed Research 39: 13-147
EU18	n	James TK, Klaffenbach P, Holland PT, Rahman A	1995	Weed Research 35: 113-120
EU19	n	Zimdahl RL, Catizone P, Butcher AC	1984	Weed Sci. 32:408-412
EFSA001	n	Batzer FR, Smith KP	2002	Dow Agro Sciences GH-C-5350
EFSA009	n	Baloch R, Grant R	1991	Dow Agro Sciences, unpublished report no. GHE-P-2398R
EFSA010	n	Mamouni A	1994	Syngenta File N° CGA219417/0258
EFSA012	n	Salmon-te Rietstap F, Jansen J, Schut M, Hansveit AO	2003	TNO Food Nutrition & Research, The Netherlands, Report No. V2438/03
EFSA017	n	Mackie JA, Hall BE	1993	Du Pont, Inveresk Research International, Report n. 9923
EFSA018	n	Burr CM	2001	Aventis CropScience UK Ltd., Report No.: C016772 (17886)
EFSA019	n	Greenslade D, Ward J, Hopkins R	1984	Hazleton Laboratories Europe. Document No. R009121
EFSA022	n	Fitzmaurice MJ, Mackenzie E	2002	Aventis CropScience UK Limited, GBR. Batelle AgriFood Limited, Ongar. Doc No: C018800
EFSA023	n	Crowe A	2001	Huntingdon Life Sciences Ltd., Report No. MAK560/003188 (Company file: R-11249).
EFSA026	n	Allan JG	1995	Hoechst Schering AgrEvo GmbH. Environmental Chemistry Frankfurt, Doc No: A55393
EFSA026	n	Stumpf K, Schink C, Schmidt E	1995	Hoechst Schering AgrEvo GmbH. Environmental Chemistry Frankfurt, Doc No: A55104

Ref Code	FOCUS	Author(s)	Year	Source
EFSA027	n	Knowles SJ	2001	Dow Agro Sciences, unpublished report no. GHE-P-9295
EFSA029	n	Gedik L, Fullard DC	2002	Inveresk Research International Ltd.
EFSA029	n	Hall BE, Lowrie C	2002	BASF Corporation Agro Research. Princeton NJ 08543-0400
EFSA034	n	Mattson LS, Smyser BP	2000	E.I. du Pont de Nemours and Company, Report no.: DuPont-2957
EFSA036	n	Diehl M	2002	RCC Ltd., Itingen, CHE. Aventis CropScience GmbH, DEU. Document No: C021783
EFSA042	n	Benwell L	1992	HUK 7054-269/42 and HUK 7203-269/42A
EFSA043	n	Burr CM	2000	Aventis CropScience UK, Limited, GBR, Document No: C019338
EFSA044	n	Lewis CJ	1995	Sumitomo Chemical Co., Ltd. Report, No. QM-0049
EFSA047	n	Hawkins DR, Elsom LF, Dighton MH, Kaur AK	1995	Huntingdon Research Centre (UK), AMR 3235-94
EFSA051	n	Schanne C	1993	RCC AG, Itingen, Switzerland RCC 315448
EFSA052	n	Simmonds MB, Hardy IJ, Ferreira EM	1996	Rhone-Poulenc Agriculture Limited, Ongar, England. Rhone-Poulenc Agro Norden, Soberg, Denmark. Document No: R012995
EFSA054	n	Steinfuehrer T	2000	Cyanamid Forschung GmbH. Schwabenheim. Germany Fed.Rep., 2000/7000151
EFSA054	n	Steinfuehrer T, Weis D	2000	Cyanamid Forschung GmbH. Schwabenheim. Germany Fed.Rep., 2000/7000150
EFSA055	n	Staudenmaier H, Schaefer C	1999	BASF, the degradation behaviour of BAS 505 F in soil
EFSA056	n	Ta CT , Lewis CJ	1997	Cyanamid, AC 299263: Soil Degradation Study
EFSA057	n	Tarara G	2000a	Aventis, Kinetics and metabolism in Soil LS 2.2 at 10°C and 20°C under aerobic conditions (2-14C-pyrimidyl) AE F130060

Ref Code	FOCUS	Author(s)	Year	Source
EFSA057	n	Tarara G	2000b	Aventis, Kinetics and metabolism in Soil LS 2.2 at 10°C and 20°C under aerobic conditions (U-14C-phenyl) AE F130061
WS1	n	Flint JL, Witt WW	1997	Weed Science 45: 586-591
WS2	n	Gottesbueren B	1991	Ph.D. thesis University of Hannover: Konzeption, Entwicklung und Validierung des wissenbasierten Harbizid-Beratungssystems HERBASYS
WS3	n	Heiermann M	1998	Ph D Dissertation Berlin, Humbold-Universität: Untersuchung zum Verhalten von Herbiziden im Boden als Grundlage für Simulationsrechnungen im Herbst und Winter. Cuvillier Verlag Göttingen. ISBN 3-89712-370-3
WS4	n	Jurado-Exposito M, Walker A	1998	Weed Research 38: 309-318
WS5	n	Krieger MS, Pillar F, Ostrander JA	2000	J. Agric. Food Chem. 48: 4757-4766
WS6	n	Lehmann RG, Fontaine DD, Olberding EL	1993	Weed Research 33: 187-195
WS7	n	Rocha F	1993	8th EWRS symposium "Quantitative approaches in weed and herbicide research and their practical application", Braunschweig, 1993, 501-508
WS8	n	Smith AE, Aubin AJ	1992	J. Agric. Food Chem. 40: 2500-2504
WS9	n	Tariq MI, Afzal S, Hussain I	2006	Environmental Research 100: 184-196
WS10	n	Vischetti C, Marini M, Businelli M, Onofri A	1996	Proc. Symp. Pestic. Chem. 1996 (10 Meet.): 287-294
WS11	n	Vischetti C, Leita L, Marucchini C, Porzi G	1998	Agronomi (Paris) 18, No. 2: 131-137
WS12	n	Walker A, Jurado-Exposito M	1998	Weed Research 38: 229-238

Ref Code	FOCUS	Author(s)	Year	Source
JJB1	n	Aden K, Richter O, Gottesbueren B	1989	Del Re, Capri, Errera, Evans, Trevisan (Eds.) 1999: Human and environmental exposure to xenobiotics - Proceedings of the XI Symposium Pesticide Chemistry, September 11-15, Cremona, Italia. 89-99
JJB2	n	Aletto L, Coquet Y, Benoit P, Bergheaud V	2006	Chemosphere 64: 1053-1061
JJB3	n	Beulke S	1998	Ph. D Dissertation Braunschweig, Technische Universität, Carolo_Wilhelmina: Untersuchung und mathematische Beschreibung ds Abbaous von Herbiziden im Boden in Abhägigkeit von Wirkstoffverfügbarkeit, mikrobieller Biomassse und Aktivität, Shaker Verlag, Aachen. ISBN 3-8265-3941-9
JJB4	n	Beulke S, Brown CD, Fryer CJ, van Beinum W	2004	Chemosphere 57: 481-490
JJB5	n	Beulke S, van Beinum W, Brown CD, Mitchell M, Walker A	2005	J. Environ. Qual. 34: 1933-1943
JJB6	n	Bromilow RH, Evans AA, Nicholls PH	1999	Pesticide Sci. 55: 1129-1134
JJB7	n	Bunte D	1991	Ph. D. thesis, University of Hannover: Abbau- und Sorptionsverhalten unterschiedlich persistenter Herbizide in Abhängigkeit von Flächenvariabilität und Alter der Rückstände
JJB8	n	Capri E, Walker A	1993	Bull. Environ. Contam. Toxicol. 50: 506-513
JJB9	n	Capri E, Ghebbioni C, Trevisan M	1995	J. Agric. Food Chem. 43: 247-253

Ref Code	FOCUS	Author(s)	Year	Source
JJB10	n	Dibbern H	1992	Zur Simulation des Ausbreitungsverhaltens der Pflanzenschutzmittel Atrazin, Chlortoluron, Isoproturon, Lindan und Terbuthylazine im Boden und Grundwasser.- Berichte des Geologisch-Paläontologischen Instituts und Museums der Christian-Albrechts-Universität Kiel Nr. 49. ISSN 0175-9302
JJB11	n	Dinelli G, Accinelli C, Vicari A., Catizone P	2000	J. Agric. Food Chem. 48: 3037-3043
JJB12	n	Düfer B	1991	Ph.D. thesis, University of Göttingen: Ursachen ungenügender Wirkungen von substituierten Phenylharnstoffen bei der Bekämpfung von Alopecurus myosuroides Huds. auf hochgradig verseuchten Standorten norddeutscher Marschböden
EC1	n	Caracciolo AB, Giuliano G, Di Corcia A, Crescenzi C, Sivestri C	2001	Bull. Environ. Contam. Toxicol. 76: 815-820
EC2	n	Beltran E, Fenet H, Cooper JF, Costoe CM	2003	J. Agric. Food Chem. 51: 146-151
EC3	n	Borek V, Morra MJ, Brown PD, McCaffrey JP	1995	J. Agric. Food Chem. 43: 1935-1940
EC4	n	Cambon JP, Bastide J, Vega D	1998	J. Agric. Food Chem. 46: 1210-1216
EC5	n	Cambon JP, Zheng Q, Bastide J	1992	Weed Research 32: 1-7
EC6	n	Dinelli G, Di Martino E, Vicari A.	1998	Agrochimica Vol. XLII - N. 1-2
EC7	n	Dungan RS, Gan J, Yates SR	2003	Water, Air, and Soil Pollution 142: 299-310
EC8	n	Gaillardon P, Sabar M.	1994	Weed Research 34: 243-250
EC9	n	Gan J, Papiernik SK, Yates SR, Jury WA	1999	J. Environ. Qual. 28:1436-1441
EC10	n	Grover R, Wolt D, Cessna AJ, Schiefer HB	1997	Rev. Environ. Contam. Toxicol. 15: 1-64
EC11	n	Hanummantharaju TH, Awasthi MD	2002	Pesticide Research Journal 14: 292-298
EC12	n	Kempson-Jones GF, Hance RJ	1979	Pesticide Sci. 10: 449-454
EC13	n	Khouey R, Coste CM, Kawar NS	2006	J. Environ. Sciences Health Part B. 41:795-806

Ref Code	FOCUS	Author(s)	Year	Source
EC14	n	Kinfe B, Peeper TF	1993	Weed Technology 7: 29-32
EC15	n	Kurt-Karakus PB, Bidleman TF, Jones KC	2005	Environ. Sci. Technol. 39: 8671-8677
MM1	n	Ma QL, Gan J., Papiernik SK, Becker JO, Yates SR	2001	J. Environ. Qual. 30: 1278-1286
MM2	n	Oppong FK, Sagar GR	1992	Weed Research 32: 167-173
MM3	n	Smith AE, Sharma MP, Aubin AJ	1990	Can. J. Soil Sci. 70: 485-491
MM4	n	Vink JPM, van der Zee SEATM	1996	Pesticide Sci. 46: 113-119
MM5	n	Vischetti C, Esposito A	1999	J. Agric. Food Chem.47: 3901-3904
MM6	n	Zheng SQ, Cooper JF	1996	Arch. Environ. Contam. Toxicol. 30: 15-20
MM7	n	Ahmad R, James TK, Rahman A, Holland PT	2003	J. Environ. Sciences Health B38: 683-695
MM8	n	Jordan EG, Kauffman DD, Kayser AJ	1982	J. Environ. Sciences Health B17: 1-17
MM9	n	Wolt JD, Smith JK, Sims JK, Duebelbeis DO	1996	J. Agric. Food Chem. 44: 324-332
RB1	n	Adam A (Abamectin (Avermectin B1).pdf)	2001	Syngenta Crop Protection AG Report nr. NOA 422601
RB2	n	Till CP (Amidosulfuron.pdf)	1988	Hoechst UK Report nr. M88017
RB3	n	Erzgräber B (Amidosulfuron.pdf)	2001	Aventis CropScience Report nr. OE99/098
RB4	n	Yeomans P (Asulam.pdf)	2000	Aventis CropScience Report nr. 68/171-D2142
RB5	n	Simmonds MB, Burr CM (Bifenox.pdf)	2000	Aventis CropScience Report nr. 15747
RB6	n	Lewis CJ (Buprofezin.pdf)	2002	Nihon Nohyaku Co Ltd. Report nr. 608/57-D2149
RB7	n	Ambrosi D, Desmoras J (Carbetamide.pdf)	1978	Rhone-Poulenc Agro. Report nr. 19743E
RB8	n	Mahay N, Burr CM (Diflufenican.pdf)	2001	Aventis CropScience Report nr. 16672
RB9	n	Giraud JP, Chabassol Y (Diflufenican.pdf)	1985	Rhone-Poulenc Agrochimie. Report nr. 15581.85
RB10	n	Harradine KJ, Eatherall A (Fenpropidin.pdf)	2002	Syngenta UK Report nr. RAJ0117B
RB11	n	Rümbeli R (Fenpropidin.pdf)	1991	Dr R. Maag AG Report nr. 041/9168
RB12	n	Anonymous (Hexythiazox.pdf)	1984	Nippon Soda Co. Ltd Report nr. RD-83132N
RB13	n	Doris E (Mepiquat-chloride.pdf)	2003	BASF AG Report nr. 58415

Ref Code	FOCUS	Author(s)	Year	Source
RB14	n	Gottesbüren B (Metazachlor & metabolite BH479-4.pdf)	2003	BASF AG Report nr. CALC-380
RB15	n	Keller W (Metazachlor & metabolite BH479-4.pdf)	1990	BASF AG Report nr. ABB-01-90
RB16	n	Keller W (Metazachlor & metabolite BH479-4.pdf)	1989	BASF AG Report nr. Method 293
RB17	n	Keller W (Metazachlor & metabolite BH479-4.pdf)	1990	BASF AG Report nr. Methode 303
RB18	n	Keller W (Metazachlor & metabolite BH479-4.pdf)	1991	BASF AG Report nr. ABB-02-91
RB19	n	Schneider E (Metazachlor & metabolite BH479-4.pdf)	2000	Feinchemiie Schwebda GmbH Report nr. PR97/018
RB20	n	Shaw D (Napropramide.pdf)	2001	United Phosphorus Ltd. Report nr. UPH 027/013239
RB21	n	Dyson JS, Hayes SE, Earl M (Pinoxaden & metabolites NOA407854 & NOA447204.pdf)	2004	Syngenta UK Report nr. RAJ0203B
RB22	n	Reischmann FJ (Pinoxaden & metabolite NOA407855.pdf)	2003	Syngenta Crop Protection. Report nr. NOA 407855
RB23	n	Lee DY, Corrigan NM (Proquinazid (DPX-KQ926) & 3 metabolites.pdf)	2000	E.I. du Pont de Nemours & Company. Report nr. AMR 4986-98
RB24	n	Reinken G (Sulcotrione & metabolite CMBA.pdf)	2003	Bayer CropScience AG. Report nr. MEF-179/03
RB25	n	Subba-Rao RV, Wang WW (Sulcotrione & metabolite CMBA.pdf)	1988	ICI Americas Inc. Report nr. PMS-296
RB26	n	Pluckrose J, Bewick DW (Tefluthrin.pdf)	1986	ICI Plant Protection Division. Report nr. RJ 0525B
RB27	n	Greener M (Tralkoxydim.pdf)	2003	Syngenta UK. Report nr. RAJ0111B
RB28	n	Butters CA, Gibbings EL, Mason R (Tralkoxydim.pdf)	1996	Zeneca Agrochemicals. Report nr. RJ 1965B
RB29	n	Entwistle K (Tralkoxydim.pdf)	1996	Zeneca Agrochemicals. Report nr. RJ 2040B
SB1	n	Aikens PJ (Acequinocyl.pdf)	2000	Agro-Kanesho Cà. Ltd. Report nr. AGK 053/983928
SB2	n	Oddy AM (Carbonyl DAR. pdf & Carbonyl.pdf)	2002	Bayer CropScience SA. Report nr. CX/02/048
SB3	n	Baumann J (Clomazone.pdf)	2003	FMC Chemical Sprl. Report nr. E-17-02-41
SB4	n	Hatzenbeler CJ, Lenz NR (Flonicamid (TFNA metabolite).pdf)	2002	Ishihara Sangyo Kaisha Ltd. Report nr. 012064-1

Ref Code	FOCUS	Author(s)	Year	Source
SB5	n	Lenz NR (Flonicamid (TFNA-AM metabolite).pdf)	2002	Ishihara Sangyo Kaisha Ltd. Report nr. 012696-1
SB6	n	Findak DC, Lentz NR (Flonicamid (TFNA-OH metabolite).pdf)	2002	Ishihara Sangyo Kaisha Ltd. Report nr. 012066-1
SB7	n	Lentz NR (Flonicamid (TFNG metabolite).pdf)	2002	Ishihara Sangyo Kaisha Ltd. Report nr. 012065-1
SB8	n	Lentz NR (Flonicamid (TFNG-AM metabolite).pdf)	2002	Ishihara Sangyo Kaisha Ltd. Report nr. 012697-1
SB9	n	Lentz NR (Flonicamid DAR.pdf)	2002	Ishihara Sangyo Kaisha Ltd. Report nr. 013066-1
SB10	n	Shaw D (Methomyl.pdf)	2001	E.I. du Pont de Nemours & Company. Report nr. DPT/583
SB11	n	Jackson R, Massart J, Portwood D (Penoxulam.pdf)	2001	Dow AgroSciences. Report nr. GHE-P-8899
SB12	n	Kley C (Propamocarb DAR.pdf & Propamocarb-HCL AE OE01-090.pdf)	2001	Aventis CropScience. Report nr. OE01/090
SB13	n	Kley C (Propamocarb HCL AGR20 Addendum.pdf)	2001	Aventis CropScience. Report nr. OE01/050 (Addendum to report nr. AGR20)
SB14	n	Fent G, Hein W (Propamocarb-HCL AGR20.pdf)	2001	Aventis CropScience. Report nr. AGR20
SB15	n	Fent G, Hein W (Propamocarb-HCL AGR21.pdf)	2001	Aventis CropScience. Report nr. AGR21
SB16	n	Kley C (Propamocarb HCL OE01-051 Addendum to AGR 21.pdf)	2001	Aventis CropScience. Report nr. OE01/051 (Addendum to report nr. AGR21)
SB17	n	Brühl R, Celorio J (Propamocarb-HCL PA 66752-71-6.pdf)	1978	Schering AG Report nr. PA 66 752.71/6
SB18	n	Iwan J (Propamocarb-HCL RS 58-80 nr 2.pdf	1980	Schering AG Report nr.R=S 48/80 PA 66 752.73/2
SB19	n	Brühl R, Celorio J (Propamocarb-HCL RS 58-80.pdf)	1980	Schering AG Report nr.R=S 58/80 PA 66 752.71/6
SB20	n	Brühl R, Celorio J (Propamocarb-HCL RS 71-80.pdf)	1980	Schering AG Report nr.R=S 71/80 PA 66 752.71/6
SB21	n	Brühl R, Celorio J (Propamocarb-HCL UPSR 1-86.pdf)	1986	Schering AG Report nr.UPSR 1/86 PA 66 752.71

Appendix 2

Accepted studies. Summary of experimental data selected for Q_{10} assessment

The comprehensive document detailing the assessment of all considered studies is available at the EFSA web-site. See foot-note[1]

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Soil texture	Conc (mg kg^{-1})	FC (%)	MW HC (%)	Moist (% g g^{-1})	Temp (°C)	DT_{50} (day)	R	E_a (kJ mol^{-1})
(*E*)-1,3-dichloro-propene	chlorinated hydrocarbon	996	TCMM15	MM1	Ma	Arlington	sandy loam	0.6		50	10	20	2.7	0.98	53.44
		997						0.6		50	10	30	1.31	0.99	
(*Z*)-1,3-dichloro-propene	chlorinated hydrocarbon	1012	TCMM19	MM1	Ma	Arlington	sandy loam	0.65		50	10	20	3.48	0.97	60.72
		1013						0.65		50	10	30	1.53	0.99	
alachlor	chloroacetamide	163	TCEU42	EU4	Walker	Wellesbourne 1	sandy loam	4			12	5	38.6	0.92	56.94
		164						4			12	15	16.5	0.92	
		165						4			12	25	7.4	0.92	
		175	TCEU51	EU5	Moon	Hunts Mill 2	sandy loam	8			7.9	5	119	0.99	68.33
		176						8			7.9	10	76.6	0.99	
		177						8			7.9	15	39.7	0.99	
		178						8			7.9	20	25.7	0.99	
		179						8			7.9	25	17.3	0.99	
		180	TCEU61	EU6	Walker	Cottage Field 0-20 cm	not reported	8			15.2	5	95.9	0.995	75.59
		181						8			15.2	10	60	0.997	
		182						8			15.2	15	31	0.999	
		183						8			15.2	20	17.4	0.999	
		184						8			15.2	25	11.5	0.998	
		190	TCEU63	EU6	Walker	Little Cherry 0-	not	8			13.2	5	112	0.995	80.70

[1] http://www.efsa.europa.eu/EFSA/ScientificOpinionPublicationReport/efsa_locale-1178620753812_ScientificOpinions.htm

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Soil texture	Conc (mg kg^{-1})	FC (%)	MW HC (%)	Moist (% g g^{-1})	Temp (°C)	DT_{50} (day)	R	E_a (kJ mol^{-1})
alachlor	chloroacetamide	191				20 cm	reported	8			13.2	10	58.5	0.999	
		192						8			13.2	15	28.8	0.999	
		193						8			13.2	20	16.6	0.999	
		194						8			13.2	25	11.3	0.997	
		541	TCWS411	WS4	Jurado-Exposito	Wellesbourne 3		15			20	10	79.6	0.97	79.65
		542						15			20	20	25.1	0.99	
		799	TCJJB81	JJB8	Capri	Tencara	clay loam	8			22	15	32.5	0.94	77.96
		800						8			22	20	16.7	0.98	
		801						8			22	25	9	0.96	
		802						8			22	30	6.7	0.99	
atrazine	triazine	103	TCEU36	EU3	Walker	Pump Ground 5 cm	sandy loam	4			9.8	5	178	0.81	69.19
		104						4			9.3	10	128	0.81	
		105						4			9.9	20	43.9	0.81	
		106						4			9.8	25	24.7	0.81	
		107						4			9.5	30	16.5	0.81	
		218	TCEU92	EU9	Walker	Mississippi	silt loam	4			16.9	5	179	0.919	46.10
		220						4			16.8	25	47	0.969	
		584	TCWS73	WS7	Rocha F	X9	sandy	1		60		5	81	0.99	33.70
		585						1		60		10	58	0.99	
		586						1		60		25	29	0.99	
		587						1		60		30	24	0.99	
		599	TCWS76	WS7	Rocha F	X12	sandy loam	1		60		5	74	0.99	37.80
		600						1		60		10	55	0.99	
		601						1		60		25	25	0.99	
		602						1		60		30	19	0.99	
		614	TCWS79	WS7	Rocha F	X18	silty loam	1		60		5	144	0.99	43.83
		615						1		60		10	101	0.99	
		616						1		60		25	40	0.99	
		617						1		60		30	30	0.99	
		630	TCWS712	WS7	Rocha F	X4	loam	1		60		10	181	0.99	51.83
		631						1		60		25	61	0.99	
		632						1		60		30	42	0.99	

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bentazon	benzothiadiazinone	58	TCJB82	JB8	Scorza	Andelst	not reported	1.1			21	5	166	n.a.	74.70
bentazon	benzothiadiazinone	59						1.1			21	15	56	n.a.	
		60						1.1			21	25	19	n.a.	
		64	TCJB92	JB9	Boesten	Vredepeel	not reported	1.2			15	5	206	n.a.	113.34
		65						1.2			15	15	37.6	n.a.	
		730	TCJJB52	JJB5	Beulke	Salop small	clay loam	15		70	20.6	15	36.4	acceptable Chi2 error	33.42
		731						15		70	20.6	25	22.8	acceptable Chi2 error	
carbaryl	carbamate	1203	TCSB21	SB2	Oddy	Soil 0205	clay loam	1.81		50		10	80.9	0.96	67.55
		1204						1.81		50		20	30.4	0.94	
chloridazon	pyridazinone	675	TCWS102	WS10	Vischetti	Umbria	clay loam	4.2	100			10	76	s.e. reported	52.53
		676						4.2	100			20	35.5	s.e. reported	
		805	TCJJB92	JJB9	Capri	X16	silty clay loam	2			22	10	75.6	0.85	61.52
		806						2			22	20	21.3	0.82	
		807						2			22	30	13.6	0.94	
chlorotoluron	phenylurea	845	TCJJB121	JJB12	Düfer	Altendorf		2		60		5	90.1	0.995	33.12
		846						2		60		10	55.8	0.988	
		847						2		60		20	41.5	0.982	
		848	TCJJB122	JJB12	Düfer	Norden		2		60		5	112	0.969	61.42
		849						2		60		10	55.2	0.993	
		850						2		60		20	27.5	0.969	
		851	TCJJB123	JJB12	Düfer	Simonsberkerkoog		2		60		5	76.4	0.979	54.20
		852						2		60		10	49	0.988	
		853						2		60		20	22.9	0.946	
chlorsulfuron	sulfonylurea	204	TCEU81	EU8	Walker	Wellesbourne 2	sandy loam	4			12	10	64.2	n.a.	71.70
		205						4			12	15	37.4	n.a.	
		206						4			12	20	25.6	n.a.	
		207						4			12	25	12.8	n.a.	

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chlorsulfuron		208						4			12	30	8.9	n.a.	
chlorthal-dimethyl	phthalic acid	138	TCEU317	EU3	Walker	Pump Ground 5 cm	sandy loam	4			9.1	5	295	0.81	90.15
		139						4			9.6	10	233	0.81	
chlorthal-dimethyl	phthalic acid	140						4			9.2	15	90.1	0.81	
		141						4			9.2	25	24.5	0.81	
clopyralid	pyridinecarboxylic acid	1096	TCMM71	MM7	Ahmad	Horotiu 1	silt loam	840		60		10	46.2	0.97	86.91
		1097						840		60		20	7.3	0.97	
		1098						840		60		30	4.1	0.98	
cyanazine	triazine	724	TCJJB51	JJB5	Beulke	Salop small	clay loam	15		70	20.6	15	12	acceptable Chi2 error	32.63
		725						15		70	20.6	25	7.6	acceptable Chi2 error	
cyprodinil	anilinopyrimidine	348	TCEFSA0101	EFSA010	Mamouni	Les Evouettes	silt loam	1	60		23.9	10	79.8	0.99	82.35
		349						1	60		23.9	20	24.2	0.99	
dichlorprop-p	Aryloxyphenoxy-propionate	350	TCEFSA0121	EFSA012	Salmon-te Rietstap	Massdijk Netherlands	sandy loam	1.32		40	16.9	10	37.4	0.941	111.82
		351						1.32		40	16.9	20	7.4	0.993	
dimethachlor	chloroacetamide	166	TCEU43	EU4	Walker	Wellesbourne 1	sandy loam	4			12	5	35.7	0.92	54.33
		167						4			12	15	14.4	0.92	
		168						4			12	25	7.4	0.92	
ethephon	phosphonic acid	354	TCEFSA0181	EFSA018	Burr	Boarded Barns Farm 1	clay loam	2.24		45	28.8	10	51.4	0.84	57.94
		355						2.24		45	28.8	20	22.2	0.9	
ethofumesate	benzofuran	406	TCWS21	WS2	Gottesbüren	Ahlum 1	(parabraunerde)	1.5		60		10	58	0.99	19.24
		407						1.5		60		20	35	0.98	
		408						1.5		60		30	34	0.93	
		458	TCWS39	WS3	Heiermann	Neuenkirchen	(parabraunerde)	1.79		80		1	150	0.97	58.27
		459						1.79		80		10	46	0.99	
		460						1.79		80		20	20	0.99	
		461						1.79		80		30	13	0.98	
		702	TCJJB31	JJB3	Beulke	II		1.9		60		10	107	1	48.56

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ethofumesate		703						1.9		60		20	34.7	1	
		704						1.9		60		30	27.6	0.98	
ethoprophos	organophosphate	43	TCJB71	JB7	Smelt	Wierum	silt loam	10	100		22	2	89	0.995	74.51
		44						10	100		22	6	49.5	0.994	
		45						10	100		22	10	30.1	0.991	
ethoprophos	organophosphate	46						10	100		22	20	11.7	0.986	
		47	TCJB72	JB7	Smelt	Middenmeer	sandy loam	10	100		21	2	144	0.981	82.00
		48						10	100		21	6	80	0.994	
		49						10	100		21	10	37.1	0.988	
		50						10	100		21	20	15.9	0.988	
		52	TCJB73	JB7	Smelt	Rolde	loamy sand	10	100		17	6	347	0.956	75.08
		53						10	100		17	10	198	0.978	
		54						10	100		17	20	72.2	0.983	
		61	TCJB91	JB9	Boesten	Vredepeel	not reported	5.7			15	5	349	n.a.	64.56
		62						5.7			15	15	100	n.a.	
		63						5.7			15	25	54	n.a.	
florasulam	triazolopyrimidine	561	TCWS55	WS5	Krieger	Naicom-hoodoo	clay loam	0.00256		40		5	85	0.97	105.70
		562						0.00256		40		10	46	0.97	
		563						0.00256		40		20	8.5	0.99	
fluorochloridone	pyrrolidinone	7	TCJB24	JB2	Walker	Big Cherry	sandy loam	4			13.1	10	89	0.97	55.71
		8						4			13.1	20	39.7	0.98	
imazamox	imidazolinone	396	TCEFSA0562	EFSA 056	Ta	Pontfarverger	silty clay loam	1		45	28	20	12	0.999	86.46
		397						1		45	28	10	42	0.993	
imidacloprid	neonicotinoid	55	TCJB81	JB8	Scorza	Andelst	not reported	0.8			22	5	547	n.a.	64.43
		56						0.8			22	15	153	n.a.	
		57						0.8			22	25	85	n.a.	
isoproturon	phenylurea	15	TCJB41	JB4	Berger	X5	loamy sand	1.5		40	13.1	0	46.2	0.973	40.60
		16						1.5		40	13.1	10	20.7	0.968	
		17						1.5		40	13.1	20	13.7	0.923	
		24	TCJB44	JB4	Berger	X17	silty	1.5		40	15.8	0	52	0.936	43.02

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isoproturon	phenylurea	25					loam	1.5		40	15.8	10	25.2	0.996	
		26						1.5		40	15.8	20	14.3	0.984	
		34	TCJB51	JB5	Blair	Broom's Barn	sandy clay loam	4			17.3	10	40.1	n.a.	44.97
		35						4			17.3	20	20.9	n.a.	
		38	TCJB52	JB5	Blair	Lidgate	clay	4			28.6	10	53.3	n.a.	46.68
		39						4			28.6	20	27.1	n.a.	
		487	TCWS317	WS3	Heiermann	Nienwohlde8	(braunerde)	1.07		60		10	121	0.91	40.50
		488						1.07		60		20	60	0.98	
		489						1.07		60		30	39	0.97	
		525	TCWS43	WS4	Jurado-Exposito	Wellesbourne 3		15			20	10	30.9	1	47.61
		526						15			20	20	15.5	0.99	
		685	TCWS122	WS12	Walker	Hunts Mill 1	sandy loam	10			8.9	5	82.5	0.979	45.26
		686						10			8.9	25	22.2	0.99	
		718	TCJJB42	JJB4	Beulke	Lawford		19			46	5	40.4	0.93	65.58
		719						19			46	15	15.1	0.88	
isoxaben	benzamide	5	TCJB23	JB2	Walker	Big Cherry	sandy loam	4			13.1	10	155	0.92	47.22
		6						4			13.1	20	78.2	0.89	
linuron	phenylurea	3	TCJB22	JB2	Walker	Big Cherry	sandy loam	4			13.1	10	76.2	0.9	51.56
		4						4			13.1	20	36.1	0.98	
		226	TCEU94	EU9	Walker	Colorado	loam	4			16.9	5	126	0.923	41.33
		228						4			16.8	25	38	0.968	
mepiquat chloride	quaternary ammonium	1142	TCRB131	RB13	Doris	X6	loamy sand	1		40		10	83	0.95	50.38
		1143						1		40		20	40	0.97	
mesosulfuron-methyl	sulfonylurea	398	TCEFSA0571	EFSA 057	Tarara	Lufa 2	loamy sand	0.02		50	27.7	20	49.1	0.9837	79.07
		399						0.02		50	27.7	10	154	0.9906	
		400	TCEFSA0572	EFSA 057	Tarara	Lufa 3	loamy sand	0.02		50	19.1	20	30.2	0.9962	68.77
		401						0.02		50	19.1	10	81.8	0.9956	
metamitron	triazinone	677	TCWS103	WS10	Vischetti	Umbria	clay loam	6.5	100			10	46.5	s.e. reported	60.33

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metamitron		678						6.5	100			20	19.4	s.e. reported	
		812	TCJJB95	JJB9	Capri	X16	silty clay loam	2			22	10	39.8	0.96	47.75
		813						2			22	20	15.5	0.99	
		814						2			22	30	10.5	0.98	
metazachlor	chloroacetamide	169	TCEU44	EU4	Walker	Wellesbourne 1	sandy loam	4			12	5	77	0.92	60.85
		170						4			12	15	29.2	0.92	
		171						4			12	25	13.2	0.92	
		695	TCJJB11	JJB1	Aden	Upper Rhine valley	loamy sand	1			8	10	44.6		65.57
metazachlor	chloroacetamide	696						1			8	30	7.1		
		705	TCJJB32	JJB3	Beulke	I		2		60		1	59.2	1	63.06
		706						2		60		10	24.3	1	
		707						2		60		20	8	1	
		708						2		60		30	4.5	1	
		709	TCJJB33	JJB3	Beulke	II		2.3		60		1	51.9	1	58.72
		710						2.3		60		10	29	1	
		711						2.3		60		20	9.7	1	
		712						2.3		60		30	4.8	1	
		713	TCJJB34	JJB3	Beulke	IV		3.3		60		10	53.2	1	66.06
		714						3.3		60		20	16.1	0.99	
		715						3.3		60		30	8.4	1	
		1144	TCRB 141	RB 14	Gottesbüren	Limburgerhof Bruch West	sandy loam	2 (dry wt)		40		10	19.7	0.998	66.15
		1145						2 (dry wt)		40		20	6.19	0.999	
		1146						2 (dry wt)		40		30	3.1	0.993	
metazachlor metab. BH479-4	chloroacetamide	1150	TCRB 143	RB 14	Gottesbüren	Limburgerhof Bruch West	sandy loam	2 (dry wt)		40		10	277	0.92	63.33
		1151						2 (dry wt)		40		20	70.7	0.97	
		1152						2 (dry wt)		40		30	47.5	0.99	

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Methabenz-thiazuron	urea	418	TCWS25	WS2	Gottesbüren	Ahlum 1	(parabraunerde)	2.8		60		10	137	0.98	46.85
		419						2.8		60		20	59	0.96	
		420						2.8		60		30	37	0.96	
methazole	phenylurea precursor	201	TCEU71	EU7	Walker	Sheep Pens	sandy loam	4			14.2	25	3.5	n.a.	75.43
		202						4			14.2	15	8.7	n.a.	
		203						4			14.2	5	31.1	n.a.	
methomyl	oxime carbamate	1219	TCSB101	SB10	Shaw	Nambsheim 1	sandy loam	3.8		50		10	23	1	92.74
		1220						3.8		50		20	6	0.99	
metolachlor	chloroacetamide	172	TCEU45	EU4	Walker	Wellesbourne 1	sandy loam	4			12	5	108	0.92	51.97
		173						4			12	15	47.4	0.92	
metolachlor	chloroacetamide	174						4			12	25	23.9	0.92	
		222	TCEU93	EU9	Walker	New York	sandy loam	4			16.9	5	135	0.861	46.54
		224						4			16.8	25	35	0.99	
		679	TCWS111	WS11	Vischetti	Udine		1.6	75			10	46.2	r = 1	58.48
		680						1.6	75			20	19.8	r = 0.94	
metribuzin	triazinone	9	TCJB31	JB3	Pestemer	Braunschweig 1	not reported	0.3		90	21.2	10	60	0.92	54.52
		10						0.3		90	21.2	20	29	0.992	
		11						0.3		90	21.2	30	13	0.97	
		130	TCEU314	EU3	Walker	Pump Ground 5 cm	sandy loam	4			9.1	5	209	0.81	60.63
		131						4			9.6	10	150	0.81	
		132						4			9.2	15	110	0.81	
		133						4			9.2	25	36.3	0.81	
oxamyl	oxime carbamate	372	TCEFSA0341	EFSA 034	Mattson	Commerce	silt loam	2		45	15	10	16.4	0.992	117.23
		373						2		45	15	20	3	0.988	
pendimethalin	dinitroaniline	421	TCWS26	WS2	Gottesbüren	Ahlum 1	(parabraunerde)	1.65		60		10	135	0.89	53.85
		422						1.65		60		20	50	0.94	
		423						1.65		60		30	30	0.95	
Penoxulam		1221	TCSB111	SB11	Jackson	Greggio	silty clay loam	0.2		40		6	137	0.96	66.47
		1222						0.2		40		20	24	0.99	
		1223						0.2		40		30	15	0.97	

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primisulfuron-methyl	sulfonylurea	901	TCEC62	EC6	Dinelli	Bologna	SILT LOAM	5	80		22.4	15	88.8	0.898	134.47
		902						5	80		22.4	20	38	0.967	
		903						5	80		22.4	25	13.5	0.959	
prometryne	triazine	232	TCEU102	EU10	Walker	Gravel Pits 2	sandy loam	8			11.2	15	112	0.982	70.60
		233						8			11.4	25	41.5	0.995	
propachlor	chloroacetamide	160	TCEU41	EU4	Walker	Wellesbourne 1	sandy loam	4			12	5	21.7	0.92	56.62
		161						4			12	15	9.2	0.92	
		162						4			12	25	4.2	0.92	
propiconazole	triazole	748	TCJJB65	JJB6	Bromilow	Rothamsted	clay loam	1	80			5	408	accurate rate constant s	65.72
propiconazole	triazole	749						1	80			10	195	accurate rate constant s	
		750						1	80			15	135	accurate rate constant s	
		751						1	80			18	113	accurate rate constant s	
propyzamide	benzamide	1	TCJB21	JB2	Walker	Big Cherry	sandy loam	4			13.1	10	63.4	0.84	52.57
		2						4			13.1	20	29.6	0.96	
		113	TCEU39	EU3	Walker	Pump Ground 5 cm	sandy loam	4			9.8	5	264	0.81	73.91
		114						4			9.3	10	136	0.81	
		115						4			9.9	20	55.5	0.81	
		116						4			9.8	25	36.1	0.81	
		117						4			9.5	30	15.9	0.81	
		234	TCEU111	EU11	Walker	Gravel Pits 1	sandy loam	6.4	100		11.7	15	76	n.a.	61.79
		235						6.4	100		11.9	25	32	n.a.	
		236	TCEU112	EU11	Walker	Little Cherry	sandy loam	6.4	100		12	15	70	n.a.	60.52
		237						6.4	100		12.1	25	30	n.a.	

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propyzamide		238	TCEU113	EU11	Walker	Gallas Leys	clay	6.4	100		16.7	15	112	n.a.	70.06
		239						6.4	100		16.7	25	42	n.a.	
		240	TCEU114	EU11	Walker	Water Meadows	clay loam	6.4	100		29.5	15	85	n.a.	63.38
		241						6.4	100		29.1	25	35	n.a.	
		533	TCWS47	WS4	Jurado-Exposito	Wellesbourne 3		15			20	10	77.9	0.98	113.23
		534						15			20	20	15.1	0.89	
proquinazid metab. IN-MM986		1179	TCRB232	RB23	Lee	Nambsheim 2	silt loam	0.2		40-50% (of 0 bar)		10	38	0.866	59.70
		1180						0.2		40-50% (of 0 bar)		20	16	0.929	
proquinazid metab. IN-MM991		1181	TCRB233	RB23	Lee	Nambsheim 2	silt loam	0.2		40-50% (of 0 bar)		10	121	0.954	120.86
		1182						0.2		40-50% (of 0 bar)		20	21	0.9	
rimsulfuron	sulfonylurea	905	TCEC64	EC6	Dinelli	Bologna	SILT LOAM	5	80		22.4	5	25.3	0.977	70.45
		906						5	80		22.4	10	15	0.986	
		907						5	80		22.4	15	9.7	0.959	
		908						5	80		22.4	20	6	0.993	
		909						5	80		22.4	25	3.1	0.927	
simazine	triazine	93	TCEU33	EU3	Walker	Pump Ground 5 cm	sandy loam	4			9.8	5	260	0.81	69.65
		94						4			9.3	10	125	0.81	
		95						4			9.9	20	47.8	0.81	
		96						4			9.8	25	29.4	0.81	
		97						4			9.5	30	21.5	0.81	
		230	TCEU101	EU10	Walker	Gravel Pits 2	sandy loam	8			11.5	15	112	0.963	80.54
		231						8			11.4	25	36.3	0.98	
terbuthylazine	triazine	681	TCWS11 2	WS11	Vischetti	Udine		0.8	75			10	148	r = 0.93	112.54
		682						0.8	75			20	28.9	r = 0.92	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Soil texture	Conc (mg kg^{-1})	FC (%)	MW HC (%)	Moist (% g g^{-1})	Temp (^{o}C)	DT_{50} (day)	R	E_a (kJ mol^{-1})
TFNA-AM (metabolite of flonicamid)		1209	TCSB51	SB5	Lenz	Bedfordshire 2	loamy sand	0.01		50		10	4.5	0.99	91.22
		1210						0.01		50		20	1.2	0.99	
triadimefon	triazole	756	TCJJB67	JJB6	Bromilow	Rothamsted	clay loam	1	80			5	35.7	accurate rate constant s	84.76
		757						1	80			10	16.9	accurate rate constant s	
		758						1	80			15	9.8	accurate rate constant s	
triadimefon	triazole	759						1	80			18	6.8	accurate rate constant s	
		760	TCJJB68	JJB6	Bromilow	Woburn	sandy loam	1	80			5	58.8	accurate rate constant s	76.42
		761						1	80			10	29	accurate rate constant s	
triadimefon	triazole	762						1	80			15	17.4	accurate rate constant s	
		763						1	80			18	13.4	accurate rate constant s	
triallate	thiocarbamate	427	TCWS28	WS2	Gottesbüren	Ahlum 1	(parabra unerde)	1.2		60		10	109	0.91	37.58
		428						1.2		60		20	65	0.97	
		429						1.2		60		30	38	0.96	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Soil texture	Conc (mg kg^{-1})	FC (%)	MW HC (%)	Moist (% g g^{-1})	Temp (^{o}C)	DT_{50} (day)	R	E_a (kJ mol^{-1})
triasulfuron	sulfonylurea	895	TCEC61	EC6	Dinelli	Bologna	silt loam	5	80		22.4	15	90.5	0.921	83.05
		896						5	80		22.4	20	49.4	0.921	
		897						5	80		22.4	25	28.3	0.951	
trifluralin	dinitroaniline	123	TCEU312	EU3	Walker	Pump Ground 5 cm	sandy loam	4			9.8	5	453	0.81	52.42
		124						4			9.3	10	321	0.81	
		125						4			9.9	20	149	0.81	
		126						4			9.8	25	101	0.81	
		127						4			9.5	30	71	0.81	

Conc = Initial test substance concentration in soil (mg kg^{-1})

FC = Experimental soil moisture content (% of FC)

MWHC = Experimental soil moisture content (% of MWHC)

Moist = Experimental soil moisture content (% g g^{-1})

Temp = Incubation temperature (^{0}C)

DT_{50} = DT_{50} (days)

R = Square of Pearson moment (from regression analysis) (r^2)

E_a = Activation energy (kJ mol^{-1}) calculated from the above data (sometimes reported as kcal mol^{-1} in the older literature)

Appendix 3

Rejected studies. Summary of experimental data rejected for Q_{10} assessment

The comprehensive document detailing the assessment of all considered studies is available at the EFSA web-site. See foot-note[2]

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
(*E*)-1,3-dichloropropene	chlorinated hydrocarbon	930	TCEC94	EC9	Gan	Arlington sandy loam	20	2.7	no	yes	yes	no	
		931					30	1.31	no	yes	yes	no	
		932					35	1.02	no	yes	yes	no	
		933					40	0.84	no	yes	yes	no	
		934	TCEC95	EC9	Gan	Arlington sandy loam	20	5.16	no	yes	yes	no	
		935					30	3.17	no	yes	yes	no	
		936					35	2.02	no	yes	yes	no	
		937					40	1.57	no	yes	yes	no	
		938	TCEC96	EC9	Gan	Arlington sandy loam	20	7.22	no	yes	yes	no	
		939					30	3.32	no	yes	yes	no	
		940					35	2.86	no	yes	yes	no	
		941					40	1.83	no	yes	yes	no	
		942	TCEC97	EC9	Gan	Arlington sandy loam	20	11.11	no	yes	yes	no	
		943					30	3.11	no	yes	yes	no	
		944					35	3.11	no	yes	yes	no	
		945					40	1.76	no	yes	yes	no	
		998	TCMM15	MM1	Ma	Arlington sandy loam	35	1.02	yes	yes	yes	no	Above 30ºC
		999					40	0.84	yes	yes	yes	no	Half life below 1 day
		1000	TCMM16	MM1	Ma	Arlington	20	5.16	yes	yes	yes	no	Fumigant, biocidal action not dismissed

[2] http://www.efsa.europa.eu/EFSA/ScientificOpinionPublicationReport/efsa_locale-1178620753812_ScientificOpinions.htm

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
(*E*)-1,3-dichloropropene	chlorinated hydrocarbon	1001				sandy loam	30	3.17	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1002					35	2.02	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1003					40	1.57	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1004	TCMM17	MM1	Ma	Arlington sandy loam	20	7.22	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1005					30	3.32	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1006					35	2.86	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1007					40	1.83	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1008	TCMM18	MM1	Ma	Arlington sandy loam	20	11.11	yes	yes	yes	no	Authors did not investigate sterile degradation at this dosage. excluded because of suspected biocidal action
		1009					30	3.11	yes	yes	yes	no	Authors did not investigate sterile degradation at this dosage. excluded because of suspected biocidal action
		1010					35	3.11	yes	yes	yes	no	Authors did not investigate sterile degradation at this dosage. excluded because of suspected biocidal action
		1011					40	1.76	yes	yes	yes	no	Authors did not investigate sterile degradation at this dosage. excluded because of suspected biocidal action
(*Z*)-1,3-dichloropropene	chlorinated hydrocarbon	946	TCEC98	EC9	Gan	Arlington sandy loam	20	3.48	no	yes	yes	no	
		947					30	1.53	no	yes	yes	no	
		948					35	1.16	no	yes	yes	no	
		949					40	0.91	no	yes	yes	no	
		950	TCEC99	EC9	Gan	Arlington sandy loam	20	5.07	no	yes	yes	no	
		951					30	2.89	no	yes	yes	no	
		952					35	1.9	no	yes	yes	no	
		953					40	1.31	no	yes	yes	no	
		954	TCEC910	EC9	Gan	Arlington sandy loam	20	6.88	no	yes	yes	no	
		955					30	2.86	no	yes	yes	no	
		956					35	2.37	no	yes	yes	no	
(*Z*)-1,3-	chlorinated	957					40	1.44	no	yes	yes	no	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (⁰C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
dichloropropene	hydrocarbon												
		958	TCEC911	EC9	Gan	Arlington sandy loam	20	10.31	no	yes	yes	no	
		959					30	2.7	no	yes	yes	no	
		960					35	2.27	no	yes	yes	no	
		961					40	1.33	no	yes	yes	no	
		1014	TCMM19	MM1	Ma	Arlington sandy loam	35	1.16	yes	yes	yes	no	Above 30ºC
		1015					40	0.91	yes	yes	yes	no	Half life below 1 day
		1016	TCMM110	MM1	Ma	Arlington sandy loam	20	5.07	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1017					30	2.89	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1018					35	1.9	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1019					40	1.31	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1020	TCMM111	MM1	Ma	Arlington sandy loam	20	6.88	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1021					30	2.86	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1022					35	2.37	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1023					40	1.44	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		1024	TCMM112	MM1	Ma	Arlington sandy loam	20	10.31	yes	yes	yes	no	Authors did not investigate sterile degradation at this dosage. excluded because of suspected biocidal action
		1025					30	2.7	yes	yes	yes	no	Authors did not investigate sterile degradation at this dosage. excluded because of suspected biocidal action
		1026					35	2.27	yes	yes	yes	no	Authors did not investigate sterile degradation at this dosage. excluded because of suspected biocidal action
		1027					40	1.33	yes	yes	yes	no	Authors did not investigate sterile degradation at this dosage. excluded because of suspected biocidal action

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
1,3-dichloropropene	chlorinated hydrocarbon	340	TCEFSA 0011	EFS A001	Batzer	Marcham 3	10	24.9	no	yes	yes	no	RMS recalculated DT_{50}. after storage of soil for an unknown period under unknown conditions soils were moistened and pre-incubated for 10 days at 20°C before addition of the test substance
		341					20	9.3	no	yes	yes	no	
2,4,5-T	phenoxyacetate	313	TCEU15 1	EU15	Walker	Regina 2	10	57.7	no	yes	yes	no	r given in the paper! Data seem ok
		314					25	11	no	yes	yes	no	Using first-order kinetics
		315					35	6.8	no	yes	yes	no	DT_{50} values were calculated from the rate constants (*k*) provided
		316	TCEU15 2	EU15	Walker	Regina 2	10	62.9	no	yes	yes	no	
		317					15	26.6	no	yes	yes	no	
		318					20	19.8	no	yes	yes	no	
		319					25	7.7	no	yes	yes	no	
		320					30	4.4	no	yes	yes	no	
		321					35	3.9	no	yes	yes	no	
5-0H-florasulam	triazolopyrimidine	548	TCWS52	WS5	Krieger	Cuckney	5	49	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
		549					15	29	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
		550					25	11	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
		556	TCWS54	WS5	Krieger	Marcham 2	5	78	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
		557					10	54	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (⁰C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
5-0H-florasulam	triazolopyrimidine	558					15	23	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
		559					20	15	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
5-0H-florasulam	triazolopyrimidine	560					25	8.1	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
		565	TCWS56	WS5	Krieger	Naicom-hoodoo	5	43	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
		566					10	48	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
		567					20	27	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
		568					35	16	yes	n.a.	not evaluated	no	Not evaluated because of data quality issues (metabolite)
abamectin	avermectin	1107	TCRB11	RB1	Adam	Gartenacker Switzerland 2	8.6	59.4 (52.4)	no	yes	yes	no	Recalculated DT_{50} (original in brackets)
		1108					19.5	23.3 (21.3)	no	yes	yes	no	Recalculated DT_{50} (original in brackets)
		1109					30	16.6 (16.0)	no	yes	yes	no	Recalculated DT_{50} (original in brackets)
acequinocyl	naphthaquinone	1201	TCSB11	SB1	Aikens	Evesham 1	10	4.7	no	yes	no	no	Rejected because: DT_{50} calc by RMS in DAR 1.9 days. This reflects measurements on page 48 better, but not possible to evaluate goodness of fit in DAR. No information on storage time.

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
acequinocyl	naphthaquinone	1202					20	2.3	no	yes	no	no	Rejected because: DT_{50} calc by RMS in DAR 1.1 days. This reflects measurements on page 49 better, but not possible to evaluate goodness of fit in DAR. No information on storage time.
alachlor	chloroacetamide	185	TCEU62	EU6	Walker	Hunts Mill 2	5	119.1	yes	yes	yes	no	No forced air flow, rejected because same as TCEU51
		186					10	76.6	yes	yes	yes	no	No forced air flow, rejected because same as TCEU51
		187					15	39.7	yes	yes	yes	no	No forced air flow, rejected because same as TCEU51
		188					20	25.7	yes	yes	yes	no	No forced air flow, rejected because same as TCEU51
		189					25	17.3	yes	yes	yes	no	No forced air flow, rejected because same as TCEU51
		195	TCEU64	EU6	Walker	Little Cherry 20-40 cm	5	170.9	yes	yes	yes	no	Other dataset for same soil and pesticide was preferred
		196					15	50	yes	yes	yes	no	Other dataset for same soil and pesticide was preferred
		197					25	19.9	yes	yes	yes	no	Other dataset for same soil and pesticide was preferred
		198	TCEU65	EU6	Walker	Little Cherry 40-60 cm	5	279.6	yes	yes	yes	no	Other dataset for same soil and pesticide was preferred
		199					15	91.6	yes	yes	yes	no	Other dataset for same soil and pesticide was preferred
		200					25	34.8	yes	yes	yes	no	Other dataset for same soil and pesticide was preferred
		537	TCWS49	WS4	Jurado-Exposito	Wellesbourne 3	10	118.8	yes	yes	yes	no	Volatile, but no forced air flow. rejected because: 20% moisture preferred (shorter half-lives)
		538					20	38.5	yes	yes	yes	no	Volatile, but no forced air flow. rejected because: 20% moisture preferred (shorter half-lives)

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^0C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
alachlor	chloroacetamide	539	TCWS410	WS4	Jurado-Exposito	Wellesbourne 3	10	115.5	yes	yes	no	no	Volatile, but no forced air flow. Rejected because: 20% moisture preferred (shorter half-lives) 1st sample only 80% of theoretically applied, slow degradation after that, fit under-estimates true DT_{50}
		540					20	38.7	yes	yes	yes	no	Volatile, but no forced air flow. rejected because: 20% moisture preferred (shorter half-lives)
		543	TCWS412	WS4	Jurado-Exposito	Wellesbourne 3	10	69.3	yes	yes	no	no	Volatile, but no forced air flow Rejected because visual fit not very good and replication of other study at same conditions
		544					20	20.4	yes	yes	no	no	Volatile, but no forced air flow. Rejected because visual fit not very good and replication of other study at same conditions
alpha-hexachlorocyclohexane	chlorinated hydrocarbon	978	TCEC151	EC15	Lemley	X8			no	no	no	no	65 soils collected in different ecosystems. paper not suitable for this scope because missing a large amount of information
allyl isothiocyanate	isothiocyanate	869	TCEC31	EC3	Borek	Latahco	10	1.46	no	no	no	no	Visual inspection for DT_{50}. storage time missed
		870					15	1.08	no	no	no	no	Visual inspection for DT_{50}. storage time missed
		871					20	0.96	no	no	no	no	Visual inspection for DT_{50}. storage time missed
		872					25	0.83	no	no	no	no	Visual inspection for DT_{50}. storage time missed
allylnitrile	nitrile	873	TCEC32	EC3	Borek	Latahco	10	4.17	no	no	no	no	Visual inspection for DT_{50}. storage time missed
		874					15	4.42	no	no	no	no	Visual inspection for DT_{50}. storage time missed
		875					20	4.5	no	no	no	no	Visual inspection for DT_{50}. storage time missed
		876					25	4.63	no	no	no	no	Visual inspection for DT_{50}. storage time missed

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (⁰C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
amidosulfuron	sulfonylurea	634	TCWS81	WS8	Smith	Indian head	10	63	yes	n.a.	no	no	Rejected because only 3 data points
		635					20	45	yes	n.a.	yes	no	Rejected: day 0 not measured but set to 100% in fitting, conc. of 1st sample well below 100%
		636					30	33	yes	n.a.	yes	no	Rejected: day 0 not measured but set to 100% in fitting, conc. of 1st sample well below 100%
		637	TCWS82	WS8	Smith	Regina 1	10	231	yes	n.a.	no	no	Extrapolated too far beyond the study period (84 days) r2<0.8, only 3 data points
		638					20	79	yes	n.a.	no	no	Rejected: only 4 data points
amidosulfuron	sulfonylurea	639					30	46	yes	n.a.	yes	no	Rejected: day 0 not measured but set to 100% in fitting, conc. of 1st sample well below 100%
		640	TCWS83	WS8	Smith	White city	10	44	yes	n.a.	no	no	Rejected because only 3 data points
		641					20	26	yes	n.a.	yes	no	Rejected: day 0 not measured but set to 100% in fitting, conc. of 1st sample well below 100%
		642					30	14	yes	n.a.	yes	no	Rejected: day 0 not measured but set to 100% in fitting, conc. of 1st sample well below 100%
		1110	TCRB21	RB2	Till	Speyer 4	10	21	no	yes	yes	no	Different soil samples for the two temperatures
		1111					20	3	no	yes	yes	no	Different soil samples for the two temperatures
		1112	TCRB31	RB3	Erzgräber	Speyer 4	10	23.2	no	yes	yes	no	Recalculation of RB2 (Till) using TopFit, but MFO kinetics not helpful
		1113					20	2.2	no	yes	yes	no	Recalculation of RB2 (Till) using TopFit, but MFO kinetics not helpful
asulam	carbamate	1114	TCRB41	RB4	Yeomans	X14	20	3.89	no	yes	yes	no	
		1115					10	9.35	no	yes	yes	no	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (⁰C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
atrazine	triazine	98	TCEU34	EU3	Walker	Pump Ground 5 cm	5	209	yes	yes	yes	no	Data not used because soil moisture below 5%
		99					15	99.3	yes	yes	yes	no	Data not used because soil moisture below 5%
		100					25	31.7	yes	yes	yes	no	Data not used because soil moisture below 5%
		101	TCEU35	EU3	Walker	Pump Ground 5 cm	15	83.6	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		102					25	25.9	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		214	TCEU91	EU9	Walker	Colorado	5	181	yes	yes	no	no	No visual inspection possible, decide fit quality on n/r2 ratio
atrazine	triazine	215					15	87	yes	yes	yes	no	No visual inspection possible, decide fit quality on n/r2 ratio
		216					25	41	yes	yes	yes	yes	No visual inspection possible, decide fit quality on n/r2 ratio
		217					35	22	yes	yes	yes	no	^{14}C-Labelled compounds were used. excluded because temperature above 30ºC
		219	TCEU92	EU9	Walker	Mississip pi	15	100	yes	yes	yes	no	No visual inspection possible, decide fit quality on n/r2 ratio
		221					35	27	yes	yes	yes	no	No visual inspection possible, decide fit quality on n/r2 ratio. excluded because temperature above 30ºC
		247	TCEU13 1	EU13	Smith	Regina 2	5	206	no	yes	no	no	r2>0.84. quality criterion depends on n/r2 ratio
		248					10	79	no	yes	yes	no	r2>0.84. quality criterion depends on n/r2 ratio
		249					15	71	no	yes	yes	no	r2>0.84. quality criterion depends on n/r2 ratio
		250					20	56	no	yes	yes	no	r2>0.84. quality criterion depends on n/r2 ratio
		251					25	51	no	yes	yes	no	r2>0.84. quality criterion depends on n/r2 ratio

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (°C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
atrazine	triazine	252					30	44	no	yes	yes	no	r2>0.84. quality criterion depends on n/r2 ratio
		574	TCWS71	WS7	Rocha F	X9	5	87	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		575					10	70	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		576					25	33	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		577					30	27	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		578					40	17	yes	yes	yes	no	Rejected because - temperature > 30°C - 60% moisture preferred (shorter half-lives)
		579	TCWS72	WS7	Rocha F	X9	5	82	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		580					10	65	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		581					25	31	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		582					30	25	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		583					40	16	yes	yes	yes	no	Rejected because - temperature > 30°C - 60% moisture preferred (shorter half-lives)
		588	TCWS73	WS7	Rocha F	X9	40	15	yes	yes	yes	no	Rejected because temperature > 30oC
		589	TCWS74	WS7	Rocha F	X12	5	92	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		590					10	73	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		591					25	32	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		592					30	25	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
atrazine	triazine	593					40	16	yes	yes	yes	no	Rejected because - temperature > 30^{o}C - 60% moisture preferred (shorter half-lives)
		594	TCWS75	WS7	Rocha F	X12	5	83	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		595					10	63	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		596					25	23	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		597					30	22	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		598					40	14	yes	yes	yes	no	Rejected because - temperature > 30^{o}C - 60% moisture preferred (shorter half-lives)
		603	TCWS76	WS7	Rocha F	X12	40	12	yes	yes	yes	no	Rejected because temperature > 30^{o}C
		604	TCWS77	WS7	Rocha F	X18	5	201	yes	yes	yes	no	Rejected because: - 60% moisture preferred (shorter half-lives) - DT_{50} exceeds 2 x study period (= 100 d, from Rocha and Walker, Weed Res. 1995)
		605					10	144	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		606					25	58	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		607					30	43	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		608					40	24	yes	yes	yes	no	Rejected because - temperature > 30^{o}C - 60% moisture preferred (shorter half-lives)
		609	TCWS78	WS7	Rocha F	X18	5	167	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		610					10	121	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		611					25	48	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (°C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
atrazine	triazine	612					30	35	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		613					40	20	yes	yes	yes	no	Rejected because - temperature > 30°C - 60% moisture preferred (shorter half-lives)
		618	TCWS79	WS7	Rocha F	X18	40	17	yes	yes	yes	no	Rejected because temperature > 30°C
		619	TCWS710	WS7	Rocha F	X4	5	390	yes	yes	yes	no	Rejected because: - 60% moisture preferred (shorter half-lives) - DT_{50} exceeds 2 x study period (= 100 d, from Rocha and Walker, Weed Res. 1995)
		620					10	261	yes	yes	yes	no	Rejected because: - 60% moisture preferred (shorter half-lives) - DT_{50} exceeds 2 x study period (= 100 d, from Rocha and Walker, Weed Res. 1995)
		621					25	90	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		622					30	59	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		623					40	27	yes	yes	yes	no	Rejected because - temperature > 30°C - 60% moisture preferred (shorter half-lives)
		624	TCWS711	WS7	Rocha F	X4	5	324	yes	yes	yes	no	Rejected because: - 60% moisture preferred (shorter half-lives) - DT_{50} exceeds 2 x study period (= 100 d, from Rocha and Walker, Weed Res. 1995)
		625					10	215	yes	yes	yes	no	Rejected because: - 60% moisture preferred (shorter half-lives) - DT_{50} exceeds 2 x study period (= 100 d, from Rocha and Walker, Weed Res. 1995)
		626					25	74	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		627					30	52	yes	yes	yes	no	Rejected because 60% moisture preferred (shorter half-lives)
		628					40	25	yes	yes	yes	no	Rejected because - temperature > 30°C - 60% moisture preferred (shorter half-lives)

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
atrazine	triazine	629	TCWS712	WS7	Rocha F	X4	5	265	yes	yes	yes	no	Rejected because: DT_{50} exceeds 2 x study period (= 100 d, from Rocha and Walker, Weed Res. 1995)
		633					40	21	yes	yes	yes	no	Rejected because temperature > 30^{o}C
		821	TCJJB111	JJB11	Dinelli	Ozzano	5	366.9	no	yes	no	no	
		822					10	173	no	yes	yes	no	
		823					15	50.5	no	yes	yes	no	
		824					20	39.5	no	yes	yes	no	
		825					25	31.2	no	yes	yes	no	
		826					35	20.2	no	yes	yes	no	
		827	TCJJB112	JJB11	Dinelli	Ozzano	15	70.8	no	yes	yes	no	
		828					25	39.6	no	yes	yes	no	
		829					35	25.2	no	yes	yes	no	
		830	TCJJB113	JJB11	Dinelli	Ozzano	15	88.2	no	yes	yes	no	
		831					25	45.5	no	yes	yes	no	
		832					35	27.1	no	yes	yes	no	
bentazon	benzothiadiazinone	726	TCJJB52	JJB5	Beulke	Salop clay loam small	15	37.6	yes	yes	no	no	No forced air flow, rejected because 70% MWHC data from same soil preferred
bentazon	benzothiadiazinone	727					25	21.3	yes	yes	yes	no	No forced air flow, rejected because 70% MWHC data from same soil preferred
		728					15	58.2	yes	yes	no	no	No forced air flow, rejected because 70% MWHC data from same soil preferred
		729					25	31.4	yes	yes	yes	no	No forced air flow, rejected because 70% MWHC data from same soil preferred
bifenox	diphenyl ether	1116	TCRB51	RB5	Simmonds	Aldhams Farm	20	36.8 (16.6)	yes	yes	no	no	Note SFO or KIM 2-compartment model
		1117					10	55.6 (34.6)	yes	yes	no	no	Note SFO or KIM 2-compartment model
buprofezin		1118	TCRB61	RB6	Lewis	Ipswich	10	170	yes	yes	yes	no	Two-compartment model, not useful
		1119					20	99	yes	yes	yes	no	Two-compartment model, not useful

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
cadusafos	organophosphate	1072	TCMM67	MM6	Zheng	Martinique Paquemar	25	42.1	no	no	no	no	
		1073					35	33.6	no	no	no	no	
		1074	TCMM68	MM6	Zheng	Martinique St Anne	25	42.6	no	no	no	no	
		1075					35	37.8	no	no	no	no	
		1076	TCMM69	MM6	Zheng	Martinique Bochet	25	38.9	no	no	no	no	
		1077					35	30.4	no	no	no	no	
		1078	TCMM610	MM6	Zheng	Martinique Leyritz	25	38.2	no	no	no	no	
		1079					35	32.5	no	no	no	no	
		1080	TCMM611	MM6	Zheng	Martinique Eden	25	40.4	no	no	no	no	
		1081					35	31.3	no	no	no	no	
		1082	TCMM612	MM6	Zheng	France Marsillargues	25	37.3	no	no	no	no	
		1083					35	27	no	no	no	no	
carbetamide	carbamate	1120	TCRB71	RB7	Ambrosi	Emerainville	12	35	no	yes	no	no	Graphical analysis, 1978 study, soil air dried
		1121					25	9	no	yes	no	no	Graphical analysis, 1978 study, soil air dried
		1122					25	8	no	yes	no	no	Graphical analysis, 1978 study, soil air dried
		1123	TCRB72	RB7	Ambrosi	Le Mort	12	40	no	yes	no	no	Graphical analysis, 1978 study, soil air dried
		1124					25	7	no	yes	no	no	Graphical analysis, 1978 study, soil air dried
		1125					25	4	no	yes	no	no	Graphical analysis, 1978 study, soil air dried
		649	TCWS93	WS9	Tariql	Pakistan	15	69.3	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (°C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
carbetamide	carbamate	650					25	57.8	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		651					35	43.3	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		652	TCWS94	WS9	Tariql	Pakistan	15	63.2	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
carbosulfan	carbamate	653					25	51.3	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
carbosulfan	carbamate	654					35	34.7	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		643	TCWS91	WS9	Tariql	Pakistan	15	5.33	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		644					25	3.85	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		645					35	1.98	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		646	TCWS92	WS9	Tariql	Pakistan	15	6.13	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
carbosulfan	carbamate	647					25	3.85	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		648					35	1.41	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
chloridazon	pyridazinone	803	TCJJB91	JJB9	Capri	X16	10	133.7	yes	yes	no	no	
		804					30	12.2	yes	yes	yes	no	Rejected because data at 22% moisture preferred (larger number of temperatures)
		808	TCJJB93	JJB9	Capri	X16	10	41	yes	yes	no	no	
		809					30	7.9	yes	yes	yes	no	Rejected because data at 22% moisture preferred (larger number of temperatures)
chlorotoluron	phenylurea	430	TCWS31	WS3	Heiermann	Neuenkirchen	1	269	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures extrapolated too far beyond end of study period (85 d)
		431					10	106	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		432					20	40	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (°C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
chlorotoluron	phenylurea	433	TCWS32	WS3	Heiermann	Neuenkirchen	1	147	no	yes	yes	no	Rejected because storage period too long
		434					10	48	no	yes	yes	no	Rejected because storage period too long
		435					20	13	no	yes	yes	no	Rejected because storage period too long
		436					30	11	no	yes	yes	no	Rejected because storage period too long
		437	TCWS33	WS3	Heiermann	Neuenkirchen	1	111	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		438					10	41	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		439					20	11	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		440	TCWS34	WS3	Heiermann	Nienwohlde8	1	222	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		441					10	124	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		442					20	61	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (⁰C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
chlorotoluron	phenylurea	443	TCWS35	WS3	Heiermann	Nienwohlde8	1	239	no	yes	yes	no	Rejected because: storage period too long extrapolated too far beyond end of study period (85 d)
		444					10	109	no	yes	yes	no	Rejected because storage period too long
		445					20	54	no	yes	yes	no	Rejected because storage period too long
		446					30	50	no	yes	yes	no	Rejected because storage period too long
		447	TCWS36	WS3	Heiermann	Nienwohlde8	1	233	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures extrapolated too far beyond end of study period (85 d)
		448					10	107	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		449					20	50	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		716	TCJJB41	JJB4	Beulke	Lawford heavy clay	5	73.5	yes	yes	no	no	
		717					15	39.2	yes	yes	no	no	
chlorsulfuron	sulfonylurea	209	TCEU82	EU8	Walker	Wellesbourne 2	10	54.2	yes	yes	no	no	
		210					20	31.9	yes	yes	no	no	
		211					30	9.7	yes	yes	no	no	
		212	TCEU83	EU8	Walker	Wellesbourne 2	20	56	yes	yes	no	no	
		213					30	26.5	yes	yes	no	no	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
chlorsulfuron	sulfonylurea	324	TCEU17 1	EU17	James	Horotiu 2	10	38.1	yes	yes	yes	no	Rejected because DT_{50} does not represent data (day 0 excluded from fitting, <50% present on first included time point day 7)
		325					22	27.9	yes	yes	yes	no	Rejected because DT_{50} does not represent data (day 0 excluded from fitting, <50% present on first included time point day 7)
		326					30	22	yes	yes	no	no	Rejected because DT_{50} does not represent data (day 0 excluded from fitting, <50% present on first included time point day 7)
		975	TCEC14 1	EC14	Kinfe	Tillman-Hollister	25	13	no	no	no	no	Long storage, bioassay estimation of the soil concentration
chlorthal-dimethyl	phthalic acid	136	TCEU31 6	EU3	Walker	Pump Ground 5 cm	20	197	yes	yes	yes	no	Data not used because soil moisture below 5%
		137					30	66	yes	yes	yes	no	Data not used because soil moisture below 5%
		142	TCEU31 8	EU3	Walker	Pump Ground 5 cm	10	155	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		143					20	40.5	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
cis-chlordane	chlorinated hydrocarbon	977	TCEC15 1	EC15	Lemley	X8			no	no	no	no	65 soils collected in different ecosystems. paper not suitable for this scope because missing a large amount of information
cis-permethrin	pyrethroid	1099	TCMM81	MM8	Jordan	Dubbs	10	29	no	yes	yes	no	Storage not reported is the only problem
		1100					25	9.7	no	yes	yes	no	1982 paper. could not find author
		1101					40	14.7	no	yes	yes	no	
clomazone	isoxazolidinone	1205	TCSB31	SB3	Bauman n	Speyer 3	10	19.8	yes	no	no	no	19.8 day is the recalculated agreed EU endpoint (page 60) Rejected because - day zero conc. 61-76% of applied. applied amount 10x target amount of 0.08 mg/kg. the 'target rate', had it been achieved, would have been below the stated limit of determination

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
clomazone	isoxazolidinone	1206					20	26.7	yes	no	no	no	26.7 day is the recalculated agreed EU endpoint (page 2) Rejected because - day zero conc. 56-79% of applied. applied amount 10x the target rate of 0.08 mg/kg. the 'target rate', had it been achieved, would have been below the stated limit of determination
clopyralid	pyridinecarboxylic acid	342	TCEFSA 0091	EFS A009	Baloch	Marcham 4	10	100	no	yes	yes	no	
		343					20	36	no	yes	yes	no	
		344	TCEFSA 0092	EFS A009	Baloch	Parabraunerde Germany	10	198	no	yes	yes	no	
		345					20	45	no	yes	yes	no	
		346	TCEFSA 0093	EFS A009	Baloch	Castle Rising UK	10	73	no	yes	yes	no	
		347					20	28	no	yes	yes	no	
cloransulam	triazolopyrimidine	1105	TCMM91	MM9	Wolt	Hanford loam	5	10180	no	no	no	no	Degradation only clear after 397 days. DT_{50} recalculated non-linear SFO
		1106					25	16	no	no	yes	no	DT_{50} recalculated non-linear SFO
cyanazine	triazine	253	TCEU132	EU13	Smith	Regina 2	5	19	no	yes	yes	no	r2>0.9. quality criterion depends on n/r2 ratio
		254					10	12.8	no	yes	yes	no	r2>0.9. quality criterion depends on n/r2 ratio
		255					15	7.6	no	yes	yes	no	r2>0.9. quality criterion depends on n/r2 ratio
		256					20	4.8	no	yes	yes	no	r2>0.9. quality criterion depends on n/r2 ratio
		257					25	3.5	no	yes	yes	no	r2>0.9. quality criterion depends on n/r2 ratio
		258					30	2.6	no	yes	yes	no	r2>0.9. quality criterion depends on n/r2 ratio

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
cyanazine	triazine	720	TCJJB51	JJB5	Beulke	Salop clay loam small	15	19.1	yes	yes	yes	no	Rejected because 70% MWHC data from same soil preferred
		721					25	10.4	yes	yes	yes	no	Rejected because 70% MWHC data from same soil preferred
		722					15	25.1	yes	yes	no	no	Rejected because 70% MWHC data from same soil preferred
		723					25	20.1	yes	yes	yes	no	Rejected because 70% MWHC data from same soil preferred
diflufenican	pyridinecarboxamide	1126	TCRB81	RB8	Mahay	X15	10	182 (193)	yes	yes	no	no	Soil storage. SFO correlation poor, Kim 1-compartment model not very helpful
		1127					20	137 (82.2)	yes	yes	no	no	Soil storage: SFO correlation ok. Kim 2-compartment model not very helpful
		1128	TCRB91	RB9	Giraud	X13	10	975	no	yes	no	no	Air-dried soil. large extrapolation as long half-life
		1129					22	294	no	yes	yes	no	Air-dried soil
		1130	TCRB92	RB9	Giraud	X1	10	728	no	yes	yes	no	Air-dried soil
		1131					22	168	no	yes	yes	no	Air-dried soil
dimoxystrobin	strobilurin	392	TCEFSA 0551	EFS A055	Staudenmaier	Lufa 1	5	1203	no	yes	no	no	Soil-storage according to BBA guidelines
		393					30	200	no	yes	yes	no	Soil-storage according to BBA guidelines
diuron	phenylurea	352	TCEFSA 0171	EFS A017	Mackie	Mogenstrupvej	10	143	no	no	no	no	4 weeks soil storage after field collection under non-defined conditions
		353					20	51	no	no	no	no	4 weeks soil storage after field collection under non-defined conditions
		687	TCWS123	WS12	Walker	Cottage fields	5	103.5	yes	yes	yes	no	Rejected because DT_{50} > 2x study period (35 d)
		688					25	48.1	yes	yes	yes	yes	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
diuron	phenylurea	689	TCWS124	WS12	Walker	Hunts Mill 1	5	247.6	yes	yes	yes	no	Rejected because DT_{50} > 2x study period (42 d)
		690					25	48.1	yes	yes	yes	yes	
endosulfan	chlorinated hydrocarbon	661	TCWS97	WS9	Tariql	Pakistan	15	130.8	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		662					25	106.6	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		663					35	86.6	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		664	TCWS98	WS9	Tariql	Pakistan	15	115.5	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
endosulfan	chlorinated hydrocarbon	665					25	88.9	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		666					35	63	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
epoxiconazole	triazole	740	TCJJB63	JJB6	Bromilow	Rothamsted clay loam	5	1507	yes	yes	no	no	
		741					10	1332	yes	yes	no	no	
		742					15	1100	yes	yes	no	no	
		743					18	1004	yes	yes	no	no	
		744	TCJJB64	JJB6	Bromilow	Woburn sandy loam	5	1540	yes	yes	no	no	
		745					10	1066	yes	yes	yes	yes	
		746					15	815	yes	yes	no	no	
		747					18	737	yes	yes	no	no	
ethofumesate	benzofuran	409	TCWS22	WS2	Gottesbüren	Ahlum 1	10	88	yes	yes	no	no	Storage information from Beulke, diploma thesis 1991 Rejected because - same soil as study ethofumesate, Ahlum 1987 - only 4 sampling points
		410					20	28	yes	yes	yes	no	Storage information from Beulke, diploma thesis 1991 Rejected because same soil as study ethofumesate, Ahlum 1987
		411					30	26	yes	yes	yes	no	Storage information from Beulke, diploma thesis 1991 Rejected because same soil as study ethofumesate, Ahlum 1988

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
ethofumesate	benzofuran	412	TCWS23	WS2	Gottesbüren	Braunschweig 1	10	248	yes	yes	no	no	Storage information from Beulke, diploma thesis 1991 rRejected because - DT_{50} > 2 x study period (84 days) - only 4 sampling points
		413					20	65	yes	yes	yes	no	Storage information from Beulke, diploma thesis 1991. Rejected because Ea above 20°C is very low, whereas appears high at lower temp.
		414					30	64	yes	yes	yes	no	Storage information from Beulke, diploma thesis 1991. Rejected because Ea above 20°C is very low, whereas appears high at lower temp.
		415	TCWS24	WS2	Gottesbüren	Salzdahlum	10	152	yes	yes	no	no	Storage information from Beulke, diploma thesis 1991 Rejected because only 4 sampling points
		416					20	42	yes	yes	yes	no	Storage information from Beulke, diploma thesis 1991. Rejected because Ea above 20°C is very low, whereas appears high at lower temp.
		417					30	33	yes	yes	yes	no	Storage information from Beulke, diploma thesis 1991. Rejected because Ea above 20°C is very low, whereas appears high at lower temp.
		450	TCWS37	WS3	Heiermann	Neuenkirchen	1	393	yes	yes	no	no	Rejected because: 80% MWHC preferred because fits are better extrapolated too far beyond end of study period (85 d) r2 < 0.8 note: this is the SFO value, wrong way round in table A1
		451					10	86	yes	yes	no	no	Rejected because: 80% MWHC preferred because fits are better see p 48 for first-order value (ECPA recalculated SFO value = 76 d) SB recalculated SFO DT_{50} = 76 days, visual fit poor

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
ethofumesate	benzofuran	452					20	36	yes	yes	yes	no	Rejected because: 80% MWHC preferred because fits are better
		453					30	36	yes	yes	yes	no	Rejected because: 80% MWHC preferred because fits are better
		454	TCWS38	WS3	Heiermann	Neuenkirchen	1	202	yes	yes	no	no	Rejected because: 80% MWHC preferred because fits are better extrapolated too far beyond end of study period (85 d) r2 < 0.8
		455					10	36	yes	yes	no	no	Rejected because: 80% MWHC preferred because fits are better
		456					20	21	yes	yes	yes	no	Rejected because: 80% MWHC preferred because fits are better
		457					30	19	yes	yes	no	no	Rejected because: 80% MWHC preferred because fits are better
		462	TCWS310	WS3	Heiermann	Nienwohlde7	1	467	yes	yes	no	no	Rejected because: extrapolated too far beyond end of study period (84 d) r2 <0.8 60% MWHC preferred because larger no of temperatures
		463					20	105	yes	yes	yes	no	Rejected because: 60% MWHC preferred because larger no of temperatures
		464	TCWS311	WS3	Heiermann	Nienwohlde7	1	374	yes	yes	yes	no	Rejected because extrapolated too far beyond end of study period (84 d)
		465					10	212	yes	yes	yes	no	Rejected because extrapolated too far beyond end of study period (84 d)
		466					20	78	yes	yes	yes	no	Rejected because Ea above 20°C is negative, whereas appears high at lower temp.

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre- ssion QC	Over- all QC	Remarks
ethofumesate	benzofuran	467					30	93	yes	yes	yes	no	Rejected because Ea above 20°C is negative, whereas appears high at lower temp.
		468	TCWS312	WS3	Heiermann	Nienwohlde7	1	192	yes	yes	yes	no	Rejected because extrapolated too far beyond end of study period (84 d)
		469					10	146	yes	yes	yes	no	Rejected because: 60% MWHC preferred because larger no of temperatures
		470					20	62	yes	yes	yes	no	Rejected because: 60% MWHC preferred because larger no of temperatures
		701	TCJJB31	JJB3	Beulke	II	1	198.1	yes	yes	yes	no	Rejected because incubation time shorter than 0.5 * DT_{50}
ethoprophos	organophosphate	51	TCJB73	JB7	Smelt	Rolde	2	1386	yes	yes	no	no	Inaccurate because experiment lasted only 214 d
		356	TCEFSA0191	EFSA019	Greenslade	X10	10	36	yes	yes	no	no	
		357					22	27	yes	yes	no	no	
		358	TCEFSA0192	EFSA019	Greenslade	X11	10	54	yes	no	no	no	
		359					22	23	yes	no	no	no	
Ethylenethiourea	dithiocarbamate	1240	TCEC111	EC11	Hanummantharaju	Bangalore soil	15	18.48	no	no	yes	no	Missing data on storage time. metabolite
		1241					25	14.75	no	no	yes	no	Missing data on storage time. metabolite
		1242	TCEC112	EC11	Hanummantharaju	Chettali soil	15	17.99	no	no	yes	no	Missing data on storage time. metabolite
		1243					25	12.9	no	no	yes	no	Missing data on storage time. metabolite
Ethylenethiourea	dithiocarbamate	1244	TCEC113	EC11	Hanummantharaju	Hiriyuri soil	15	15.47	no	no	yes	no	Missing data on storage time. metabolite
		1245					25	12.17	no	no	yes	no	Missing data on storage time. metabolite
fenpropidin	piperidine	1132	TCRB101	RB10	Harradine	Dielsdrof	8	217	no	yes	yes	no	Recalculation of RB 10 (Rumbeli) using SFO by ModelMaker

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
fenpropidin	piperidine	1133					22	68	no	yes	yes	no	Recalculation of RB 10 (Rumbeli) using SFO by ModelMaker
		1134					22	98	no	yes	yes	no	Recalculation of RB 10 (Rumbeli) using SFO by ModelMaker
		1135	TCRB111	RB11	Rümbeli	Dielsdrof	8	187	no	yes	yes	no	Soil storage (?)
		1136					22	59	no	yes	yes	no	Soil storage (?), unhelpful kinetics
		1137					22	93	no	yes	yes	no	Low application rate. soil storage (?), unhelpful kinetics
fipronil	phenylpyrazole	360	TCEFSA 0221	EFS A022	Fitzmaurice	Chazay	10	747	yes	yes	no	no	Soils handled according to International Standard on Soil Quality
		361					20	382	yes	yes	yes	yes	
		362	TCEFSA 0222	EFS A022	Fitzmaurice	Ongar	10	515	yes	yes	no	no	
		363					20	123	yes	yes	yes	yes	
flonicamid		1217	TCSB91	SB9	Lentz	Bedfordshire 2	10	2.4	yes	yes	no	no	Log-transformation results in poor fit, initial conc. too low, DT_{50} too slow, true DT_{50} 1.6 days
		1218					20	0.702	yes	yes	yes	no	Rejected because DT_{50} < 1 day
florasulam	triazolopyrimidine	545	TCWS51	WS5	Krieger	Cuckney	5	6.4	yes	n.a.	yes	no	Rejected because - only 2-3 samples incl. day zero up to DT_{50} - data in Table 2 suggest that DT_{50} shorter than calculated - measurements between day 3 and 14 not consistent
		546					15	3.3	yes	n.a.	yes	no	Rejected because - only 2-3 samples incl. day zero up to DT_{50} - data in Table 2 suggest that DT_{50} shorter than calculated - measurements between day 3 and 14 not consistent
		547					25	1	yes	n.a.	yes	no	Rejected because - only 1 sample incl. day zero up to DT_{50} - DT_{50} 1 day uncertain

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (°C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
florasulam	triazolopyrimidine	551	TCWS53	WS5	Krieger	Marcham 2	5	18	yes	n.a.	yes	no	Rejected because - measurements between day 3 and 14 not consistent
		552					10	23	yes	n.a.	yes	no	Rejected because - measurements between day 3 and 14 not consistent
		553					15	7.4	yes	n.a.	yes	no	Rejected because - measurements between day 3 and 14 not consistent
		554					20	4.1	yes	n.a.	yes	no	Rejected because - measurements between day 3 and 14 not consistent
		555					25	1.3	yes	n.a.	yes	no	Rejected because - measurements between day 3 and 14 not consistent - only 2 samples incl. day zero up to DT_{50}
		564	TCWS55	WS5	Krieger	Naicom-hoodoo	35	1.7	yes	n.a.	yes	no	Rejected because temperature > 30°C
flumetsulam	triazolopyrimidine	569	TCWS61	WS6	Lehmann	Hoytville clay	7.5	246	no	no	yes	no	Rejected because: storage period too long
		570					15	115	no	no	no	no	Rejected because: storage period too long - visual fit poor (initial fast drop, then slower decline)
		571					26.1	49	no	no	yes	no	Rejected because: storage period too long
		572					35.9	34	no	no	yes	no	Rejected because: storage period too long temperature>30°C
		573					44	27	no	no	yes	no	Rejected because: storage period too long temperature>30°C

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (°C)	DT_{50} (day)	Storage QC	Test QC	Regression QC	Overall QC	Remarks
flupyrsulfuron-methyl	sulfonylurea	322	TCEU161	EU16	Singles	Somersham Uk	10	58	yes	yes	no	no	^{14}C-Labelled compound was used. First-order fit was performed,
		323					20	26	yes	yes	no	no	But fit (r2) not shown, only for the field data. still data seem ok
flutriafol	triazole	732	TCJJB61	JJB6	Bromilow	Rothamsted clay loam	5	2310	yes	yes	no	no	
		733					10	2888	yes	yes	no	no	
		734					15	2038	yes	yes	no	no	
		735					18	1650	yes	yes	no	no	
		736	TCJJB62	JJB6	Bromilow	Woburn sandy loam	5	3850	yes	yes	no	no	
		737					10	3013	yes	yes	no	no	
		738					15	1575	yes	yes	no	no	
		739					18	1444	yes	yes	no	no	
folpet	phthalimide	364	TCEFSA0231	EFSA023	Crowe	Farditch farm	10	3.8	no	yes	yes	no	
folpet	phthalimide	365					20	0.8	no	yes	yes	no	DT_{50} < 1 day --> not to be included for statistical analyses
glufosinate	phosphinic acid	366	TCEFSA0261	EFSA026	Allan	Frankfurt	10	18	yes	yes	yes	no	Soil stored in open containers under natural conditions after field sampling Rejected because separate study
		367					20	5.9	yes	yes	yes	no	Soil stored in open containers under natural conditions after field sampling Rejected because separate study
haloxyfop-R	aryloxyphenoxy propionate	368	TCEFSA0271	EFSA027	Knowles	Marcham 1	10	20.6	yes	yes	no	no	DT_{50} of the main metabolite, the corresponding acid, is used
		369					20	9.4	yes	yes	no	no	Soil storage according to ISO 103381-6 guideline
hexythiazox		1138	TCRB121	RB12	Anonymous	X2	15	8	no	yes	no	no	Graphical analysis only
		1139					25	6	no	yes	no	no	Graphical analysis only
		1140	TCRB122	RB12	Anonymous	X3	15	25	no	yes	no	no	Graphical analysis only
		1141					25	14	no	yes	no	no	Graphical analysis only
imazamox	imidazolinone	394	TCEFSA0561	EFSA056	Ta	Boissy	20	44	yes	yes	no	no	Soil-storage conditions follow ISO 10381-6. kinetic fit only with data up to day 27 --> extrapolation to DT_{50} = 44 days not possible

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
imazamox	imidazolinone	395					10	113	yes	yes	yes	yes	Soil-storage conditions follow ISO 10381-7
imazaquin	imidazolinone	402	TCWS11	WS1	Flint	Maury silt loam	15	49	yes	no	yes	no	Rejected because bioassay was used for analysis
		403					30	22	yes	no	yes	no	Rejected because bioassay was used for analysis
imazethapyr	imidazolinone	404	TCWS12	WS1	Flint	Maury silt loam	15	53	yes	no	yes	no	Rejected because bioassay was used for analysis
		405					30	24	yes	no	yes	no	Rejected because bioassay was used for analysis
isoproturon	phenylurea	18	TCJB42	JB4	Berger	X5	0	38.6	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		19					10	15.5	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
isoproturon	phenylurea	20					20	12.7	yes	yes	yes	no	Fitting to other kinetics: DT_{50} = 5.4 d. other dataset for same soil and pesticide is preferred
		21	TCJB43	JB4	Berger	X5	0	38.5	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		22					10	14	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		23					20	11.2	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		27	TCJB45	JB4	Berger	X17	0	45.5	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		28					10	18.5	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		29					20	12	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		30	TCJB46	JB4	Berger	X17	0	52.8	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		31					10	15.7	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
isoproturon	phenylurea	32					20	12.5	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		33	TCJB51	JB5	Blair	Broom's Barn	5	61.2	yes	yes	no	no	
		36					25	15	yes	yes	no	no	
		37	TCJB52	JB5	Blair	Lidgate	5	85.1	yes	yes	no	no	
		40					25	19	yes	yes	no	no	
		41	TCJB61	JB6	Mudd	Lankets	20	14.7	no	yes	no	no	
		42					30	14.8	no	yes	no	no	
		471	TCWS313	WS3	Heiermann	Neuenkirchen	1	65	no	yes	yes	no	Rejected because storage period too long
		472					10	25	no	yes	yes	no	Rejected because storage period too long
		473					20	9	no	yes	yes	no	Rejected because storage period too long
isoproturon	phenylurea	474	TCWS314	WS3	Heiermann	Neuenkirchen	1	39	no	yes	yes	no	Rejected because storage period too long
		475					10	13	no	yes	yes	no	Rejected because storage period too long
		476					20	5	no	yes	yes	no	Rejected because storage period too long
		477					30	5	no	yes	yes	no	Rejected because storage period too long
		478	TCWS315	WS3	Heiermann	Neuenkirchen	1	34	no	yes	yes	no	Rejected because storage period too long
		479					10	11	no	yes	yes	no	Rejected because storage period too long
		480					20	5	no	yes	yes	no	Rejected because storage period too long
		481	TCWS316	WS3	Heiermann	Nienwohlde8	1	281	yes	yes	yes	no	Rejected because: 60% MWHC preferred (medium moisture) extrapolated too far beyond end of study period (84 d)

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
isoproturon	phenylurea	482					10	115	yes	yes	yes	no	Rejected because: 60% MWHC preferred (medium moisture)
		483					20	84	yes	yes	yes	no	Rejected because: 60% MWHC preferred (medium moisture)
		484					30	51	yes	yes	yes	no	Rejected because: 60% MWHC preferred (medium moisture)
		485					40	9	yes	yes	yes	no	Rejected because: 60% MWHC preferred (medium moisture) temperature > 30^{o}C
		486	TCWS317	WS3	Heiermann	Nienwohlde8	1	262	yes	yes	yes	no	Rejected because: extrapolated too far beyond end of study period (84 d)
		490					40	25	yes	yes	yes	no	Rejected because: temperature >30^{o}C
		491	TCWS318	WS3	Heiermann	Nienwohlde8	1	313	yes	yes	yes	no	Rejected because: 60% MWHC preferred (medium moisture) extrapolated too far beyond end of study period (84 d)
		492					10	128	yes	yes	yes	no	Rejected because: 60% MWHC preferred (medium moisture)
		493					20	53	yes	yes	yes	no	Rejected because: 60% MWHC preferred (medium moisture)
		494					30	38	yes	yes	yes	no	Rejected because: 60% MWHC preferred (medium moisture)
		495					40	27	yes	yes	yes	no	Rejected because: 60% MWHC preferred (medium moisture) temperature > 30^{o}C
		521	TCWS41	WS4	Jurado-Exposito	Wellesbourne 3	10	55.5	yes	yes	yes	no	Rejected because: 20% moisture preferred (shorter half-lives)
		522					20	30	yes	yes	yes	no	Rejected because: 20% moisture preferred (shorter half-lives)

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
isoproturon	phenylurea	523	TCWS42	WS4	Jurado-Exposito	Wellesbourne 3	10	52.5	yes	yes	yes	no	Rejected because: 20% moisture preferred (shorter half-lives)
		524					20	29	yes	yes	yes	no	Rejected because: 20% moisture preferred (shorter half-lives)
		527	TCWS44	WS4	Jurado-Exposito	Wellesbourne 3	10	29.6	yes	yes	no	no	Rejected because visual fit not very good and replication of other study at same conditions
		528					20	14.4	yes	yes	yes	no	Rejected because replication of other study at same conditions
		683	TCWS121	WS12	Walker	Cottage fields	5	77.9	yes	yes	yes	no	Rejected because DT_{50} > 2x study period (35 d)
		684					25	12.7	yes	yes	yes	yes	
		697	TCJJB21	JJB2	Aletto	LA1	10	223	yes	yes	no	no	Rejected because incubation time shorter than 0.5 * DT_{50}
		698					22	157	yes	yes	yes	no	
		699	TCJJB22	JJB2	Aletto	LA1	10	23	yes	yes	no	no	
		700					22	11	yes	yes	no	no	
		1254	TCEC81	EC8	Gaillardon	not reported	11	not reported	no	no	no	no	Radioactive measurements
		1255					18	not reported	no	no	no	no	Radioactive measurements
isoxaflutole	isoxazolyl	858	TCEC21	EC2	Beltran	South France	30	2.79	no	no	no	no	Sampling points missed. visual inspection for DT_{50}
		859					30	2.04	no	no	no	no	Sampling points missed. visual inspection for DT_{50}
		860					30	1.38	no	no	no	no	Sampling points missed. visual inspection for DT_{50}
		861	TCEC22	EC2	Beltran	West France	30	not reported	no	no	no	no	Sampling points missed. visual inspection for DT_{50}

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
isoxaflutole	isoxazolyl	862	TCEC23	EC2	Beltran	Martinique	30	not reported	no	no	no	no	Sampling points missed. visual inspection for DT_{50}
		863	TCEC24	EC2	Beltran	Med Area 1	10	not reported	no	no	no	no	Sampling points missed. visual inspection for DT_{50}
		864					20	not reported	no	no	no	no	Sampling points missed. visual inspection for DT_{50}
		865					30	not reported	no	no	no	no	Sampling points missed. visual inspection for DT_{50}
		866					40	not reported	no	no	no	no	Sampling points missed. visual inspection for DT_{50}
		867					60	not reported	no	no	no	no	Sampling points missed. visual inspection for DT_{50}
isoxaflutole	isoxazolyl	868	TCEC25	EC2	Beltran	Med Area 2	30	not reported	no	no	no	no	Sampling points missed. visual inspection for DT_{50}
lambda-cyhalothrin	pyrethroid	655	TCWS95	WS9	TariqI	Pakistan	15	173.3	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil. -not first-order

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
lambda-cyhalothrin	pyrethroid	656					25	138.6	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil. -not first-order
		657					35	99.3	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil. -Sudy temp >30^{0}C -not first-order
		658	TCWS96	WS9	Tariql	Pakistan	15	161.2	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil. -not first-order
		659					25	147.5	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil. -not first-order
		660					35	77	no	yes	no	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil. -Sudy temp >30^{0}C and not first-order

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
linuron	phenylurea	66	TCJB101	JB10	Usoroh	Cockle Park	4	292	no	yes	no	no	r given in paper
		67					22	87.5	no	yes	yes	no	
		68	TCJB102	JB10	Usoroh	Cockle Park	4	276	no	yes	no	no	
		69					22	64	no	yes	yes	no	
		70	TCJB103	JB10	Usoroh	Cockle Park	4	188	no	yes	yes	no	
		71					22	56	no	yes	yes	no	
		144	TCEU319	EU3	Walker	Pump Ground 5 cm	20	178	yes	no	yes	no	Data not used because soil moisture below 5%
		145					30	not reported	yes	no	yes	no	Data not used because soil moisture below 5%
		146	TCEU320	EU3	Walker	Pump Ground 5 cm	5	not reported	yes	no	yes	no	DT_{50} not reported
		147					10	147	yes	no	yes	no	6.88+0.91 kcal/mol
		148					15	not reported	yes	no	yes	no	DT_{50} not reported
		149					25	not reported	yes	no	yes	no	DT_{50} not reported
		150	TCEU321	EU3	Walker	Pump Ground 5 cm	10	not reported	yes	no	yes	no	DT_{50} not reported
		151					20	87.9	yes	no	yes	no	
		227	TCEU94	EU9	Walker	Colorado	15	87	yes	yes	yes	no	No visual inspection possible, decide fit quality on n/r2 ratio. water content too different from previous and next study
		229					35	28	yes	yes	yes	no	No visual inspection possible, decide fit quality on n/r2 ratio.excluded because temperature above 30ºC
		962	TCEC121	EC12	Kempson-Jones	Deal soil	10	60	no	no	no	no	Missing data on storage time. incubation time longer than 90 days. data reported as example at 10% moisture content and top soil

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
linuron	phenylurea	1246					22	24	no	no	no	no	Missing data on storage time. incubation time longer than 90 days. data reported as example at 10% moisture content and top soil
		1247	TCEC122	EC12	Kempson-Jones	Limekilns soil	10	215	no	no	no	no	Missing data on storage time. incubation time longer than 90 days. data reported as example at 10% moisture content and top soil
		1248					22	147	no	no	no	no	Missing data on storage time. incubation time longer than 90 days. data reported as example at 10% moisture content and top soil
metamitron	triazinone	77	TCEU21	EU2	Walker	X7	20	93	yes	no	no	no	11.1 kcal/mol. data not used because soil moisture below 5%
		78					25	43	yes	no	no	no	11.1 kcal/mol. data not used because soil moisture below 5%
		79	TCEU22	EU2	Walker	X7	20	47	yes	no	no	no	
		80					25	24	yes	no	no	no	
		81	TCEU23	EU2	Walker	X7	5	91	yes	no	no	no	Data at 5ºC were taken from Bond and Roberts (1976 and the rest from Walker 1978 ((Weed research)
		82					10	53	yes	no	no	no	Residue data were also estimated by use of bioassays
		83					20	30	yes	no	no	no	
metamitron	triazinone	84					25	14	yes	no	no	no	
		85					30	14	yes	no	no	no	
		86	TCEU24	EU2	Walker	X7	20	21	yes	no	no	no	
		87					25	8.5	yes	no	no	no	
		152	TCEU322	EU3	Walker	Pump Ground 5 cm	20	93	yes	no	yes	no	Data not used because soil moisture below 5%
		153					30	not reported	yes	no	yes	no	Data not used because soil moisture below 5%. DT_{50} not reported
		154	TCEU323	EU3	Walker	Pump Ground 5 cm	5	not reported	yes	no	yes	no	DT_{50} not reported

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
metamitron	triazinone	155					10	52.5	yes	no	yes	no	11.14+1.22 kcal/mol
		156					15	not reported	yes	no	yes	no	DT_{50} not reported
		157					25	not reported	yes	no	yes	no	DT_{50} not reported
		158	TCEU324	EU3	Walker	Pump Ground 5 cm	10	not reported	yes	no	yes	no	DT_{50} not reported
		159					20	21	yes	no	yes	no	
		772	TCJJB71	JJB7	Bunte	Eisenbach S-1	10	24	no	yes	yes	no	
		773					20	5	no	yes	no	no	Regression rejected because only 4 sampling points
		774					30	5	no	yes	no	no	Regression rejected because only 4 sampling points
		775	TCJJB72	JJB7	Bunte	Eisenbach S-2	10	157	no	yes	yes	no	
		776					20	30	no	yes	yes	no	
		777					30	26	no	yes	yes	no	
		778	TCJJB73	JJB7	Bunte	Krummbach-L	10	12	no	yes	yes	no	
		779					20	5	no	yes	no	no	Regression rejected because only 4 sampling points
		780					30	6	no	yes	no	no	Regression rejected because only 4 sampling points
		810	TCJJB94	JJB9	Capri	X16	10	46.4	yes	yes	yes	no	Rejected because data at 22% moisture preferred (larger number of temperatures)
		811					30	12.1	yes	yes	yes	no	Rejected because data at 22% moisture preferred (larger number of temperatures)
		815	TCJJB96	JJB9	Capri	X16	10	20.7	yes	yes	yes	no	Rejected because data at 22% moisture preferred (larger number of temperatures)
		816					30	9.7	yes	yes	yes	no	Rejected because data at 22% moisture preferred (larger number of temperatures)
		1043	TCMM41	MM4	Vink	North-	5	61	no	no	no	no	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
metamitron	triazinone	1044				east polder layer 1	15	9	no	no	no	no	
		1045	TCMM42	MM4	Vink	North-east polder layer 2	5	140	no	no	no	no	
		1046					15	5	no	no	no	no	
		1047	TCMM43	MM4	Vink	North-east polder layer 3	5	>1 y	no	no	no	no	
		1048					15	41	no	no	no	no	
		1049	TCMM44	MM4	Vink	North-east polder layer 4	5	>1 y	no	no	no	no	
		1050					15	68	no	no	no	no	
metazachlor	chloroacetamide	1153	TCRB15 1	RB15	Keller	Limburgerhof Bruch West	10	23	yes	yes	no	no	Kinetics?
		1154					20	3	yes	yes	no	no	Not SFO (Timme & Frehse), impossible to compare
		1155					30	1	yes	yes	no	no	Not SFO (Timme & Frehse), impossible to compare
		1156	TCRB16 1	RB16	Keller				n.a.	n.a.	n.a.	no	Analytical method only
		1161	TCRB19 1	RB19	Schneider	LUFA Speyer	10	17.3	no	yes	no	no	Soil storage. differing kinetics impossible to compare
		1162					20	10.1	no	yes	no	no	Soil storage. differing kinetics impossible to compare
metazachlor metab. BH479-4	chloroacetamide	1147	TCRB 142	RB 14	Gottesbüren	Limburgerhof Bruch West	10	NS	yes	yes	no	no	
		1148					20	90.1	yes	yes	yes	no	Kinetics? Recalculation of RB15/RB18
		1149					30	59.3	yes	yes	yes	no	Kinetics? Recalculation of RB15/RB18
		1157	TCRB17 1	RB17	Keller				n.a.	n.a.	n.a.	no	Analytical method only
		1158	TCRB18 1	RB18	Keller	Limburgerhof	10	264	yes	yes	yes	no	Uncertainty over kinetics analysis

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
metazachlor metab. BH479-4	chloroacetamide	1159				Bruch West	20	69	yes	yes	yes	no	Uncertainty over kinetics analysis
		1160					30	41	yes	yes	yes	no	Uncertainty over kinetics analysis
metconazole	triazole	370	TCEFSA 0291	EFS A029	Gedik	Levingto n 1	10	564	yes	yes	yes	no	Different soil samples for the two temperatures. study duration was 120 days
		371					20	84	yes	yes	yes	no	Different soil samples for the two temperatures
methabenzthiaz uron	urea	12	TCJB32	JB3	Pesteme r	Braunsc hweig 1	10	1274	yes	yes	yes	no	Unreliable DT_{50} because experiment lasted 128 d only. single soil-moisture/temperature data
		13					20	127	yes	yes	no	no	
		14					30	42	yes	yes	no	no	
		496	TCWS31 9	WS3	Heierma nn	Neuenkir chen	1	359	no	yes	no	no	Rejected because: storage period too long extrapolated too far beyond end of study period (85 d) r2 <0.8 60% MWHC preferred because larger no of temperatures
		497					10	217	no	yes	yes	no	Rejected because: storage period too long extrapolated too far beyond end of study period (85 d) 60% MWHC preferred because larger no of temperatures
methabenzthiaz uron	urea	498					20	91	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		499	TCWS32 0	WS3	Heierma nn	Neuenkir chen	1	501	no	yes	no	no	Rejected because: storage period too long extrapolated too far beyond end of study period (85 d) r2 <0.8

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
methabenzthiazuron	urea	500					10	120	no	yes	yes	no	Rejected because: storage period too long extrapolated too far beyond end of study period (85 d)
		501					20	46	no	yes	yes	no	Rejected because: storage period too long
		502					30	37	no	yes	yes	no	Rejected because: storage period too long
		503	TCWS321	WS3	Heiermann	Neuenkirchen	1	264	no	yes	yes	no	Rejected because: storage period too long extrapolated too far beyond end of study period (85 d) 60% MWHC preferred because larger no of temperatures
		504					10	123	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		505					20	45	no	yes	yes	no	Rejected because: storage period too long 60% MWHC preferred because larger no of temperatures
		506	TCWS322	WS3	Heiermann	Nienwohlde8	1	289	yes	yes	yes	no	Rejected because: extrapolated too far beyond end of study period (84 d) 80% MWHC preferred (shorter half-lives)
		507					10	300	yes	yes	yes	no	Rejected because: extrapolated too far beyond end of study period (84 d) 80% MWHC preferred (shorter half-lives)
		508					20	192	yes	yes	yes	no	Rejected because: extrapolated too far beyond end of study period (84 d) 80% MWHC preferred (shorter half-lives)
		509					30	135	yes	yes	no	no	Rejected because: 80% MWHC preferred (shorter half-lives) r2<0.8
		510					40	73	yes	yes	yes	no	Rejected because: 80% MWHC preferred (shorter half-lives)

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
methabenzthiazuron	urea	511	TCWS323	WS3	Heiermann	Nienwohlde8	1	598	yes	yes	yes	no	Rejected because: 80% MWHC preferred (shorter half-lives) extrapolated too far beyond end of study period (84 d)
		512					10	287	yes	yes	yes	no	Rejected because: 80% MWHC preferred (shorter half-lives) extrapolated too far beyond end of study period (84 d)
		513					20	211	yes	yes	no	no	Rejected because: 80% MWHC preferred (shorter half-lives) extrapolated too far beyond end of study period (84 d) r2<0.8
		514					30	154	yes	yes	no	no	Rejected because: 80% MWHC preferred (shorter half-lives) r2<0.8
		515					40	120	yes	yes	no	no	Rejected because: 80% MWHC preferred (shorter half-lives) r2<0.8 temperature>30^{o}C
		516	TCWS324	WS3	Heiermann	Nienwohlde8	1	590	yes	yes	yes	no	Rejected because: extrapolated too far beyond end of study period (84 d)
		517					10	332	yes	yes	no	no	Rejected because: extrapolated too far beyond end of study period (84 d) r2<0.8
		518					20	167	yes	yes	yes	yes	
		519					30	136	yes	yes	no	no	Rejected because: r2<0.8
		520					40	107	yes	yes	no	no	Rejected because: r2<0.8 temperature>30^{o}C
		793	TCJJB78	JJB7	Bunte	Eisenbach S-1	10	194	no	yes	no	no	
		794					20	146	no	yes	yes	no	
		795					30	43	no	yes	yes	no	
		796	TCJJB79	JJB7	Bunte	Eisenbach S-2	10	836	no	yes	no	no	
		797					20	521	no	yes	no	no	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (°C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
methabenzthiazuron	urea	798					30	312	no	yes	no	no	
methyl ester of fusaric acid	fusaric acid	1051	TCMM51	MM5	Vischetti	Castiglione del Lago	10	41	no	yes	yes	no	No Vp. but no forced air flow. Information provided by author (personal communication): air dried 2 days after sampling and then kept at room temperature for 1 week before spiking
		1052					20	24.1	no	yes	yes	no	
		1053					30	16.3	no	yes	yes	no	
		1054	TCMM52	MM5	Vischetti	Papiano	10	44.7	no	yes	yes	no	
		1055					20	21.1	no	yes	yes	no	
		1056					30	11.1	no	yes	yes	no	
		1057	TCMM53	MM5	Vischetti	Castellamare di Stabia	10	44.4	no	yes	yes	no	
		1058					20	15.2	no	yes	yes	no	
		1059					30	6.2	no	yes	yes	no	
metolachlor	chloroacetamide	223	TCEU93	EU9	Walker	New York	15	71	yes	yes	yes	no	No visual inspection possible, decide fit quality on n/r2 ratio. water content too different from previous and next study
		225					35	22	yes	yes	yes	no	No visual inspection possible, decide fit quality on n/r2 ratio. excluded because temperature above 30ºC
		833	TCJJB114	JJB11	Dinelli	Ozzano	5	100.7	no	yes	yes	no	No forced air flow
		834					10	47.5	no	yes	yes	no	No forced air flow
		835					15	18	no	yes	yes	no	No forced air flow
		836					20	12.2	no	yes	yes	no	No forced air flow
		837					25	8.6	no	yes	yes	no	No forced air flow
		838					35	5.7	no	yes	yes	no	No forced air flow
		839	TCJJB115	JJB11	Dinelli	Ozzano	15	21.4	no	yes	yes	no	No forced air flow
		840					25	10.2	no	yes	yes	no	No forced air flow
		841					35	7.3	no	yes	yes	no	No forced air flow
		842	TCJJB116	JJB11	Dinelli	Ozzano	15	27.4	no	yes	yes	no	No forced air flow
		843					25	15.2	no	yes	yes	no	No forced air flow
		844					35	11.3	no	yes	yes	no	No forced air flow

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
metolachlor	chloroacetamide	1060	TCMM61	MM6	Zheng	Martinique Paquemar	25	46.5	no	yes	no	no	Forced air flow not mentioned. capping also not.
		1061					35	32.9	no	yes	no	no	
		1062	TCMM62	MM6	Zheng	Martinique St Anne	25	44.9	no	yes	no	no	
		1063					35	38.7	no	yes	no	no	
		1064	TCMM63	MM6	Zheng	Martinique Bochet	25	40	no	yes	no	no	
		1065					35	36.1	no	yes	no	no	
		1066	TCMM64	MM6	Zheng	Martinique Leyritz	25	44.8	no	yes	no	no	
		1067					35	29.6	no	yes	no	no	
		1068	TCMM65	MM6	Zheng	Martinique Eden	25	44.4	no	yes	no	no	
		1069					35	33.5	no	yes	no	no	
		1070	TCMM66	MM6	Zheng	France Marsillargues	25	44	no	yes	no	no	
		1071					35	27.6	no	yes	no	no	
metrafenone	dibenzoketone	390	TCEFSA 0541	EFS A054	Steinfuehrer	Sporkenheim	10	693	yes	yes	no	no	Soil sampling at the same date as study began
		391					20	182	yes	yes	yes	yes	Soil sampling at the same date as study began
metribuzin	triazinone	128	TCEU313	EU3	Walker	Pump Ground 5 cm	20	153	yes	yes	yes	no	Data not used because soil moisture below 5%
		129					30	60.3	yes	yes	yes	no	Data not used because soil moisture below 5%
		134	TCEU315	EU3	Walker	Pump Ground 5 cm	10	141	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		135					20	48.8	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		259	TCEU133	EU13	Smith	Regina 2	5	193	no	yes	yes	no	
		260					10	94	no	yes	yes	no	r2=0.86-0.94. quality criterion depends on n/r2 ratio
		261					15	62	no	yes	yes	no	r2=0.86-0.94. quality criterion depends on n/r2 ratio
		262					20	34	no	yes	yes	no	r2=0.86-0.94. quality criterion depends on n/r2 ratio

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
metribuzin	triazinone	263					25	32	no	yes	yes	no	r2=0.86-0.94. quality criterion depends on n/r2 ratio
		264					30	22	no	yes	yes	no	r2=0.86-0.94. quality criterion depends on n/r2 ratio
		963	TCEC123	EC12	Kempson-Jones	Deal soil	10	61	no	no	no	no	Missing data on storage time. incubation time larger than 90 days. data reported as example at 10% moisture content and top soil
		964	TCEC131	EC13	Khoury	Fanar soil	20	not reported	no	no	no	no	Missing data on storage time. DT_{50} reported in the graphics
		965					30	not reported	no	no	no	no	Missing data on storage time. DT_{50} reported in the graphics
		966					40	not reported	no	no	no	no	Missing data on storage time. DT_{50} reported in the graphics
		967					50	not reported	no	no	no	no	Missing data on storage time. DT_{50} reported in the graphics
		968					60	not reported	no	no	no	no	Missing data on storage time. DT_{50} reported in the graphics
		969	TCEC132	EC13	Khoury	Raouda soil	20	not reported	no	no	no	no	Missing data on storage time. DT_{50} reported in the graphics
		970					30	not reported	no	no	no	no	Missing data on storage time. DT_{50} reported in the graphics
		971					40	not reported	no	no	no	no	Missing data on storage time. DT_{50} reported in the graphics

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
metribuzin	triazinone	972					50	not reported	no	no	no	no	Missing data on storage time. DT_{50} reported in the graphics
		973					60	not reported	no	no	no	no	Missing data on storage time. DT_{50} reported in the graphics
		1249	TCEC123	EC12	Kempson-Jones	Deal soil	22	17.5	no	no	no	no	Missing data on storage time. incubation time longer than 90 days. data reported as example at 10% moisture content and top soil
		1250	TCEC124	EC12	Kempson-Jones	Limekilns soil	10	70	no	no	no	no	Missing data on storage time. incubation time longer than 90 days. data reported as example at 10% moisture content and top soil
		1251					22	43	no	no	no	no	Missing data on storage time. incubation time longer than 90 days. data reported as example at 10% moisture content and top soil
		1252	TCEC125	EC12	Kempson-Jones	Methwold soil	10	105	no	no	no	no	Missing data on storage time. incubation time lonrger than 90 days. data reported as example at 10% moisture content and top soil
		1253					22	25	no	no	no	no	Missing data on storage time. incubation time longer than 90 days. data reported as example at 10% moisture content and top soil
metsulfuron-methyl	sulfonylurea	333	TCEU182	EU18	James	Horotiu 2	10	36	yes	yes	no	no	Rejected because r2<0.8 and bi-phasic pattern
		334					22	23	yes	yes	yes	no	Rejected because strong bi-phasic pattern
		335					30	8	yes	yes	yes	no	Rejected because strong bi-phasic pattern
		691	TCWS125	WS12	Walker	Cottage fields	5	121.6	yes	yes	yes	no	Rejected because DT_{50} > 2x study period (35 d)
		692					25	13.5	yes	yes	yes	yes	
		693	TCWS126	WS12	Walker	Hunts Mill 1	5	106.6	yes	yes	yes	no	Rejected because DT_{50} > 2x study period (42 d)

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
metsulfuron-methyl	sulfonylurea	694					25	29.8	yes	yes	yes	yes	
MITC (methyl isothiocyanate)	isothiocyanate	911	TCEC71	EC7	Dungan RS, Gan J & Yates SR	Arlington sandy loam	20	5.8	no	yes	yes	no	Storage time (at 5ºC) not reported. the reference is wrong. these data are double published again in MM15 and reviewed by Mark Montfort.
		912					30	3	no	yes	yes	no	
		913					40	1.8	no	yes	yes	no	
		914	TCEC91	EC9	Gan	Arlington sandy loam	20	1.39	no	yes	yes	no	Storage not reported is the only problem
		915					30	0.64	no	yes	yes	no	
		916					35	0.6	no	yes	yes	no	
		917					40	0.56	no	yes	yes	no	
		918					20	7.41	no	yes	yes	no	
		919					30	3.21	no	yes	yes	no	
		920					35	2.45	no	yes	yes	no	
		921					40	1.75	no	yes	yes	no	
		922	TCEC92	EC9	Gan	Arlington sandy loam	20	9.63	no	yes	yes	no	
		923					30	4.13	no	yes	yes	no	
		924					35	3.4	no	yes	yes	no	
		925					40	2.53	no	yes	yes	no	
		926	TCEC93	EC9	Gan	Arlington sandy loam	20	12.56	no	yes	yes	no	
		927					30	6.42	no	yes	yes	no	
		928					35	5.07	no	yes	yes	no	
		929					40	3.36	no	yes	yes	no	
		980	TCMM11	MM1	Ma	Arlington sandy loam	20	1.39	yes	yes	yes	yes	E-mail confirmation Dr. Ma on storage. Teflon capped. rubber septum. no forced air flow
		981					30	0.64	yes	yes	yes	no	Half-life below 1 day
		982					35	0.6	yes	yes	yes	no	Half-life below 1 day
		983					40	0.56	yes	yes	yes	no	Half-life below 1 day
		984	TCMM12	MM1	Ma	Arlington sandy	20	7.41	yes	yes	yes	no	Fumigant, biocidal action not dismissed

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (⁰C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
MITC (methyl isothiocyanate)	isothiocyanate	985				loam	30	3.21	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		986					35	2.45	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		987					40	1.75	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		988	TCMM13	MM1	Ma	Arlington sandy loam	20	9.63	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		989					30	4.13	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		990					35	3.4	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		991					40	2.53	yes	yes	yes	no	Fumigant, biocidal action not dismissed
		992	TCMM14	MM1	Ma	Arlington sandy loam	20	12.56	yes	yes	yes	no	Authors report biocidal action at this dosage by comparison to sterile conditions
		993					30	6.42	yes	yes	yes	no	Authors report biocidal action at this dosage by comparison to sterile conditions
		994					35	5.07	yes	yes	yes	no	Authors report biocidal action at this dosage by comparison to sterile conditions
		995					40	3.36	yes	yes	yes	no	Authors report biocidal action at this dosage by comparison to sterile conditions
monocrotophos	organophosphate	667	TCWS99	WS9	Tariql	Pakistan	15	13.9	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (°C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
monocrotophos	organophosphate	668					25	9.9	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		669					35	2.31	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil. - Study temperature >30°C
		670	TCWS910	WS9	Tariql	Pakistan	15	11	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		671					25	7.7	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil.
		672					35	1.73	no	yes	yes	no	Rejected because: - Soils were taken from cropped lysimeters filled with sieved soil, it is not stated how long the lysimeters were kept until the soil for the deg study was collected. - DT_{50}s in sterile soil similar to those in non-sterile soil. - Study temperature >30°C
napropamide	amide	72	TCEU11	EU1	Walker	Little Cherry 5 cm	14	112	yes	no	yes	no	Visual inspection: all ok
		73					28	63	yes	no	yes	no	
		74	TCEU12	EU1	Walker	Little	14	102	yes	no	yes	no	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (°C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
napropamide	amide	75				Cherry 5 cm	28	56	yes	no	yes	no	Different initial content
		76					28	54	yes	no	yes	no	7.85 kcal/mol at 10% moisture
		1163	TCRB201	RB20	Shaw	Sheringham	20	463	yes	yes	no	no	Impossible to compare different kinetics. too short a study
		1164					10	380	yes	yes	no	no	Impossible to compare different kinetics. too short a study
o,p' - DDT	chlorinated hydrocarbon	979	TCEC151	EC15	Lemley	X8			no	no	no	no	65 soils collected in different ecosystems. paper not suitable for this scope because missing a large amount of information
pendimethalin	dinitroaniline	242	TCEU121	EU12	Walker	Sheep Pens	10	409	yes	yes	no	no	No visual inspection possible
		243					15	265	yes	yes	no	no	
		244					20	168	yes	yes	no	no	
		245					25	122	yes	yes	no	no	
		246					30	98	yes	yes	no	no	
		336	TCEU191	EU19	Zimdahl	Aridic Colorado	10	101	yes	no	yes	no	
		337					20	77	yes	no	yes	no	
		338					30	54	yes	no	yes	no	
		339					35	61	yes	no	yes	no	
		1084	TCMM613	MM6	Zheng	Martinique Paquemar	25	39.3	no	yes	no	no	
		1085					35	33.6	no	yes	no	no	
		1086	TCMM614	MM6	Zheng	Martinique StAnne	25	40.4	no	yes	no	no	
		1087					35	30.4	no	yes	no	no	
pendimethalin	dinitroaniline	1088	TCMM615	MM6	Zheng	Martinique Bochet	25	33.9	no	yes	no	no	
		1089					35	27.3	no	yes	no	no	
		1090	TCMM616	MM6	Zheng	Martinique Leyritz	25	30.8	no	yes	no	no	
		1091					35	23.4	no	yes	no	no	
		1092	TCMM617	MM6	Zheng	Martinique Eden	25	33.4	no	yes	no	no	
		1093					35	24.2	no	yes	no	no	
		1094	TCMM618	MM6	Zheng	France Marsillargues	25	34.6	no	yes	no	no	
		1095					35	21.1	no	yes	no	no	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (°C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
phenmedipham	carbamate	673	TCWS101	WS10	Vischetti	Umbria	10	26.7	yes	yes	yes	yes	Goodness of fit cannot be assessed visually - r2 not given - accepted because standard error <10%
		674					20	8.6	yes	yes	no	no	Rejected because: - goodness of fit cannot be assessed visually, lag phase - r2 not given , standard error >10%
phosalone	organophosphate	374	TCEFSA0361	EFSA036	Diehl	Speyer 1	10	8.5	yes	yes	no	no	Handling of soil according to ISO 103381-6 (Soil quality sampling guidance)
		375					20	1.9	yes	yes	yes	yes	Soil collected in June 2001 and experimental study starting date 18 July 2001
pinoxaden		1165	TCRB211	RB21	Dyson	Gartenacker Switzerland 1	10	0.55	yes	yes	yes	no	Reappraisal of RB22, half-life less than 1 d
		1166					20	0.28	yes	yes	yes	no	Reappraisal of RB22, half-life less than 1 d
		1167					30	0.13	yes	yes	yes	no	Reappraisal of RB22, half-life less than 1 d
		1171	TCRB221	RB22	Reischmann	Gartenacker Switzerland 1	10	0.4	yes	yes	no	no	Half-life less than 1 d
		1172					20	0.2	yes	yes	no	no	Half-life less than 1 d
		1173					30	0.1	yes	yes	no	no	Half-life less than 1 d
pinoxaden metab. NOA 407854 pinoxaden metab. NOA 407854		1168	TCRB212	RB21	Dyson	Gartenacker Switzerland 1	10	24.8	yes	yes	no	no	Reappraisal of RB22, rather different values
		1169					20	7.2	yes	yes	no	no	Reappraisal of RB22, rather different values
		1170					30	9.6	yes	yes	no	no	Reappraisal of RB22, rather different values
		1174	TCRB222	RB22	Reischmann	Gartenacker Switzerland 1	10	64.9	yes	yes	no	no	
		1175					20	29.9	yes	yes	no	no	
		1176					30	23.1	yes	yes	no	no	
primisulfuron-methyl	sulfonylurea	330	TCEU181	EU18	James	Horotiu 2	10	29	yes	yes	yes	no	Inconsistent reporting of recovered amounts at time zero

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
primisulfuron-methyl	sulfonylurea	331					22	20	yes	yes	yes	no	Inconsistent reporting of recovered amounts at time zero
		332					30	13	yes	yes	yes	no	Rejected because DT_{50} 13 d does not represent data (conc declined well below 50% by second sampling point. DT_{50}should be between 0 and 7 d). Inconsistent reporting of recovered amounts at time zero.
		899	TCEC62	EC6	Dinelli	Bologna	5	190	yes	yes	yes	no	Rejected because DT_{50}> 2x study period (60 d).
		900					10	129.8	yes	yes	yes	no	Rejected because DT_{50} > 2x study period (60 d).
		904					35	4.7	yes	yes	yes	no	
propamocarb		1224	TCSB12 1	SB12	Kley	Sarotti	10	25.3	no	yes	yes	no	Rejected because there is not enough information on storage No attempts were made to obtain this information because there are other quality issues with this set of studies.
		1225					20	11.7	no	yes	yes	no	Rejected because there is not enough information on storage Study performed in a different soil batch, storage periods differ and discrepancy in moisture too large.
		1226	TCSB12 2	SB12	Kley	LS 1	15	8.95	no	no	no	no	Rejected because no information on storage Very large application rate DT_{50}calculated from end of lag-phase based on the assumption that lag-phase does not occur in the field. EU agreed endpoint of 22 days is graphical DT_{50} from SB19. This value reflects overall decline better.
		1227					22	8.38	no	no	no	no	- No information on storage - Study performed with different batch of the soil, moisture outside accepted range - Lag phase over-estimated. DT_{50} calculated from end of lag-phase based on the assumption that lag-phase does not occur in the field.

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
propamocarb		1228					25	8.34	no	no	no	no	- No information on storage - Very large application rate - Separate study, not clear if same batch of soil was used - No clear lag phase, DT_{50} under-estimated. EU agreed endpoint of 14 days is graphical DT_{50} from SB17. This value reflects overall decline
		1229					25	7.43	no	no	no	no	- No information on storage - Very large application rate - Separate study, not clear if comparable with the others - DT_{50} does not include lag-phase based on the assumption that lag-phase does not occur in the field. Overall DT_{50} longer than reported value.
		1230	TCSB13 1	SB13	Kley	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	Document contains DT_{50} value of 4 soils at 20^{o}C including Sarotti. No information in addition to that in SB12
		1231	TCSB14 1	SB14	Fent	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	Document contains details of study with 4 soils at 20^{o}C including Sarotti.
		1232	TCSB15 1	SB15	Fent	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	Document contains details of studies with Sarotti soil at 10^{o}C
		1233	TCSB16 1	SB16	Kley	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	Document contains DT_{50} value for Sarotti soil at 10^{o}C. No information in addition to that in SB12
		1234	TCSB17 1	SB17	Brühl	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	Document contains details of study with LS 2.2 soil at 25^{o}C (single appl.)
		1235	TCSB18 1	SB18	Iwan	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	Document contains details of study with LS 2.2 soil at 22^{o}C
		1236	TCSB19 1	SB19	Brühl	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	Document contains details of study with LS 2.2 soil at 15^{o}C
		1237	TCSB20 1	SB20	Brühl	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	Document contains details of a study in a German soil at 25^{o}C, no data for other temperatures available

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
propamocarb		1238	TCSB21 1	SB21	Brühl	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	Document contains details of study with LS 2.2 soil at 25^{o}C (two appl.)
propiconazole	triazole	752	TCJJB66	JJB6	Bromilow	Woburn sandy loam	5	499	yes	yes	yes	no	
		753					10	215	yes	yes	yes	yes	
		754					15	117	yes	yes	yes	no	
		755					18	105	yes	yes	yes	no	
propyzamide	benzamide	108	TCEU37	EU3	Walker	Pump Ground 5 cm	5	373	yes	yes	yes	no	Data not used because soil moisture below 5%
		109					15	269	yes	yes	yes	no	Data not used because soil moisture below 5%
		110					25	73.2	yes	yes	yes	no	Data not used because soil moisture below 5%
		111	TCEU38	EU3	Walker	Pump Ground 5 cm	15	116	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		112					25	44.7	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		529	TCWS45	WS4	Jurado-Exposito	Wellesbourne 3	10	110	yes	yes	yes	no	Rejected because: 20% moisture preferred (shorter half-lives)
		530					20	32.9	yes	yes	yes	no	Rejected because: 20% moisture preferred (shorter half-lives)
		531	TCWS46	WS4	Jurado-Exposito	Wellesbourne 3	10	82.5	yes	yes	yes	no	Rejected because: 20% moisture preferred (shorter half-lives)
propyzamide	benzamide	532					20	30.4	yes	yes	no	no	Rejected because: visual fit not very good 20% moisture preferred (shorter half-lives)
		535	TCWS48	WS4	Jurado-Exposito	Wellesbourne 3	10	57.8	yes	yes	no	no	Rejected because visual fit not very good and replication of other study at same conditions
		536					20	15.6	yes	yes	yes	no	Rejected because replication of other study at same conditions
proquinazid metab. IN-MM671		1177	TCRB23 1	RB23	Lee	Nambsheim 2	10	145	yes	yes	no	no	Low r2
		1178					20	71	yes	yes	no	no	Low r2
rimsulfuron	sulfonylurea	376	TCEFSA	EFS	Benwell	Speyer 2	10	77	no	no	yes	no	Soil stored in soil shed

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rimsulfuron	sulfonylurea	377	0421	A042			20	30	no	no	yes	no	
		910	TCEC64	EC6	Dinelli	Bologna	35	1.4	yes	yes	yes	no	
simazine	triazine	88	TCEU31	EU3	Walker	Pump Ground 5 cm	5	517	yes	yes	yes	no	Data not used because soil moisture below 5%
		89					15	159	yes	yes	yes	no	Data not used because soil moisture below 5%
		90					25	44.8	yes	yes	yes	no	Data not used because soil moisture below 5%
		91	TCEU32	EU3	Walker	Pump Ground 5 cm	15	129	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		92					25	35	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		265	TCEU141	EU14	Walker	Warwick	10	120	yes	no	no	no	Fits: lines manually through log c vs t --> slopes. some data
		266					20	50	yes	no	no	no	Deviate strongly from first order kinetics
		267					30	29	yes	no	no	no	No clear indication whether bio/chem. analyses were performed
		268	TCEU142	EU14	Walker	Saskatshewan	10	274	yes	no	no	no	
		269					20	114	yes	no	no	no	
		270					30	78	yes	no	no	no	
		271	TCEU143	EU14	Walker	Firenze	10	147	yes	no	no	no	Visual inspection not available for all temperatures (only 20°C)
		272					20	39	yes	no	no	no	
		273					30	31	yes	no	no	no	
		274	TCEU144	EU14	Walker	Uppsala	10	230	yes	no	no	no	
		275					20	102	yes	no	no	no	
		276					30	76	yes	no	no	no	
		277	TCEU145	EU14	Walker	Braunschweig 2	10	214	yes	no	no	no	
		278					20	658	yes	no	no	no	
		279					30	42	yes	no	no	no	
		280	TCEU14	EU14	Walker	Alberta	10	283	yes	no	no	no	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
simazine	triazine	281	6				20	125	yes	no	no	no	
		282					25	59	yes	no	no	no	
		283	TCEU147	EU14	Walker	Oxford	10	55	yes	no	no	no	
		284					20	34	yes	no	no	no	
		285					30	26	yes	no	no	no	
		286	TCEU148	EU14	Walker	Ontario I	10	134	yes	no	no	no	
		287					20	62	yes	no	no	no	
		288					30	30	yes	no	no	no	
		289	TCEU149	EU14	Walker	Ontario II	10	123	yes	no	no	no	
		290					20	71	yes	no	no	no	
		291					30	33	yes	no	no	no	
		292	TCEU1410	EU14	Walker	Wageningen	10	74	yes	no	no	no	
		293					20	50	yes	no	no	no	
		294					30	27	yes	no	no	no	
		295	TCEU1411	EU14	Walker	Maarn	10	44	yes	no	no	no	
		296					20	21	yes	no	no	no	
		297					30	17	yes	no	no	no	
		298	TCEU1412	EU14	Walker	British Columbia	10	190	yes	no	no	no	
		299					20	42	yes	no	no	no	
		300					30	28	yes	no	no	no	
		301	TCEU1413	EU14	Walker	Haperden	5	190	yes	no	no	no	
		302					10	112	yes	no	no	no	
		303					20	46	yes	no	no	no	
		304	TCEU1414	EU14	Walker	Taipei	10	108	yes	no	no	no	
		305					20	39	yes	no	no	no	
		306					30	25	yes	no	no	no	
		307	TCEU1415	EU14	Walker	Taichung	10	153	yes	no	no	no	
		308					20	55	yes	no	no	no	
		309					30	31	yes	no	no	no	
		310	TCEU1416	EU14	Walker	Laguna	25	67	yes	no	no	no	
		311					35	24	yes	no	no	no	
		312					45	11	yes	no	no	no	
		781	TCJJB74	JJB7	Bunte	Eisenbac	10	82	no	yes	yes	no	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
simazine	triazine	782				h S-1	20	31	no	yes	yes	no	
		783					30	21	no	yes	yes	no	
		784	TCJJB75	JJB7	Bunte	Eisenbach S-2	10	86	no	yes	yes	no	
		785					20	39	no	yes	yes	no	
		786					30	19	no	yes	yes	no	
		787	TCJJB76	JJB7	Bunte	Krummbach-L	10	82	no	yes	yes	no	
		788					20	37	no	yes	yes	no	
		789					30	32	no	yes	yes	no	
		790	TCJJB77	JJB7	Bunte	Krummbach-T	10	72	no	yes	yes	no	
		791					20	45	no	yes	yes	no	
		792					30	34	no	yes	yes	no	
sulcotrione	triketone	1183	TCRB241	RB24	Reinken	Alterberry	25	24	no	yes	yes	no	Recalculation of Subba-Rao & Wang etc
		1185	TCRB251	RB25	Subba-Rao	Alterberry	5	137	no	yes	yes	no	Lack of information on soil sample storage
		1186					25	24	no	yes	yes	no	Lack of information on soil sample storage
		1187					25	66	no	yes	yes	no	Lack of information on soil sample storage
sulcotrione metab CMBA	triketone	1184	TCRB241	RB24	Reinken	Alterberry	25	23.1	no	yes	yes	no	Recalculation of Subba-Rao & Wang etc
sulfometuron-methyl	sulfonylurea	887	TCEC51	EC5	Cambon	Saint-Nazaire	20	not reported	no	no	no	no	Storage time and pair comparison missed
		888					28	not reported	no	no	no	no	Storage time and pair comparison missed
		889					35	not reported	no	no	no	no	Storage time and pair comparison missed
		890					60	not reported	no	no	no	no	Storage time and pair comparison missed

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
sulfometuron-methyl	sulfonylurea	891					68	not reported	no	no	no	no	Storage time and pair comparison missed
		892					75	not reported	no	no	no	no	Storage time and pair comparison missed
tefluthrin	pyrethroid	1188	TCRB261	RB26	Pluckrose	18 Acres 1	5	134 (179)	yes	yes	no	no	
		1189					20	26 (26)	yes	yes	no	no	Parent volatilisation of 7% (not corrected for by RMS)
		1190					20	20 (19)	yes	yes	no	no	Alternative ^{14}C label
		1191					20	13 (13)	yes	yes	no	no	Large effect of low rate
		1192					30	17 (17)	yes	yes	no	no	Parent volatilisation of 16% (not corrected for by RMS)
terbuthylazine	triazine	817	TCJJB101	JJB10	Dibbern	Ahlum 2	10	144	yes	no	no	no	No forced air flow
		818					20	109	yes	no	yes	no	No forced air flow
		819	TCJJB102	JJB10	Dibbern	Ahlum 2	10	133	yes	no	no	no	No forced air flow
		820					20	68	yes	no	yes	no	No forced air flow
		854	TCEC11	EC1	Caracciolo	Manerbio soil horizon A	15	180	no	yes	no	no	
		855					15	200	no	yes	no	no	
terbuthylazine	triazine	856	TCEC12	EC1	Caracciolo	Manerbio soil horizon A	22	30	no	yes	no	no	
		857					22	180	no	yes	no	no	
TFNA (metabolite of flonicamid		1207	TCSB41	SB4	Hatzenbeler	Bedfordshire 1	10	0.99	yes	yes	yes	no	Rejected because DT_{50}< 1 day
		1208					20	0.46	yes	yes	yes	no	Rejected because DT_{50}< 1 day
TFNA-OH (metabolite of flonicamid		1211	TCSB61	SB6	Findak	Bedfordshire 1	10	4.5	yes	yes	yes	yes	

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
TFNA-OH (metabolite of flonicamid		1212					20	1	yes	yes	no	no	Log-transformation leads to over-estimation of initial concentration (142%). DT_{50} too fast, the true value should be around 2 days.
TFNG (metabolite of flonicamid		1213	TCSB71	SB7	Lentz	Bedfordshire 1	10	0.259	yes	yes	yes	no	Rejected because DT_{50}< 1 day
TFNG-AM (metabolite of flonicamid		1214					20	0.114	yes	yes	no	no	Rejected because DT_{50}< 1 day Residues decline much more slowly between 0 and 0.25 days than between 0.25 and 0.5 days (page 44). Fit poor, DT_{50} should be around 0.25 days
TFNG-AM (metabolite of flonicamid		1215	TCSB81	SB8	Lentz	Bedfordshire 2	10	0.688	yes	yes	yes	no	Rejected because DT_{50} < 1 day
		1216					20	0.167	yes	yes	yes	no	Rejected because DT_{50} < 1 day
thiameturon	sulfonylurea	1034	TCMM31	MM3	Smith	Indian head	10	nc	no	yes	no	no	
		1035					20	nc	no	yes	yes	no	
		1036					30	nc	no	yes	no	no	
		1037	TCMM32	MM3	Smith	Regina 1	10	nc	no	yes	no	no	
		1038					20	nc	no	yes	yes	no	
		1039					30	nc	no	yes	no	no	
		1040	TCMM33	MM3	Smith	White city	10	nc	no	yes	no	no	
		1041					20	nc	no	yes	yes	no	
thiameturon	sulfonylurea	1042					30	nc	no	yes	no	no	
thifensulfuron-methyl	sulfonylurea	877	TCEC41	EC4	Cambon	Saint-Nazaire	20	not reported	no	no	no	no	Storage time and pair comparison missed
		878					35	not reported	no	no	no	no	Storage time and pair comparison missed
		879					43	not reported	no	no	no	no	Storage time and pair comparison missed

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
thifensulfuron-methyl	sulfonylurea	880					53	not reported	no	no	no	no	Storage time and pair comparison missed
		881					65	not reported	no	no	no	no	Storage time and pair comparison missed
		882	TCEC42	EC4	Cambon	Salanque	20	not reported	no	no	no	no	Storage time and pair comparison missed
		883					35	not reported	no	no	no	no	Storage time and pair comparison missed
		884					43	not reported	no	no	no	no	Storage time and pair comparison missed
		885					53	not reported	no	no	no	no	Storage time and pair comparison missed
		886					65	not reported	no	no	no	no	Storage time and pair comparison missed
thiodicarb	oxime carbamate	378	TCEFSA 0431	EFS A043	Burr	Boarded Barns Farm 2	10	1.7	yes	yes	no	no	Fitted DT_{50} cannot be found in this report, but in the monograph. poor fit for first-order kinetics. DT_{50} < 1 day --> not to be used
		379					20	0.6	yes	yes	no	no	Methomyl data cannot be used instead because the 10°C study relies only on 3 data points from which no reliable DT_{50} can be extracted.
tolclofos-methyl	organophosphate	380	TCEFSA 0441	EFS A044	Lewis	Shuttleworth	10	23	no	yes	yes	no	Date of sampling not given
		381					15	23	no	yes	yes	no	Different initial concentration of a.i. for the two temperatures
tralkoxydim	cyclohexanedione oxime	1193	TCRB271	RB27	Greener	18 Acres 2	10	12.2	no	no	n.a.	no	Different soil samples for the two temperatures

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (⁰C)	DT_{50} (day)	Stor -age QC	Test QC	Regre- ssion QC	Over- all QC	Remarks
tralkoxydim	cyclohexanedione oxime	1194					20	2.5	no	yes	n.a.	no	Different soil samples for the two temperatures
		1195	TCRB272	RB27	Greener	Frensham 1	10	10.7	no	no	n.a.	no	Different soil samples for the two temperatures
		1196					20	2.2	no	yes	n.a.	no	Different soil samples for the two temperatures
		1197	TCRB281	RB28	Butters	Frensham 2	20	2.2	no	yes	no	no	Different soil samples for the two temperatures (SFO recalculated by Greener)
		1198					20	2.5	no	yes	no	no	Different soil samples for the two temperatures (SFO recalculated by Greener)
		1199	TCRB291	RB29	Entwistle	Frensham 1	10	6	no	no	yes	no	Different soil samples for the two temperatures (SFO recalculated by Greener)
		1200					10	9	no	no	yes	no	Different soil samples for the two temperatures (SFO recalculated by Greener)
trans-chlordane	chlorinated hydrocarbon	976	TCEC151	EC15	Lemley	X8			no	no	no	no	65 soils collected in different ecosystems. paper not suitable for this scope because missing a large amount of information
trans-permethrin	pyrethroid	1102	TCMM82	MM8	Jordan	Dubbs	10	11	no	yes	yes	no	
		1103					25	4.4	no	yes	yes	no	
		1104					40	3.5	no	yes	yes	no	
triadimenol	triazole	764	TCJJB69	JJB6	Bromilow	Rothamsted clay loam	5	2003	yes	yes	no	no	
		765					10	826	yes	yes	yes	yes	
		766					15	447	yes	yes	no	no	
		767					18	363	yes	yes	no	no	
		768	TCJJB610	JJB6	Bromilow	Woburn sandy loam	5	6930	yes	yes	no	no	
		769					10	2005	yes	yes	no	no	
		770					15	805	yes	yes	no	no	
		771					18	624	yes	yes	no	no	

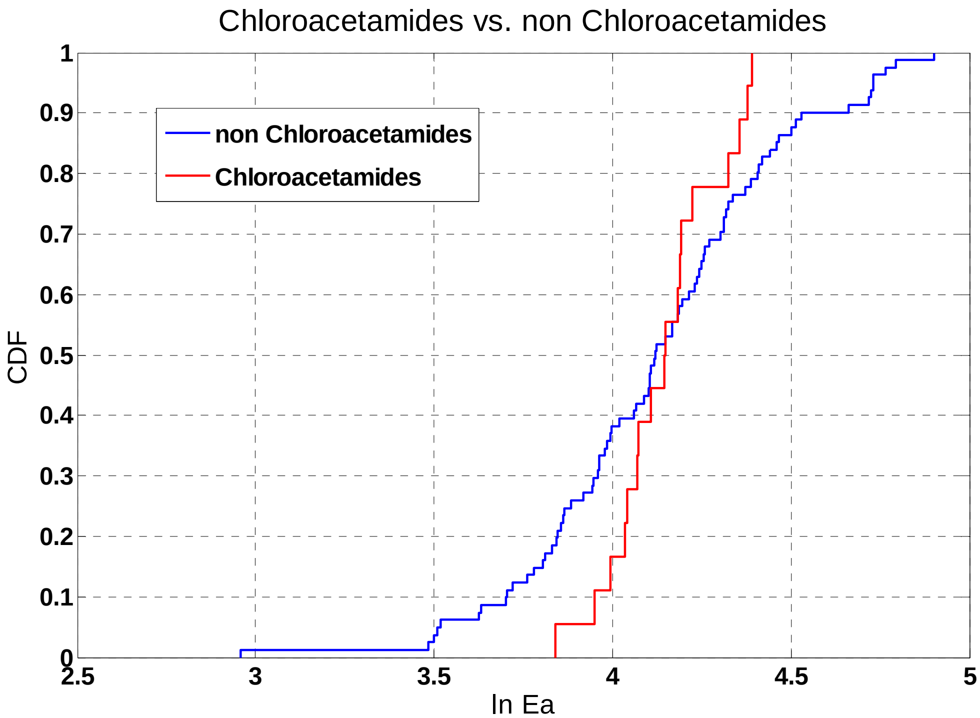
Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor -age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
triallate	thiocarbamate	424	TCWS27	WS2	Gottesbüren	Ahlum 1	10	103	yes	yes	yes	no	Volatile, but no forced air flow. Rejected because replication of other study with Ahlum soil (from subplot of same field)
		425					20	51	yes	yes	yes	no	Volatile, but no forced air flow. Rejected because replication of other study with Ahlum soil (from subplot of same field)
		426					30	34	yes	yes	yes	no	Volatile, but no forced air flow. Rejected because replication of other study with Ahlum soil (from subplot of same field)
triasulfuron	sulfonylurea	327	TCEU172	EU17	James	Horotiu 2	10	43.6	yes	yes	yes	yes	The values given are half-lives (t1/2) based on SFO excluding day zero. DT_{50} values were 10.5, 6 and 4.5days, respectively.
		328					22	44.1	yes	yes	no	no	All EU17: initial conc. 30 g a.i./ha
		329					30	39.2	yes	yes	no	no	
		893	TCEC61	EC6	Dinelli	Bologna	5	203.9	yes	yes	yes	no	Rejected because DT_{50} > 2x study period (60 d)
		894					10	148.4	yes	yes	yes	no	Rejected because DT_{50} > 2x study period (60 d)
		898					35	0.1	yes	yes	yes	no	Authors were contacted for a data requirement: data originating HL-regression lines, duration, storage time
		1028	TCMM21	MM2	Oppong	Pen-y-Ffridd	10	79	no	no	yes	no	
		1029					30	12	no	no	yes	no	
		1030	TCMM22	MM2	Oppong	Pen-y-Ffridd	10	49	no	no	yes	no	
		1031					30	11	no	no	yes	no	
		1032	TCMM23	MM2	Oppong	Pen-y-Ffridd	10	30	no	no	yes	no	
		1033					30	13	no	no	yes	no	
tribenuron	sulfonylurea	382	TCEFSA 0471	EFS A047	Hawkins	Arrow	10	11.3	no	yes	yes	no	RMS re-calculation of DT_{50} and DT90 based on first-order kinetics.
		383					20	1.9	no	yes	yes	no	RMS re-calculation of DT_{50} and DT90 based on first-order kinetics.
		384	TCEFSA 0472	EFS A047	Hawkins	Evesham 2	10	36.3	no	yes	yes	no	
		385					20	10.4	no	yes	yes	no	
trifluralin	dinitroaniline	118	TCEU310	EU3	Walker	Pump Ground 5	5	982	yes	yes	yes	no	Data not used because soil moisture below 5%

Pesticide	Pesticide family	ID	Test Code	Ref Code	First author	Soil origin	Temp (^{0}C)	DT_{50} (day)	Stor-age QC	Test QC	Regre-ssion QC	Over-all QC	Remarks
trifluralin	dinitroaniline	119				cm	15	592	yes	yes	yes	no	Data not used because soil moisture below 5%
		120					25	292	yes	yes	yes	no	Data not used because soil moisture below 5%
		121	TCEU311	EU3	Walker	Pump Ground 5 cm	15	442	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
		122					25	215	yes	yes	yes	no	Other dataset for same soil and pesticide is preferred
trifluralin	dinitroaniline	1239	TCEC101	EC10	Grover	not reported	n.a.	n.a.	no	no	no	no	The paper is a review of the environmental fate of the pesticide with a miscellanea of information but missing specific data on degradation as requested by the protocol
trinexapac-ethyl	Cyclohexanecarboxylic acid	386	TCEFSA0511	EFSA051	Schanne	Itingen Switzerland	10	0.138	yes	yes	yes	no	Soil stored in open containers under natural conditions after field collection. DT_{50} < 1 day. The acid-metabolite is formed in high amounts and is the biologically active compound. Both DT_{50} values (parent and metabolite) are reported. Trinexapac-acid was applied as parent in the same study.
		387					20	0.088	yes	yes	yes	no	
triticonazole	triazole	388	TCEFSA0521	EFSA052	Simmonds	Manningtree	10	614	yes	yes	yes	yes	DT_{50} value at 10ºC extrapolated (at DAT 365 parent distribution of radioactivity = 64.68% A.R.)
		389					25	160	yes	yes	no	no	DT_{50} value at 10ºC extrapolated (at DAT 365 parent distribution of radioactivity = 64.68% A.R.)

Appendix 4

Further analysis of distributions of activation energies for chemical classes

A4.1 Additional comparisons of E_a distribution between chemical families (Phenylureas vs. non-Phenylureas appears in the main document)

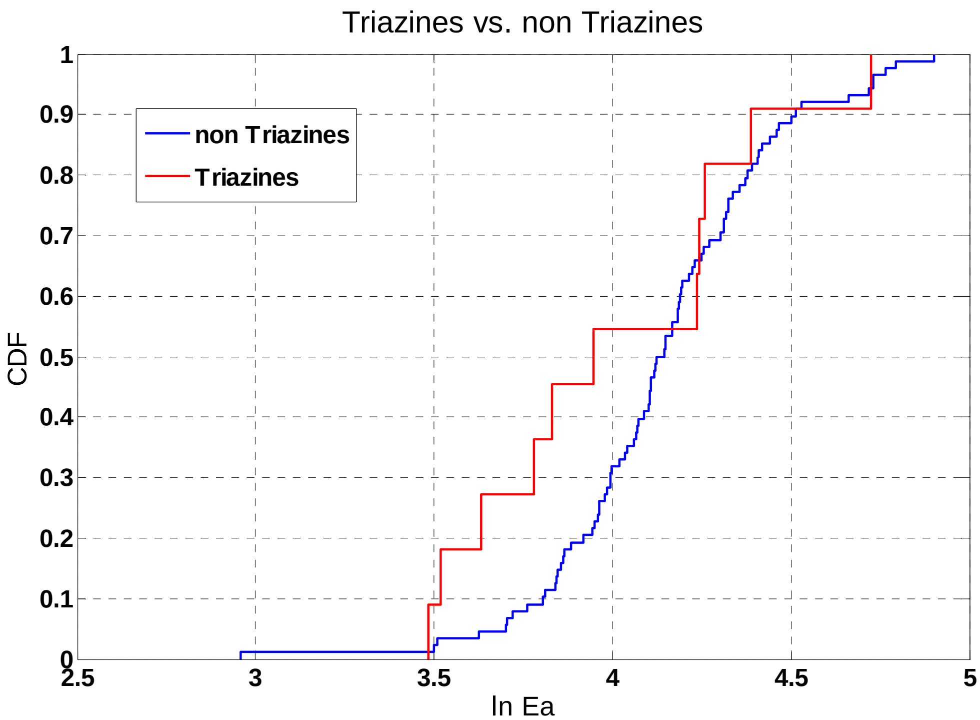


	mean	std	T-Test	Levene Test
Chloroacetamides	4.147	0.152	0.78	0.033
Non-Chloroacetamides	4.123	0.351		

Levene's test shows that the group variances are significantly different, so that non-parametric tests are the more robust:

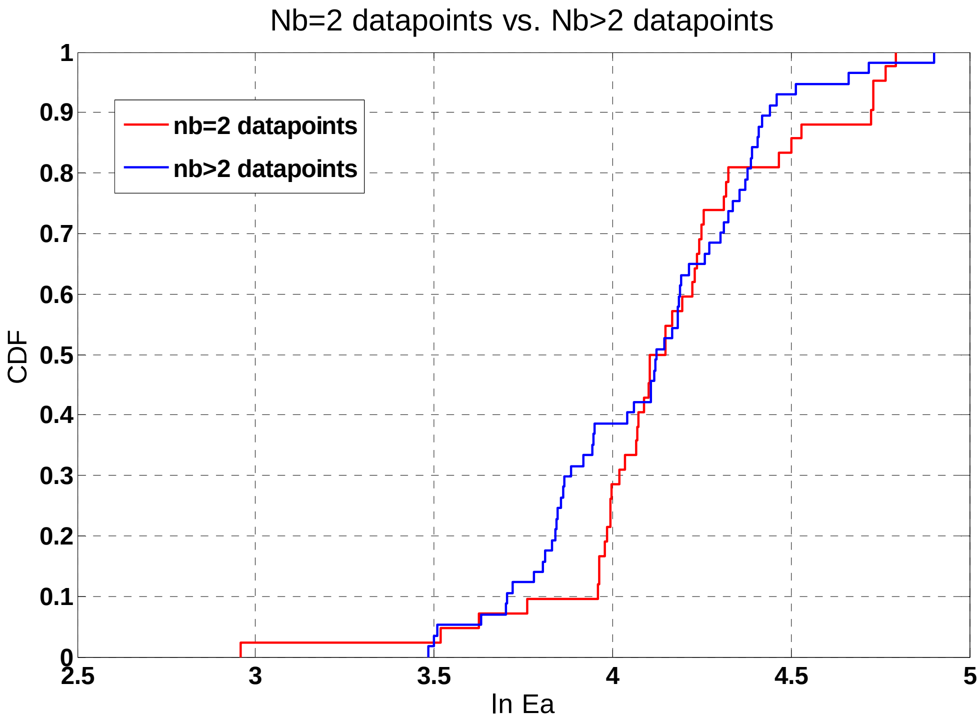
	mean	std	p-value (M-W)	p-value (K)
Chloroacetamides	4.147	0.152	0.76	0.037
Non-Chloroacetamides	4.123	0.351		

Conclusion: group means are not significantly different but the distributions (most likely the variance) are significantly different



	mean	std	T-test	Levene Test
Triazines	4.003	0.396	0.18	0.43
Non-Triazines	4.143	0.313		

Conclusion: group means and distributions are not significantly different.

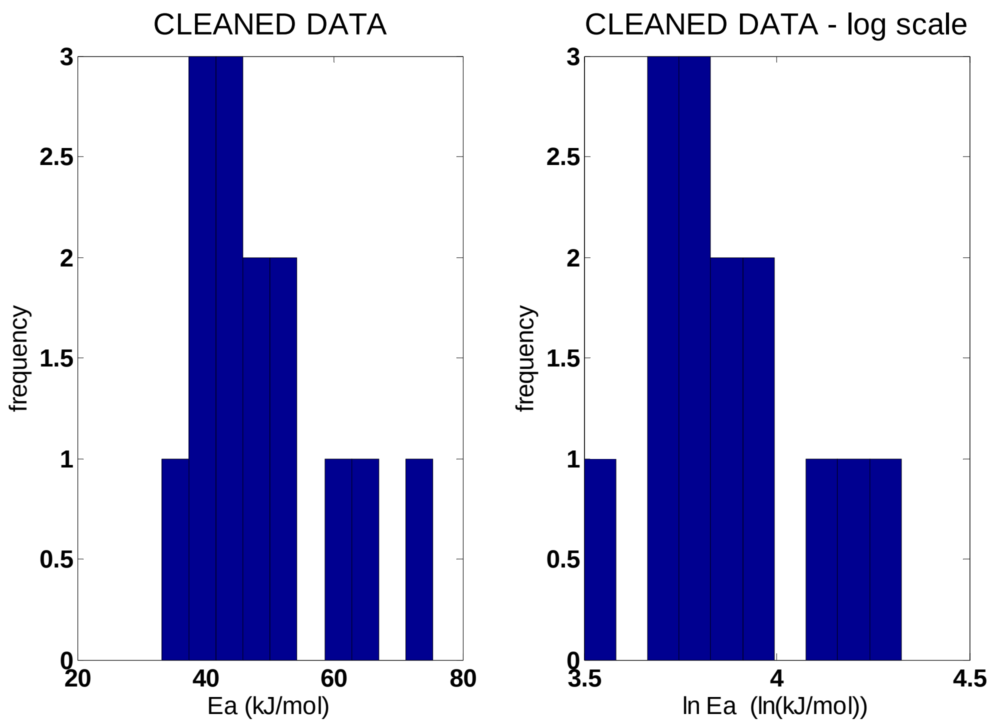


	mean	std	p-value (MW)	p-value (K)
2 data points	4.158	0.344	0.42	0.02
>2 data points	4.105	0.310		

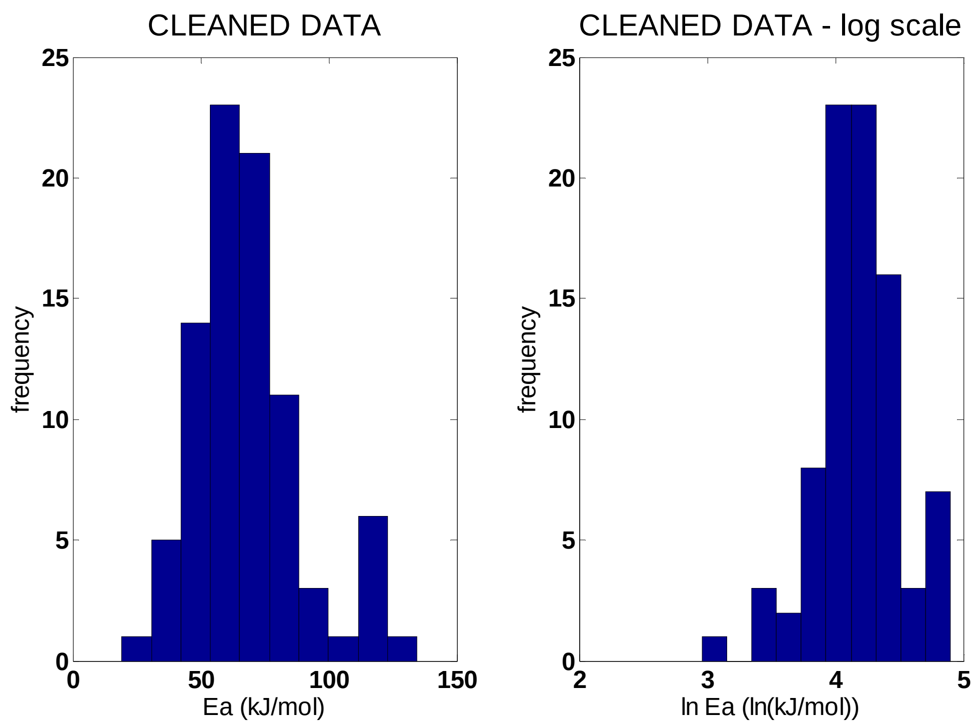
Conclusion: group means are not significantly different, but the distributions differ.

A4.2 Further analysis of the E_a distributions of Phenylureas vs. non-Phenylureas

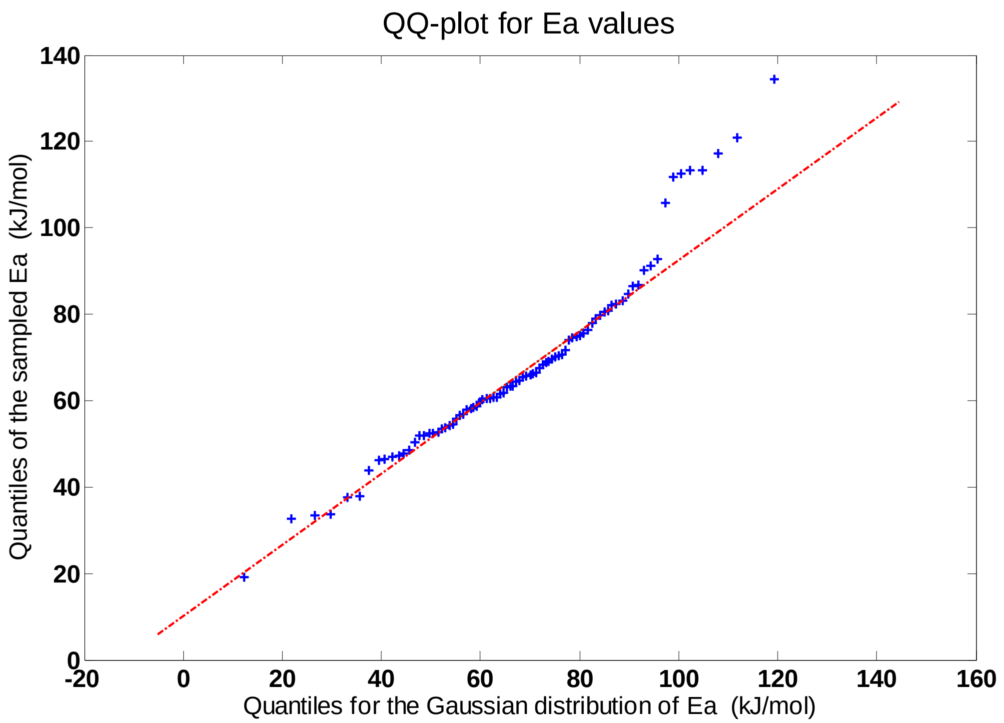
- E_a distributions for Phenylureas only:

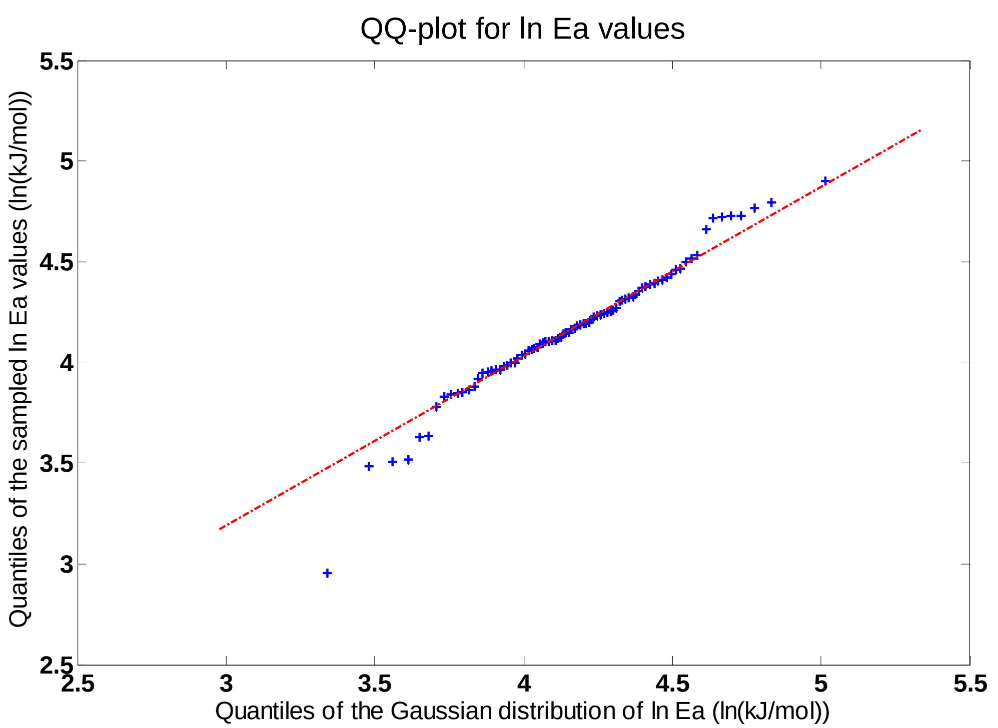


- E_a distributions for non-Phenylureas only.



- QQ plots for non-Phenylureas: respectively on linear-scaled and on log-scaled E_a values respectively:





A4.3 Measure of Association/Correlation of Soil and Chemical name (and Reference Code)

As the variables 'soil', 'chemical name' and 'reference code' are categorical and not even ordinal, it is impossible to compute any numerical correlation term such as Pearson's or Spearman's correlation factors. However, it is possible to measure the association between two of these variables. Factors reflecting the strength of association are derived from contingency tables (cross-tables of frequencies in each category). The most commonly used are the lambda and the uncertainty factors, both of which range from 0 (no association) to 1 (1-to-1 correspondence).

Lambda coefficients (based on the conditional predictive power):

	Soil	Name	Reference
Soil	1	0.59	0.90
Name	0.59	1	0.66
Reference	0.90	0.66	1

Uncertainty coefficients (based on measure of entropy):

	Soil	Name	Reference
Soil	1	0.81	0.96
Name	0.81	1	0.83
Reference	0.96	0.83	1

A4.4 Alternative to Arrhenius equation

Individual fits

In a first step, individual quadratic fits were performed on each tested compound having 3 or more data points, in order to measure the average discrepancy from linear fits. It is not possible to perform a statistical test with such limited degrees of freedom. Therefore, we replace the first-order regression:

$$\ln k = A + B/Temp$$

by the second-order regression:

$$\ln k = A + B/Temp + C/(Temp)^2$$

Where Temp=temperature in Kelvin degrees.

Out of the 98 entries, 56 of them had 3 or more data points and hence could be used in this analysis. After fitting individually each entry, both with linear and quadratic fits, the difference between the fits could be derived at various temperatures.

Hereafter we first report the descriptive statistics for the difference (linear – quadratic) between the two fits (of ln *k*), for various temperatures:

Temp (°C)	Mean	Std Dev	Minimum	Maximum
5	0.10	0.303	-1.004	1.016
10	-0.007	0.114	-0.385	0.442
20	-0.036	0.116	-0.395	0.241
30	0.154	0.358	-0.806	1.468
35	0.319	0.626	-1.380	2.353

As expected and visible on the plots, the difference is minimal between 10° and 20°C, as most data are collected in that range of temperatures. In this range, the linear fits tend to underestimate ln *k*. The situation is reversed outside that range, and differences get much higher at higher temperatures.

Then, we report the statistics for the exponential of such differences, for various temperatures:

Temp (°C)	Mean	Std Dev	Minimum	Maximum
5	1.167	0.422	0.366	2.764
10	0.999	0.119	0.679	1.556
20	0.970	0.108	0.673	1.272
30	1.256	0.605	0.446	4.342
35	1.723	1.582	0.251	10.525

This quantifies better the difference in the normal scale. Above 30°C, the approximation becomes uncertain and much less robust, with errors greater than 25%. Between 5° and 25°C, we can be confident that the difference is below 15% on the evaluation of *k*.

Random-effect modelling

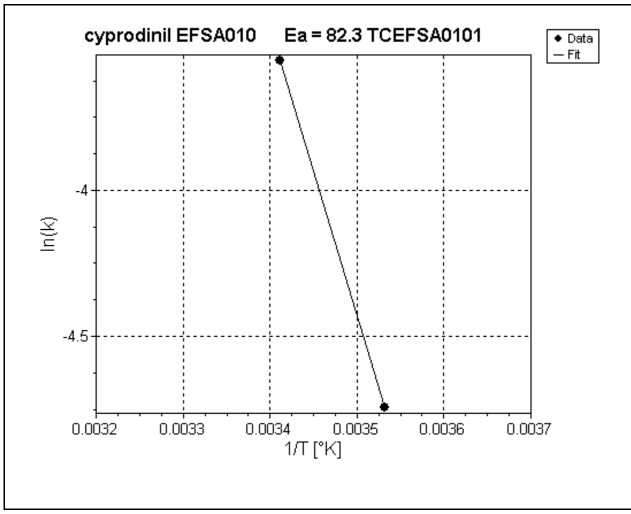
Instead of considering fits individually and independently, another approach would be to analyze all data together, using a random-effect model. The idea is to assume that for each entry, regression coefficients A, B and C can be specifically computed, but they are related to each other to each other, in the sense that all “A” coefficients can be considered as drawn from a normal distribution (or lognormal or any other), and the same for B and C and all variances parameters.

Such an approach was implemented with the quadratic model, to estimate the C parameter, and statistically investigate its size and the probability that it =0. As a software package, to fit such models, the most flexible and powerful is WinBUGS (it uses Bayesian inference). Bayesian statistics allow more flexible inference of parameters in the sense that it does not restrict the analysis to the evaluation of a single-value estimate of C and the test of C=0. Instead, it provides the whole distribution of possible Cs (and all other parameters), so that it is possible to assess the probability that C lies in any given range of values (such distributions of model parameters are called ‘posterior distributions’). WinBUGS allows simulation-based evaluation of such distributions. Let mu_C be the average C over tests, then the evaluated distribution is displayed in Figure 9 in the Opinion.

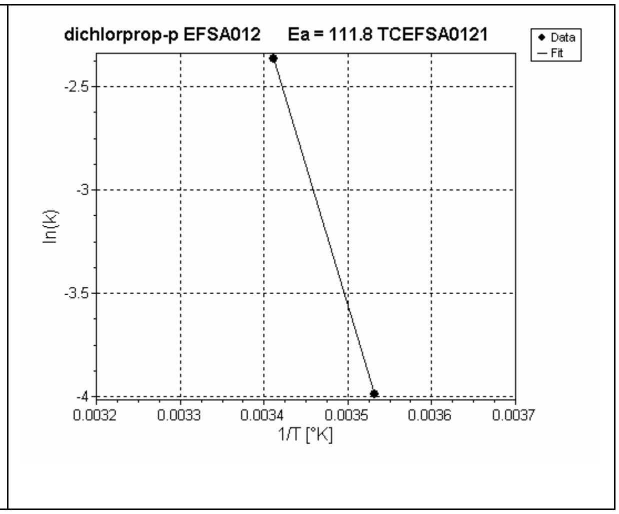
Appendix 5

Arrhenius plots for additional compounds

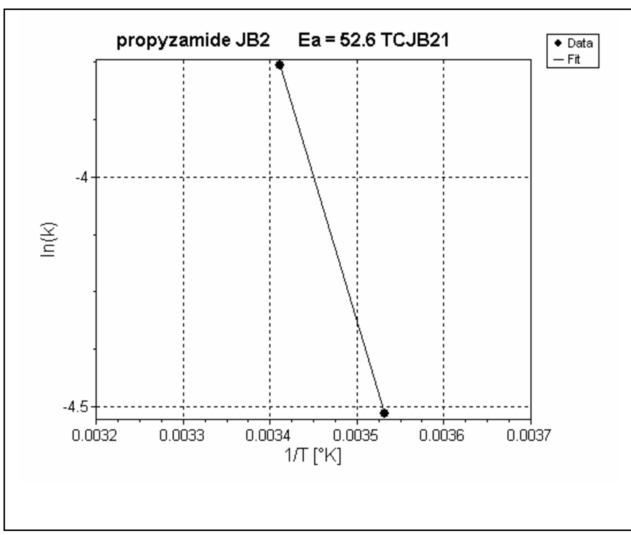
Anilinopyridine

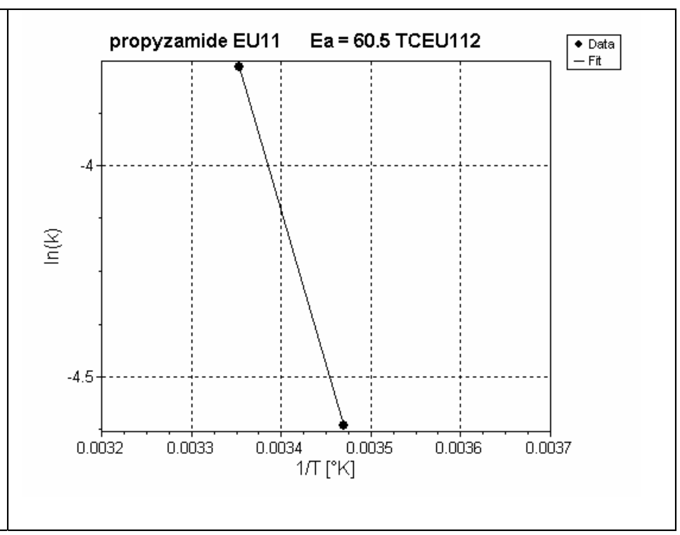


Aryloxyphenoxypropionate

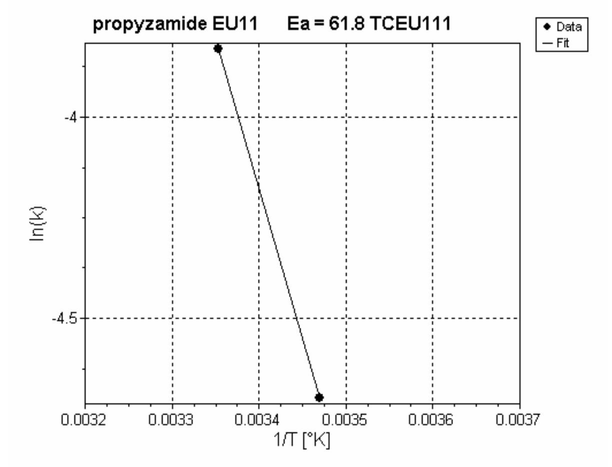


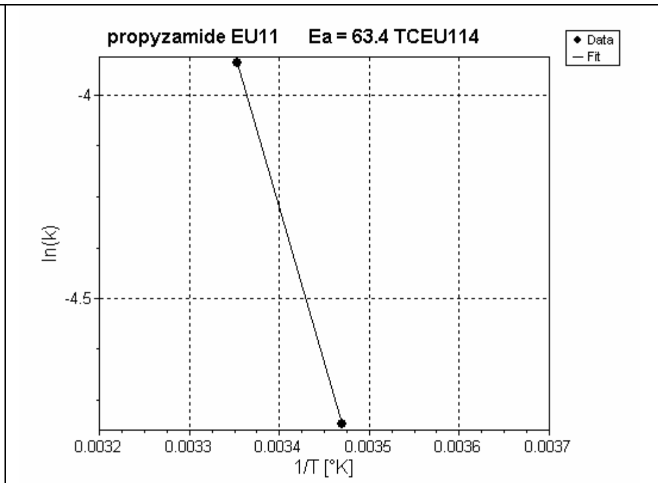
Benzamides

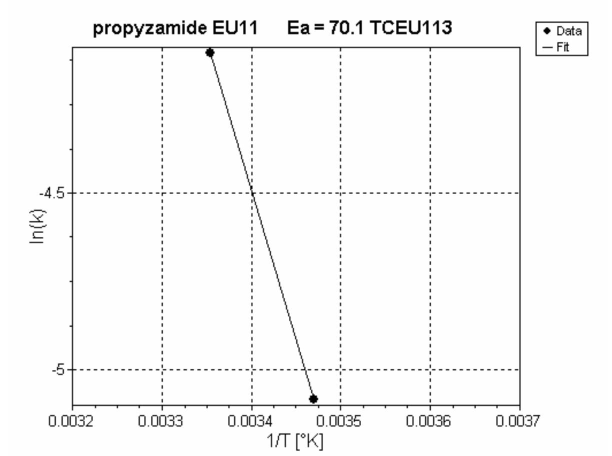


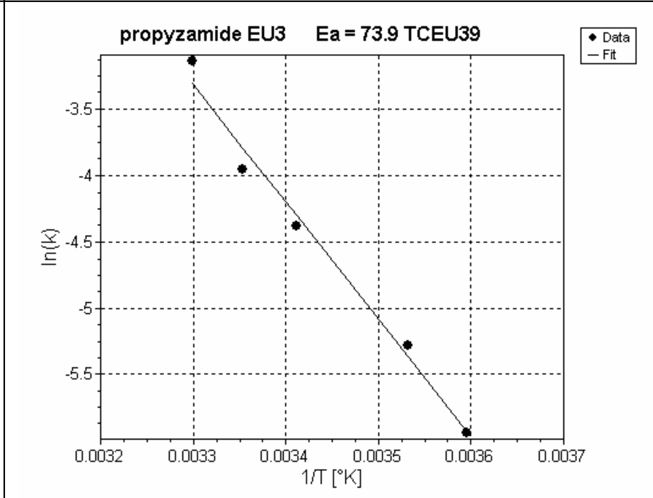


Benzamides

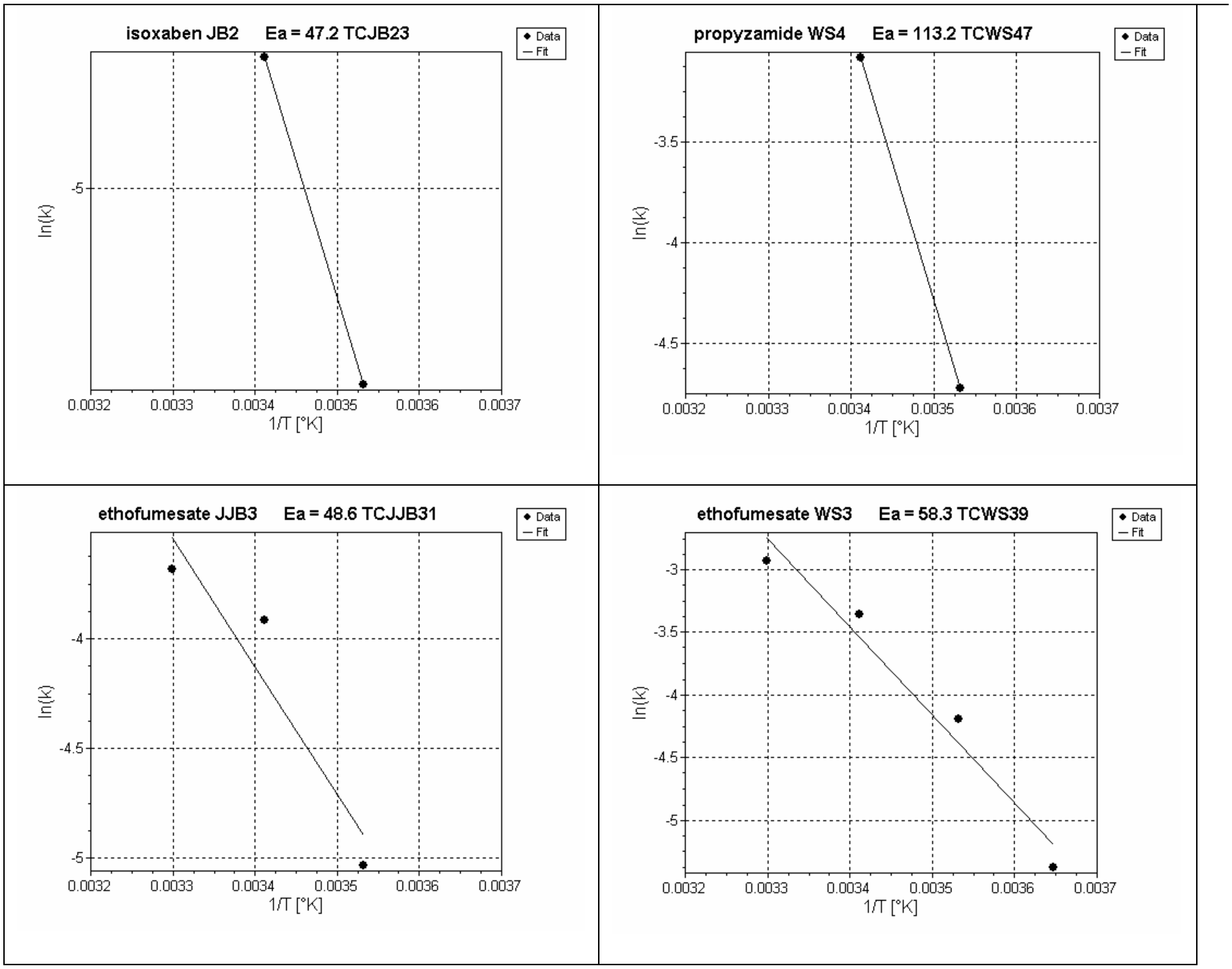

propyzamide EU11 Ea = 61.8 TCEU111
Data
Fit
ln(k)
-4
-4.5
0.0032 0.0033 0.0034 0.0035 0.0036 0.0037
1/T [°K]


propyzamide EU11 Ea = 63.4 TCEU114
Data
Fit
ln(k)
-4
-4.5
0.0032 0.0033 0.0034 0.0035 0.0036 0.0037
1/T [°K]

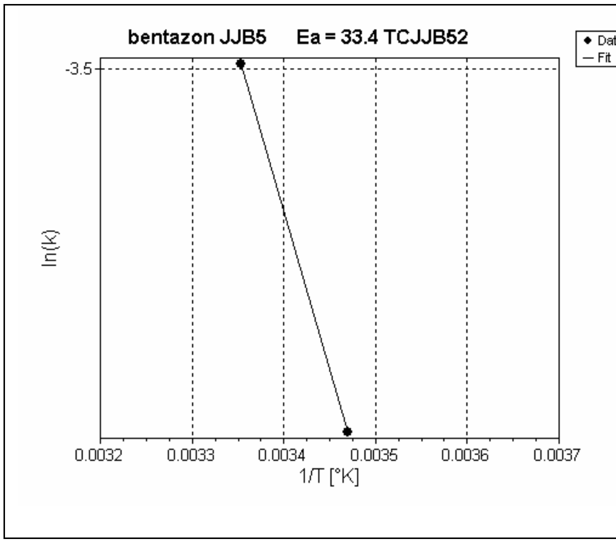

propyzamide EU11 Ea = 70.1 TCEU113
Data
Fit
ln(k)
-4.5
-5
0.0032 0.0033 0.0034 0.0035 0.0036 0.0037
1/T [°K]

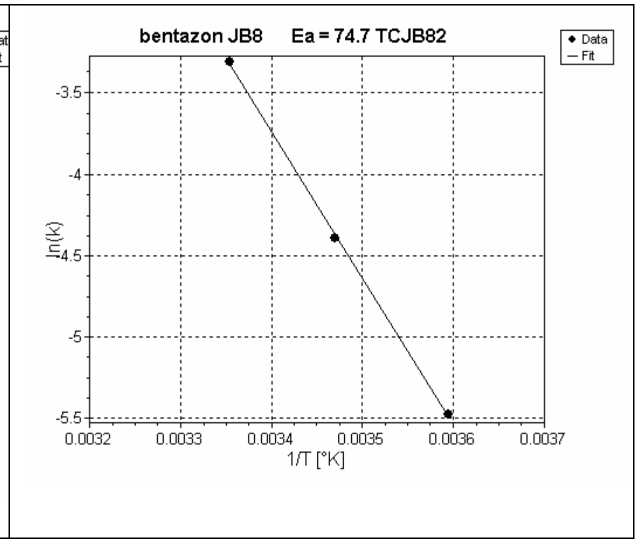

propyzamide EU3 Ea = 73.9 TCEU39
Data
Fit
ln(k)
-3.5
-4
-4.5
-5
-5.5
0.0032 0.0033 0.0034 0.0035 0.0036 0.0037
1/T [°K]

Benzamides

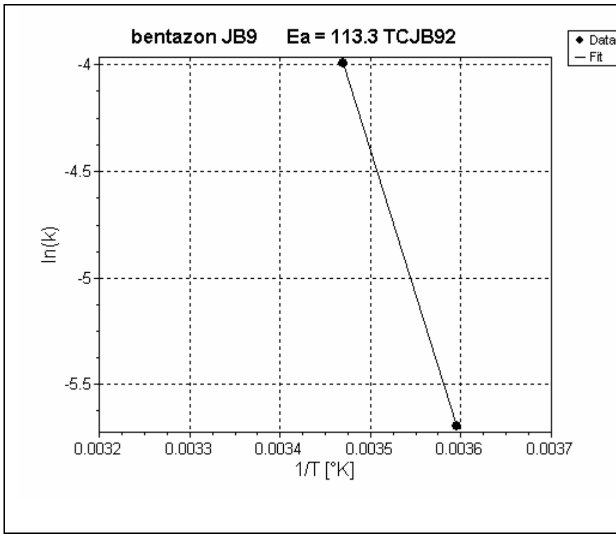

isoxaben JB2 Ea = 47.2 TCJB23
propyzamide WS4 Ea = 113.2 TCWS47
ethofumesate JJB3 Ea = 48.6 TCJJB31
ethofumesate WS3 Ea = 58.3 TCWS39
Data
Fit
ln(k)
1/T [°K]

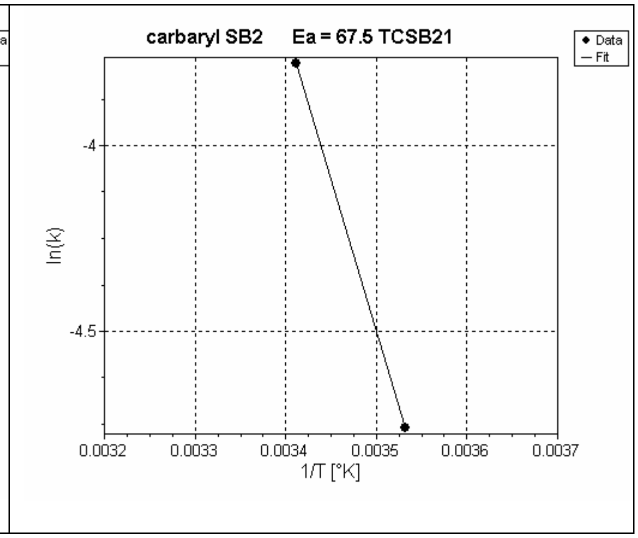
Benzothiadiazinones



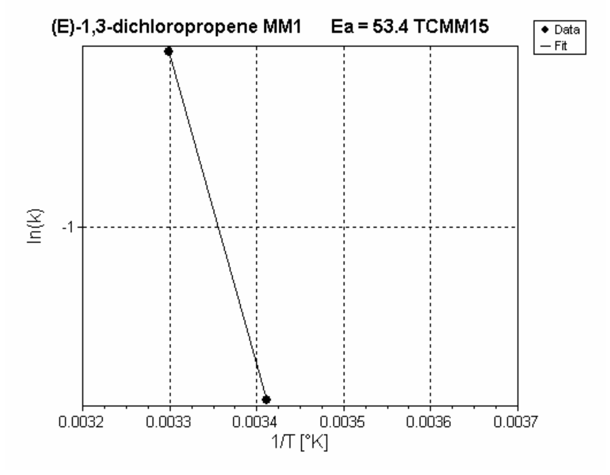


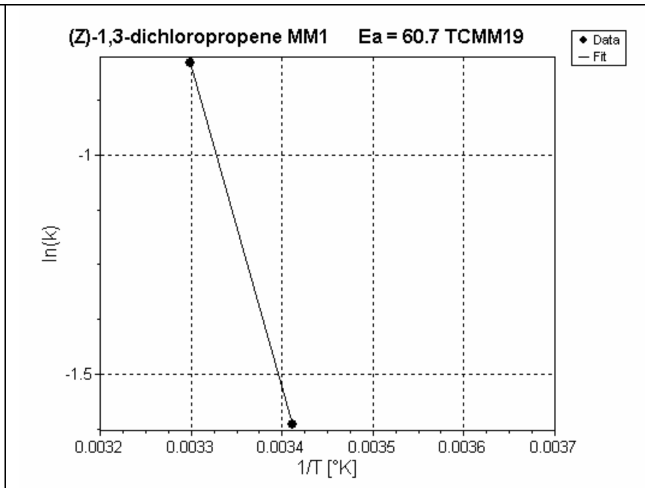
Carbamate



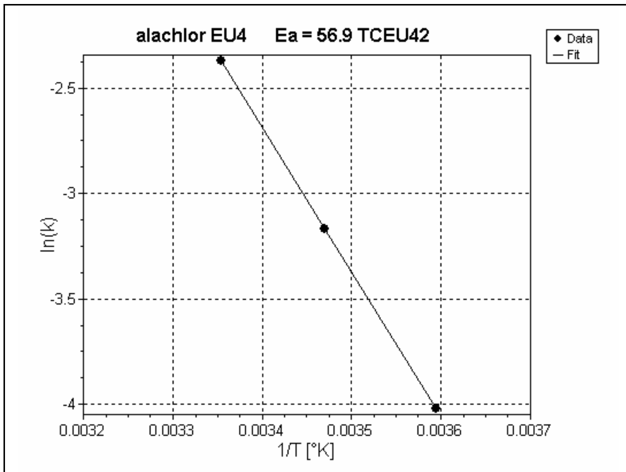


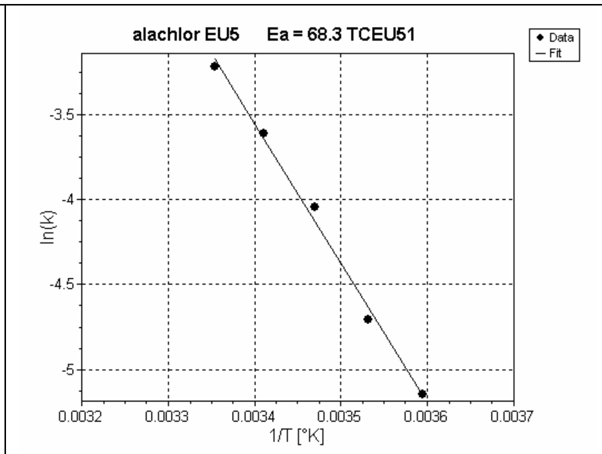
Chlorinated hydrocarbons



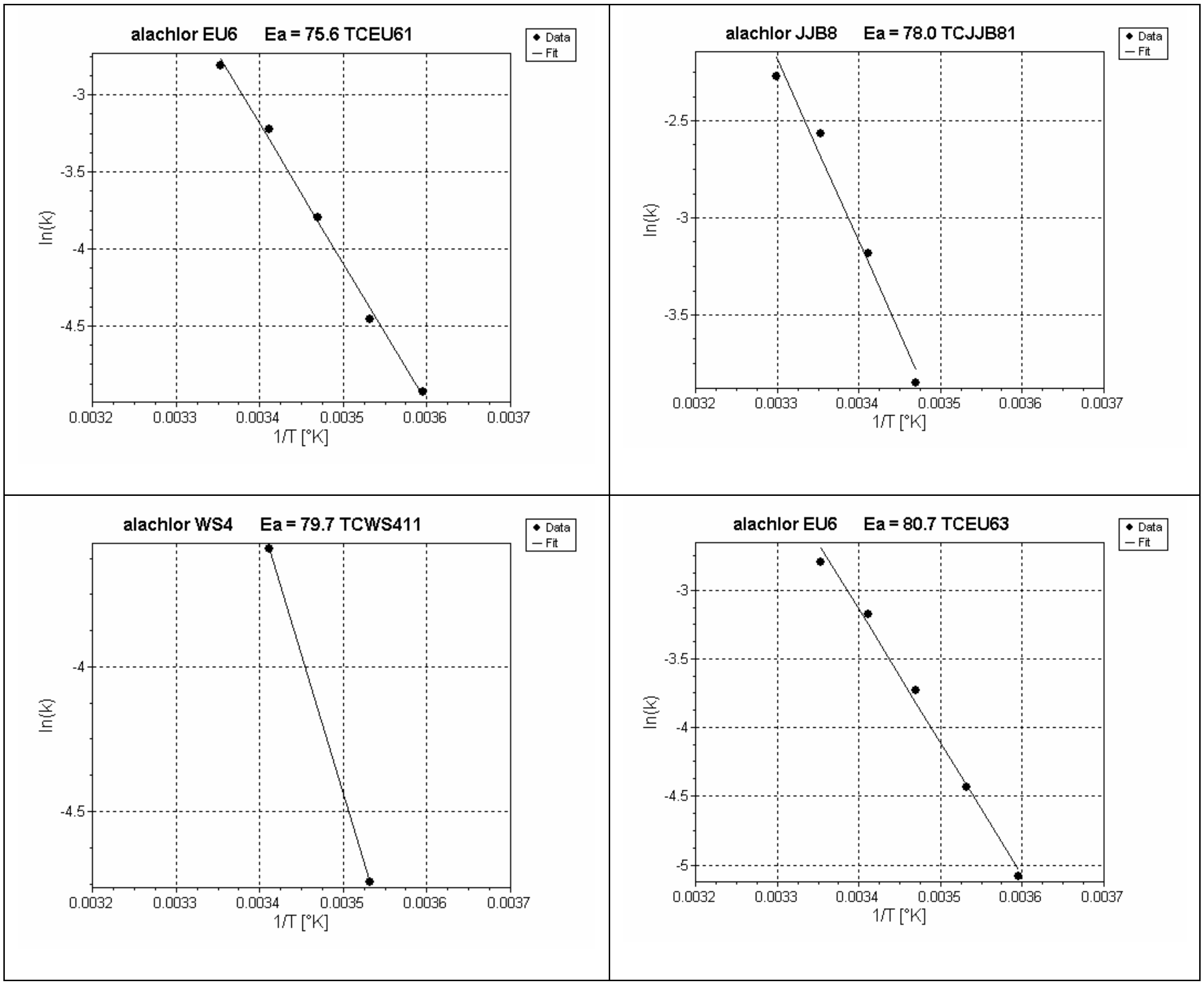


Chloroacetamides

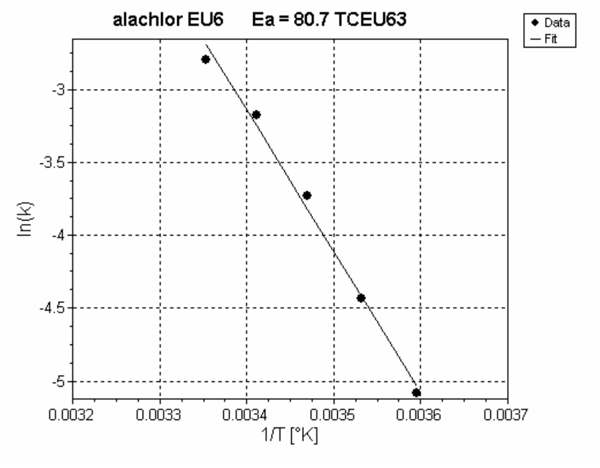


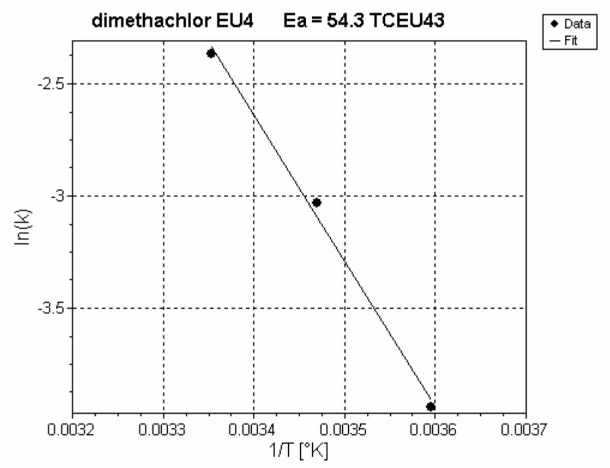


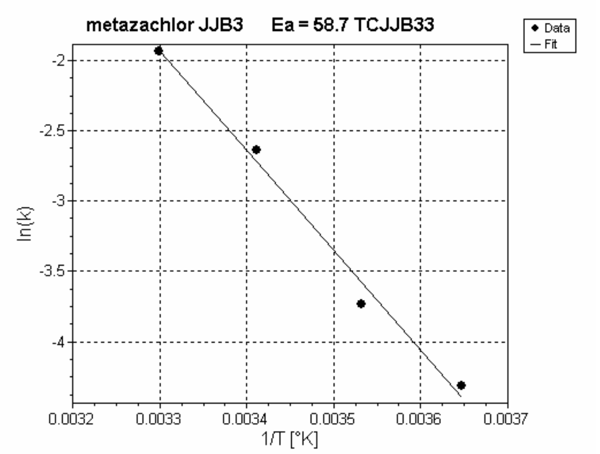
Chloroacetamides

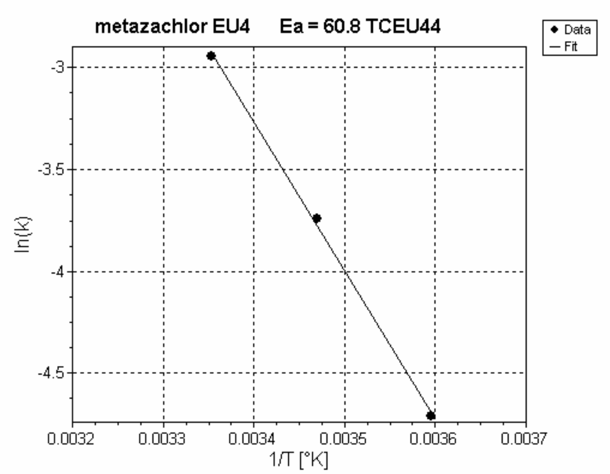


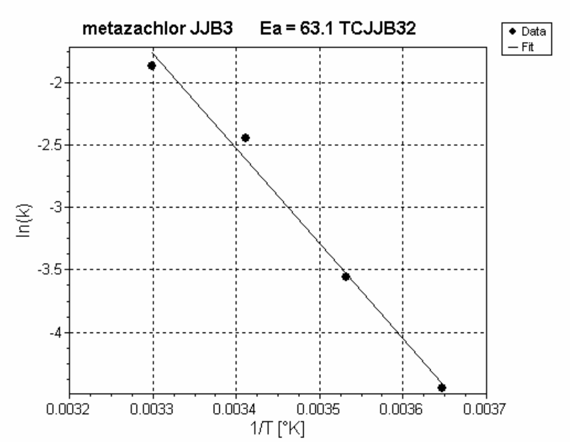
Chloroacetamides (contd.)

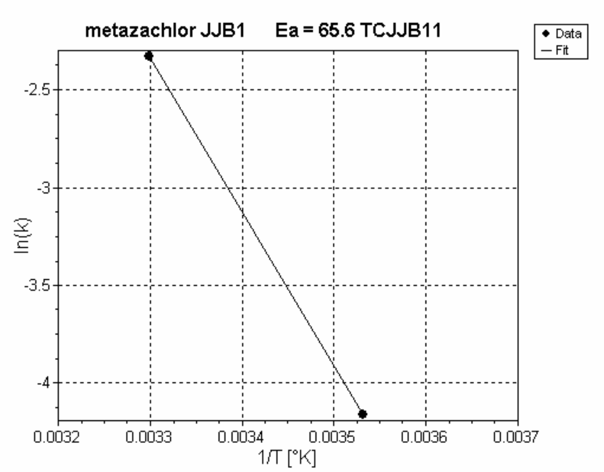




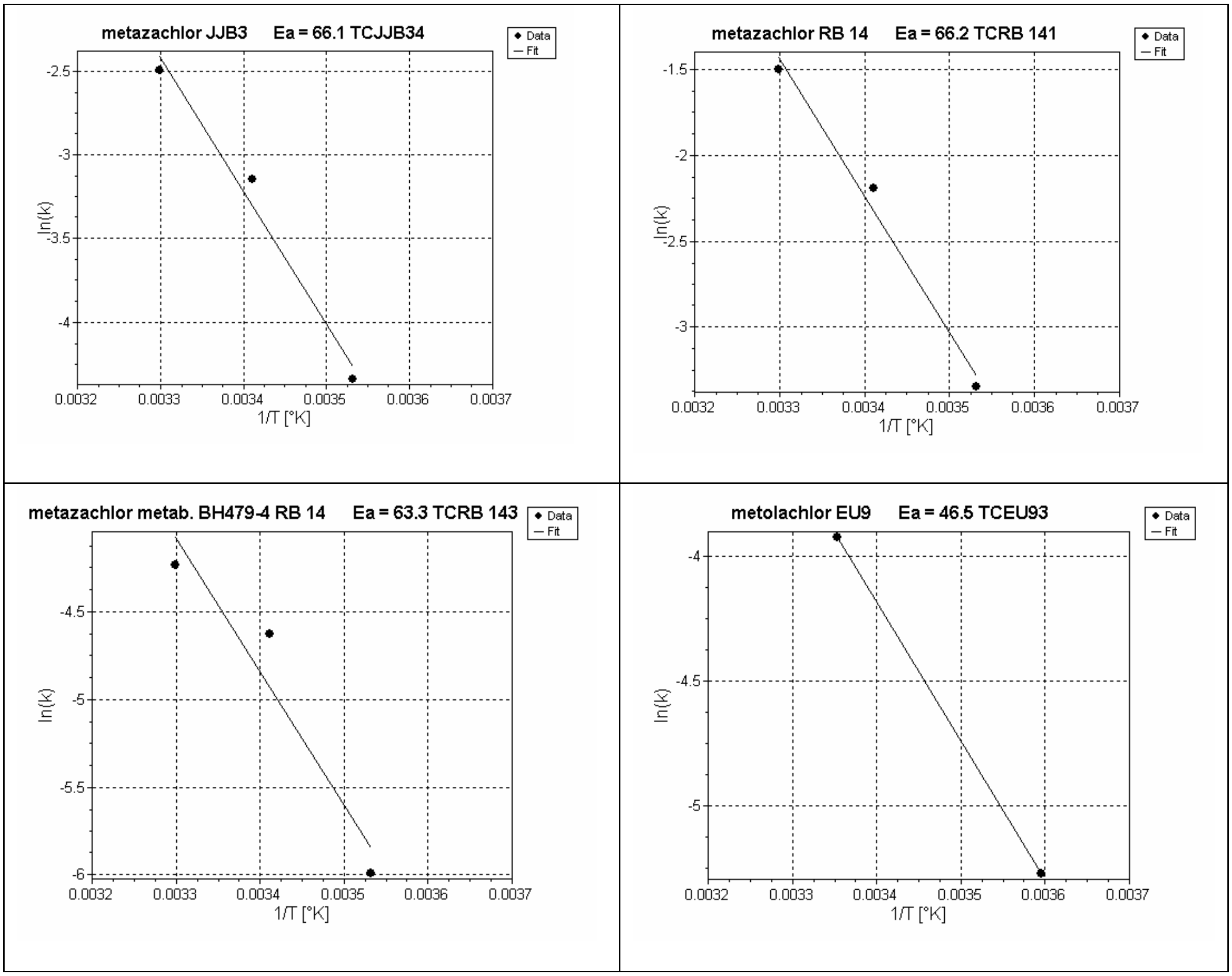




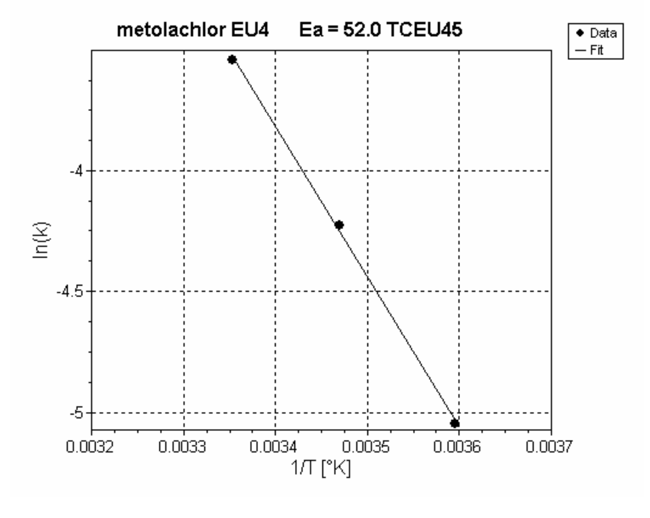


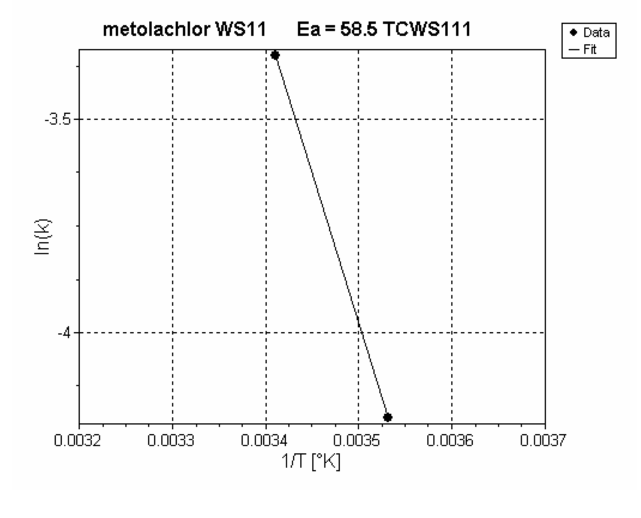


Chloroacetamides (contd.)

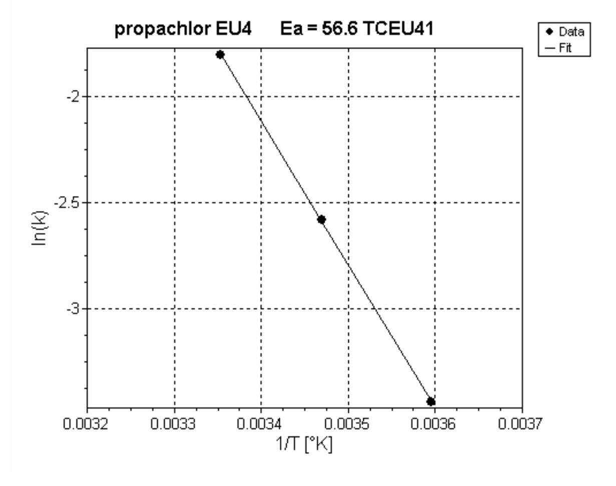


Chloroacetamides (contd.)

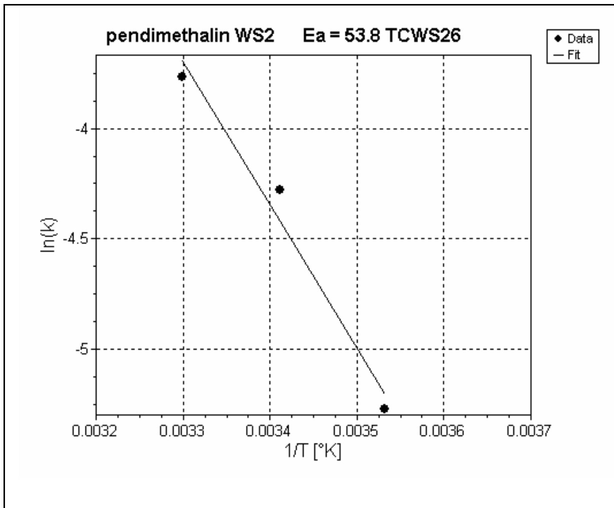


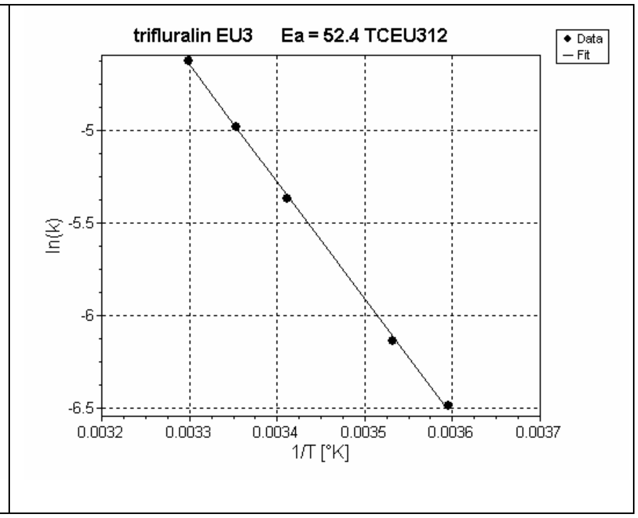


Chloroacetamides (contd.)

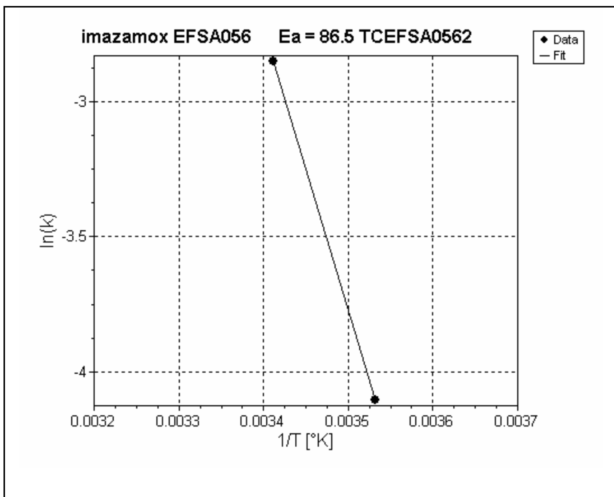


Dinitroanilines

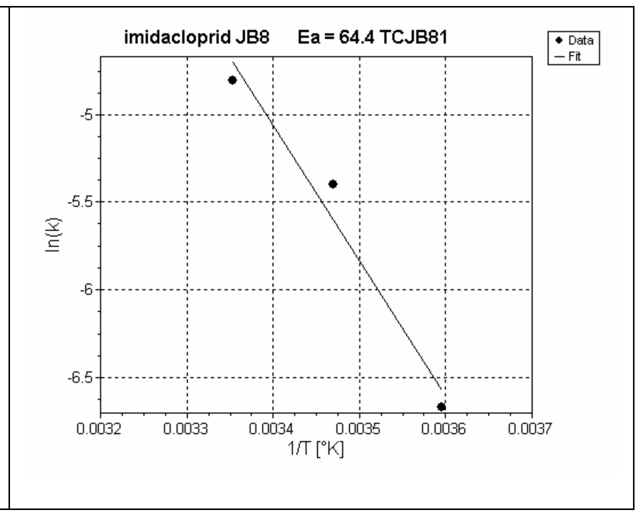




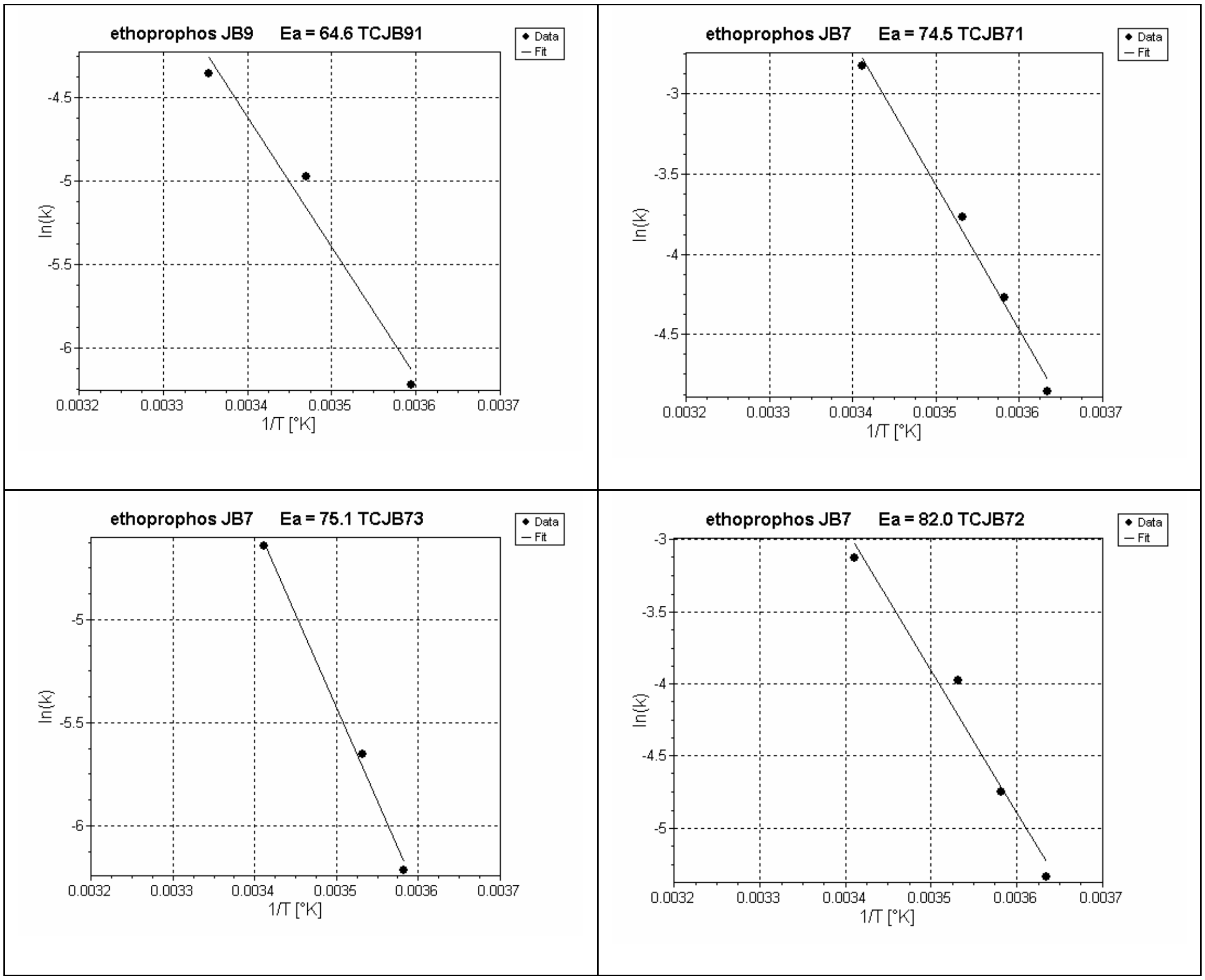
Imidazolinone



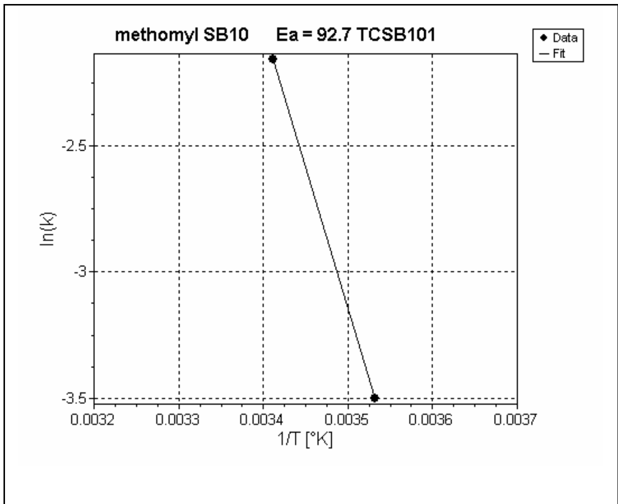
Neonicotinoid

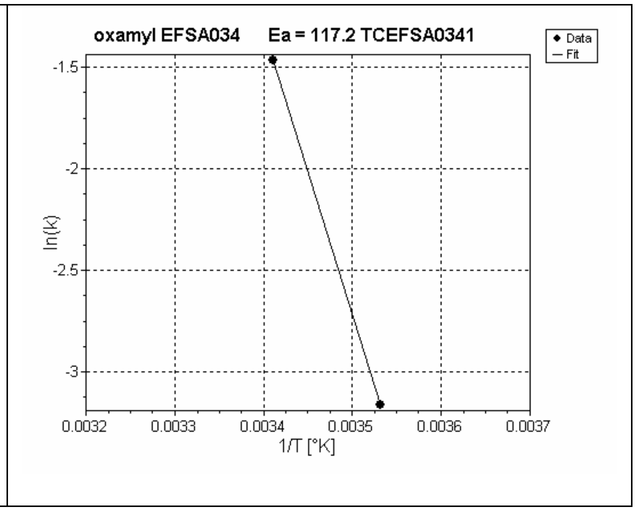


Organophosphates

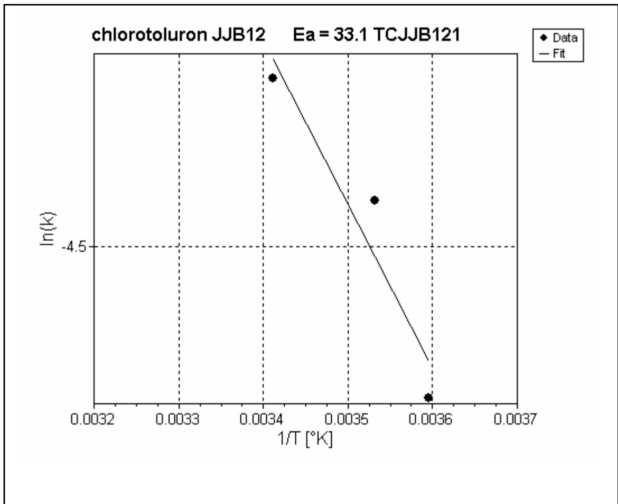


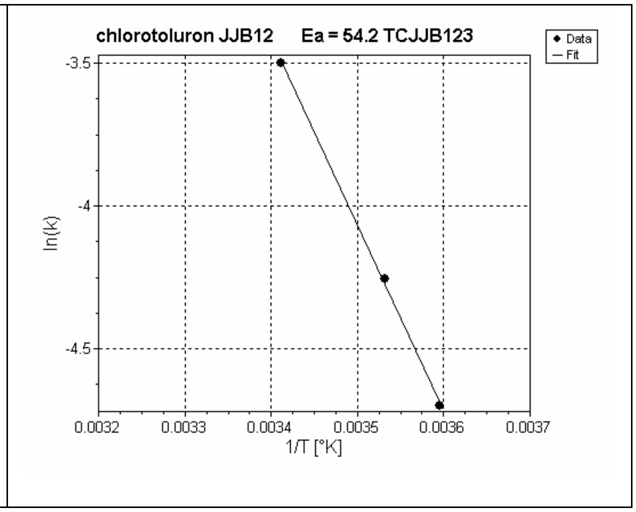
Oxime carbamates



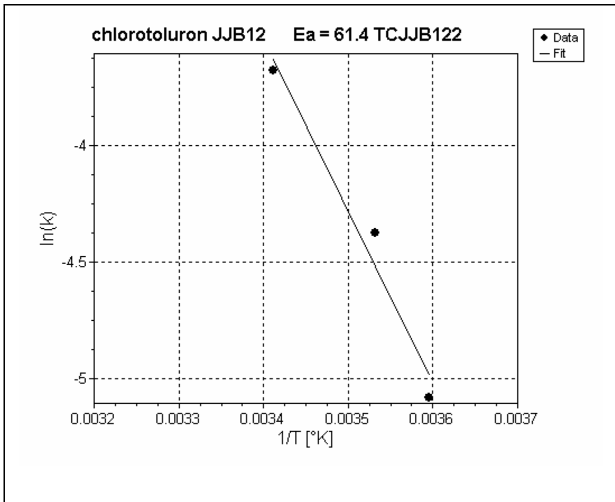


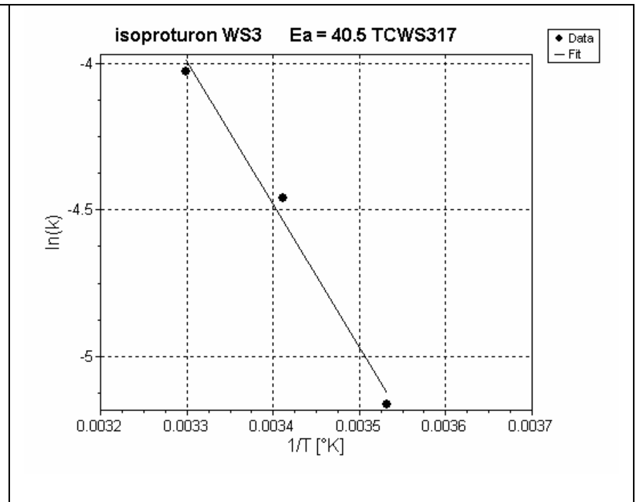
Phenylureas

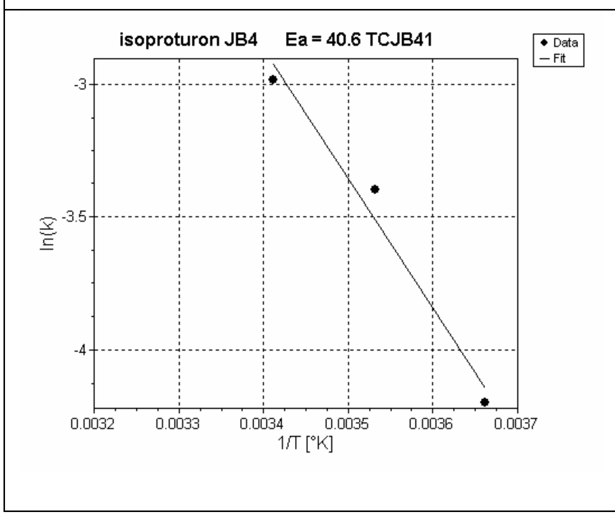


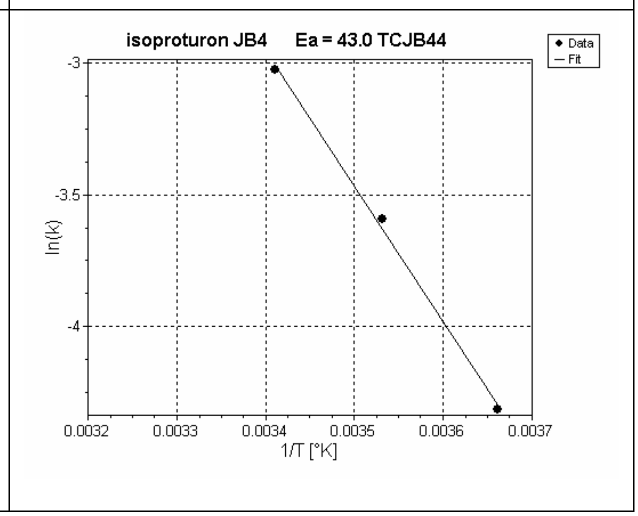


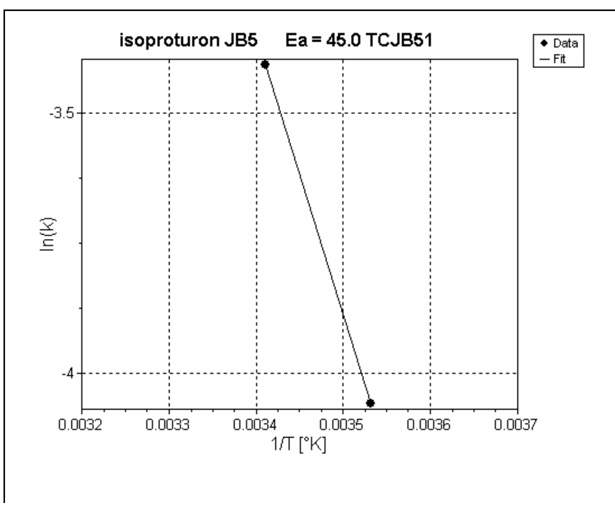
Phenylureas

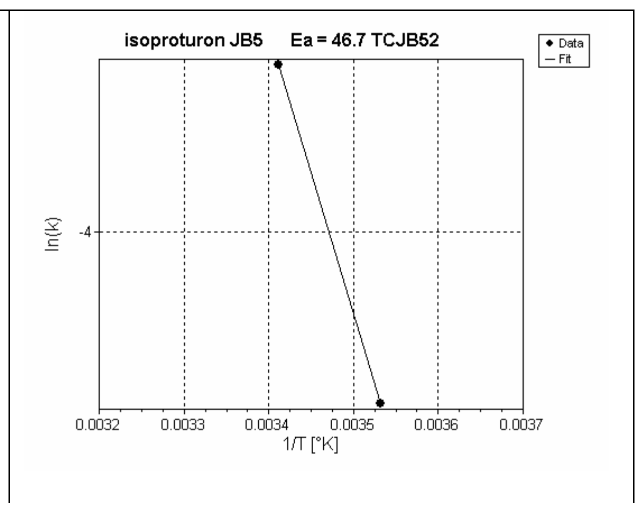




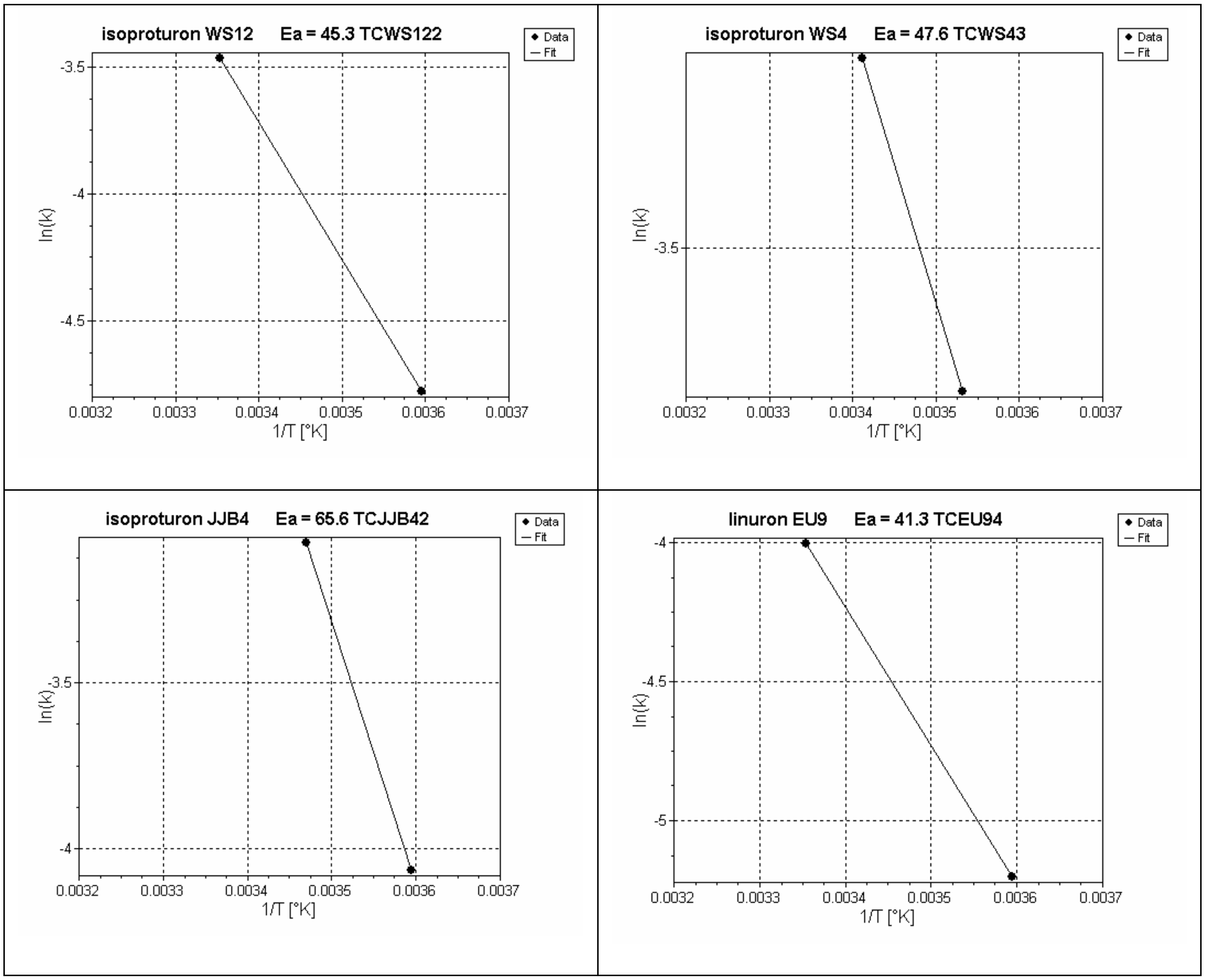




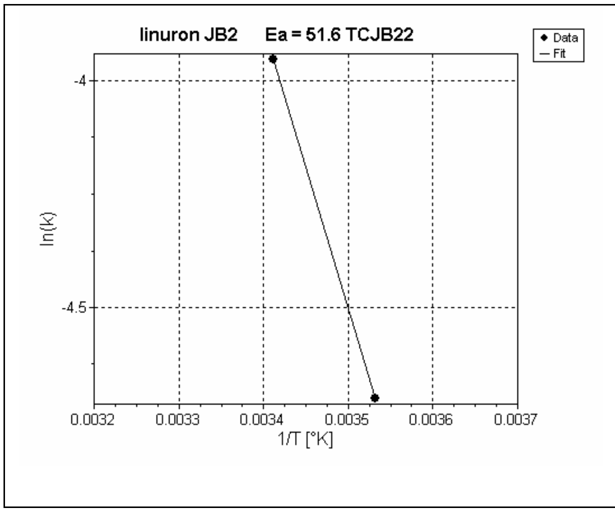




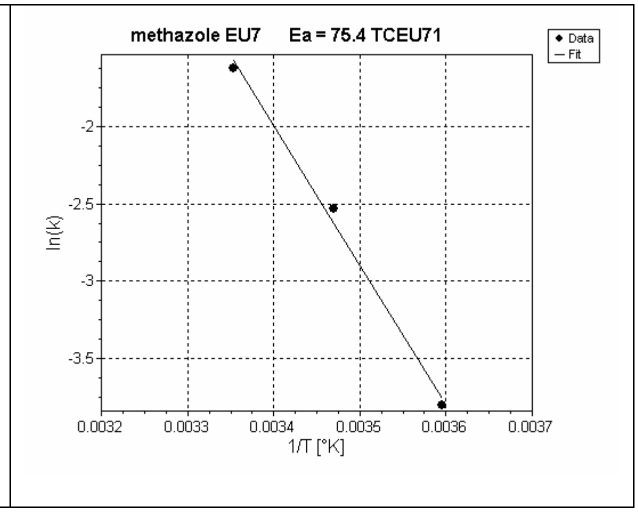
Phenylureas (contd.)



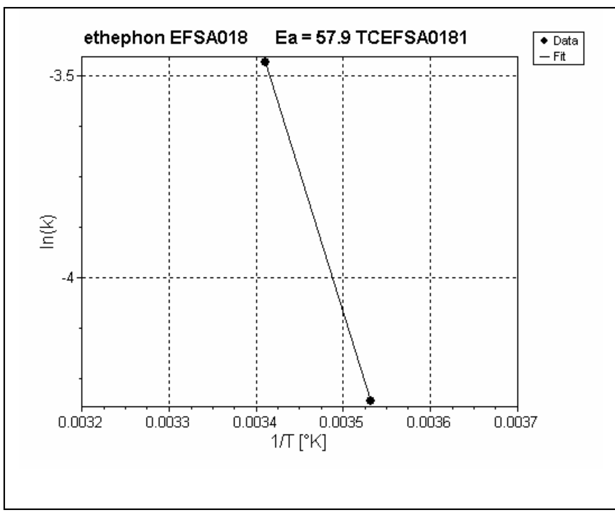
Phenylureas (contd.)



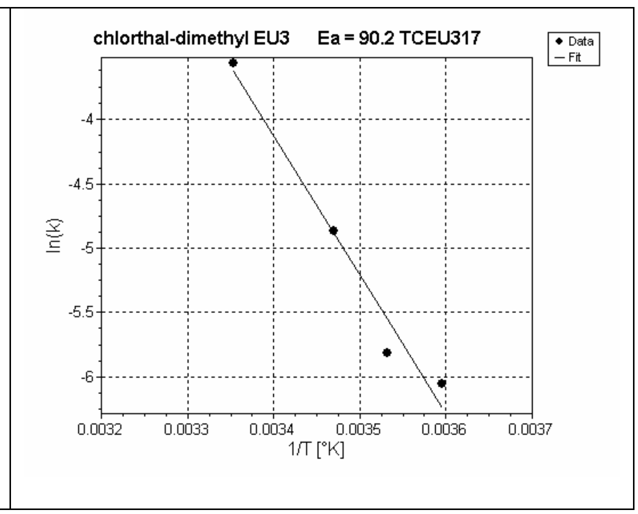
Phenylurea precursor



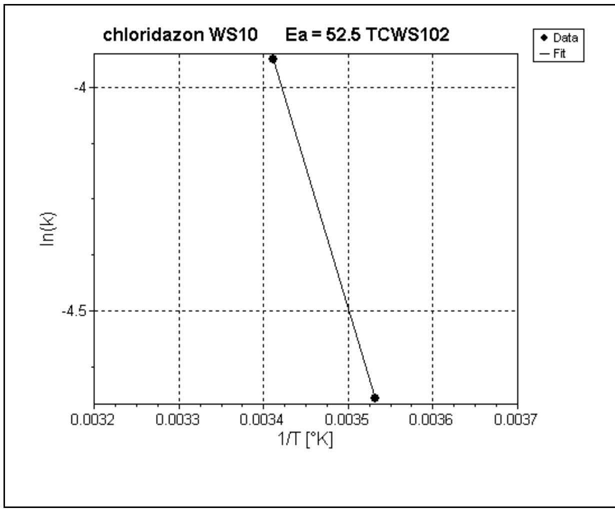
Phosphonic acid



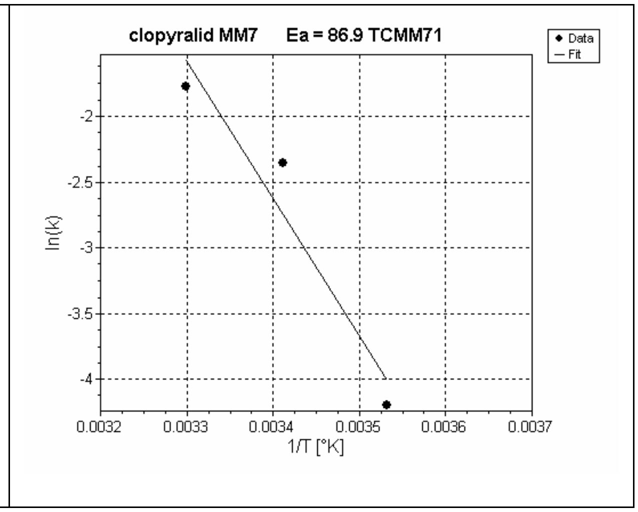
Phthalic acid



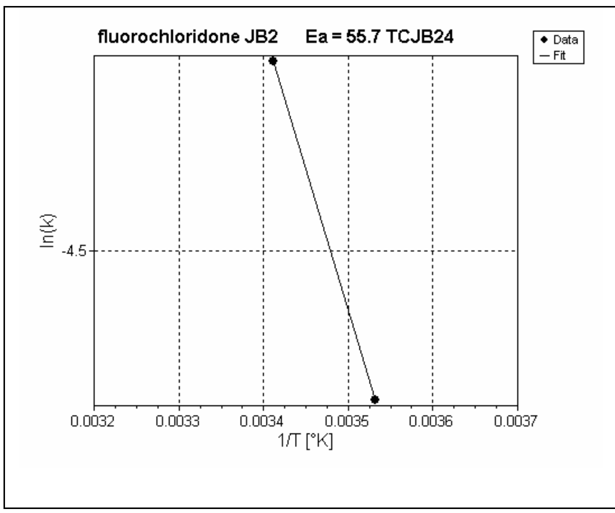
Pyridazinone



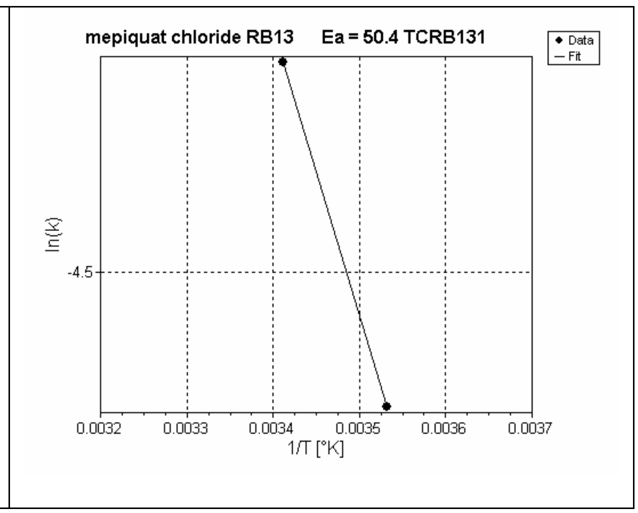
Pyridinecarboxylic acid



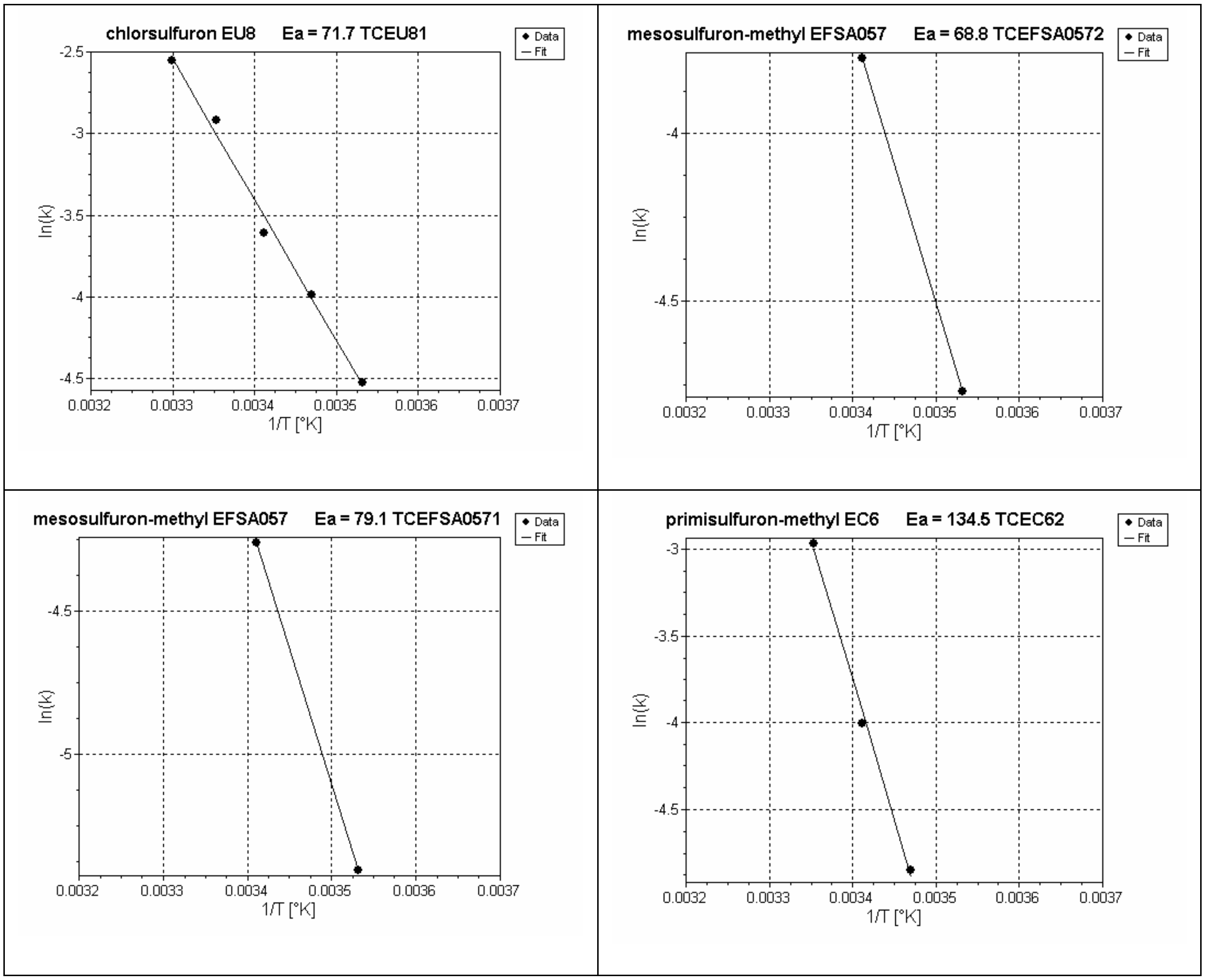
Pyrrolidinone



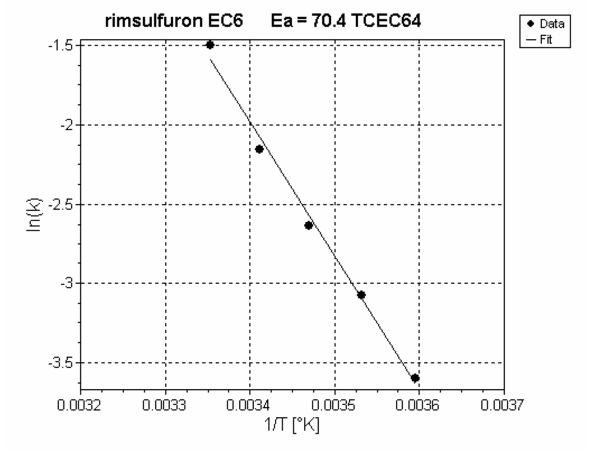
Quaternary ammonium

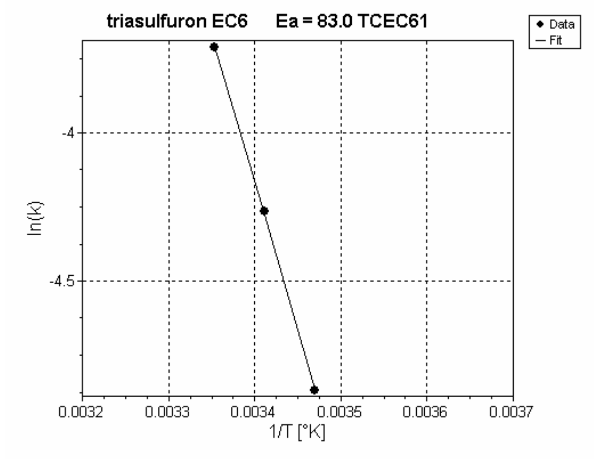


Sulfonylureas

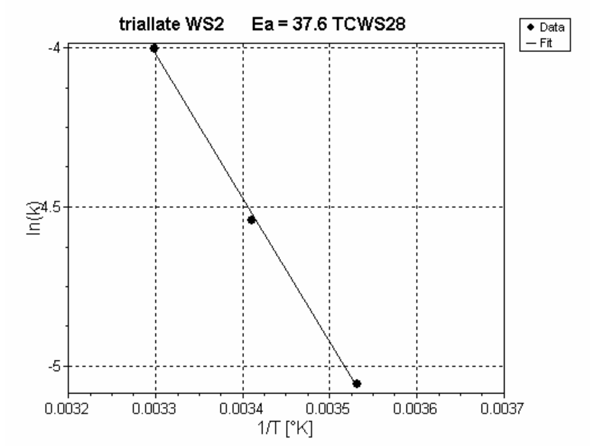


Sulfonylureas (contd.)

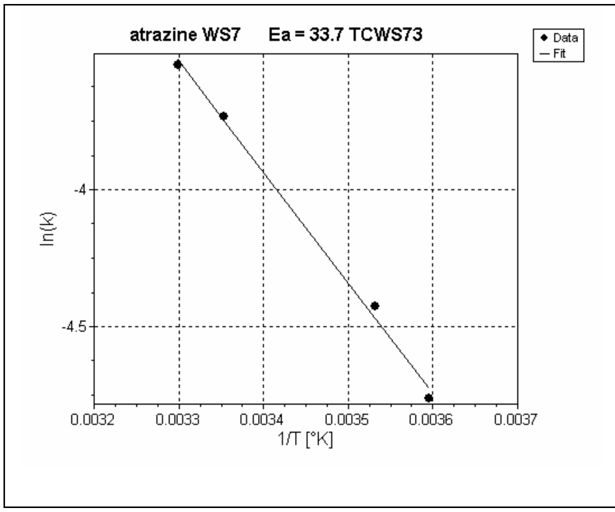


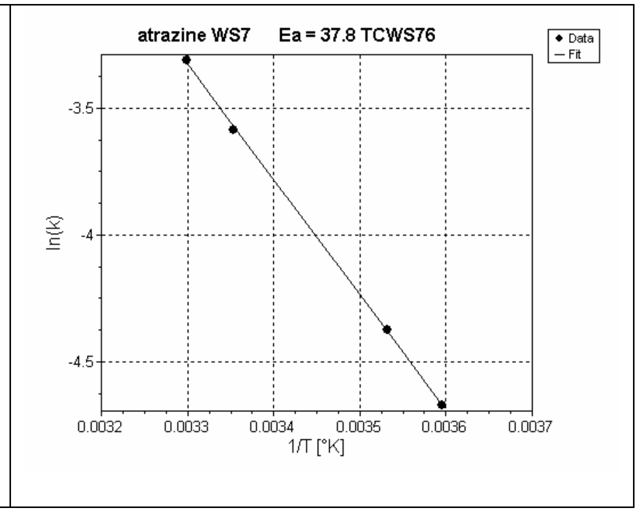


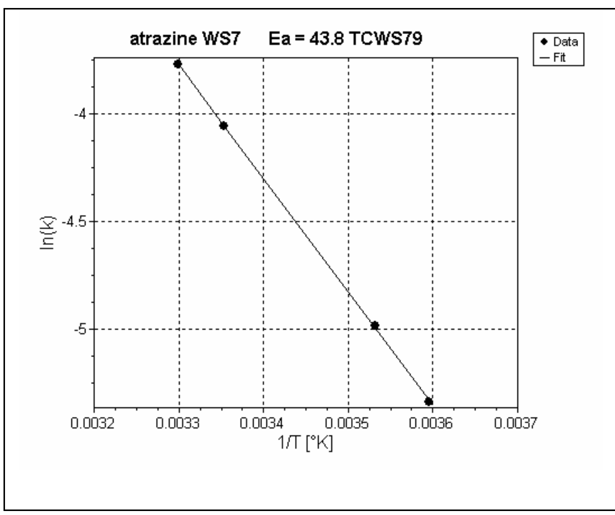
Thiocarbamate

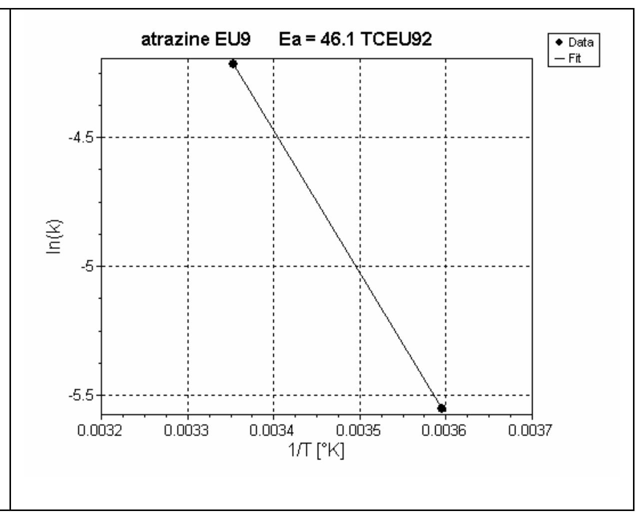


Triazines

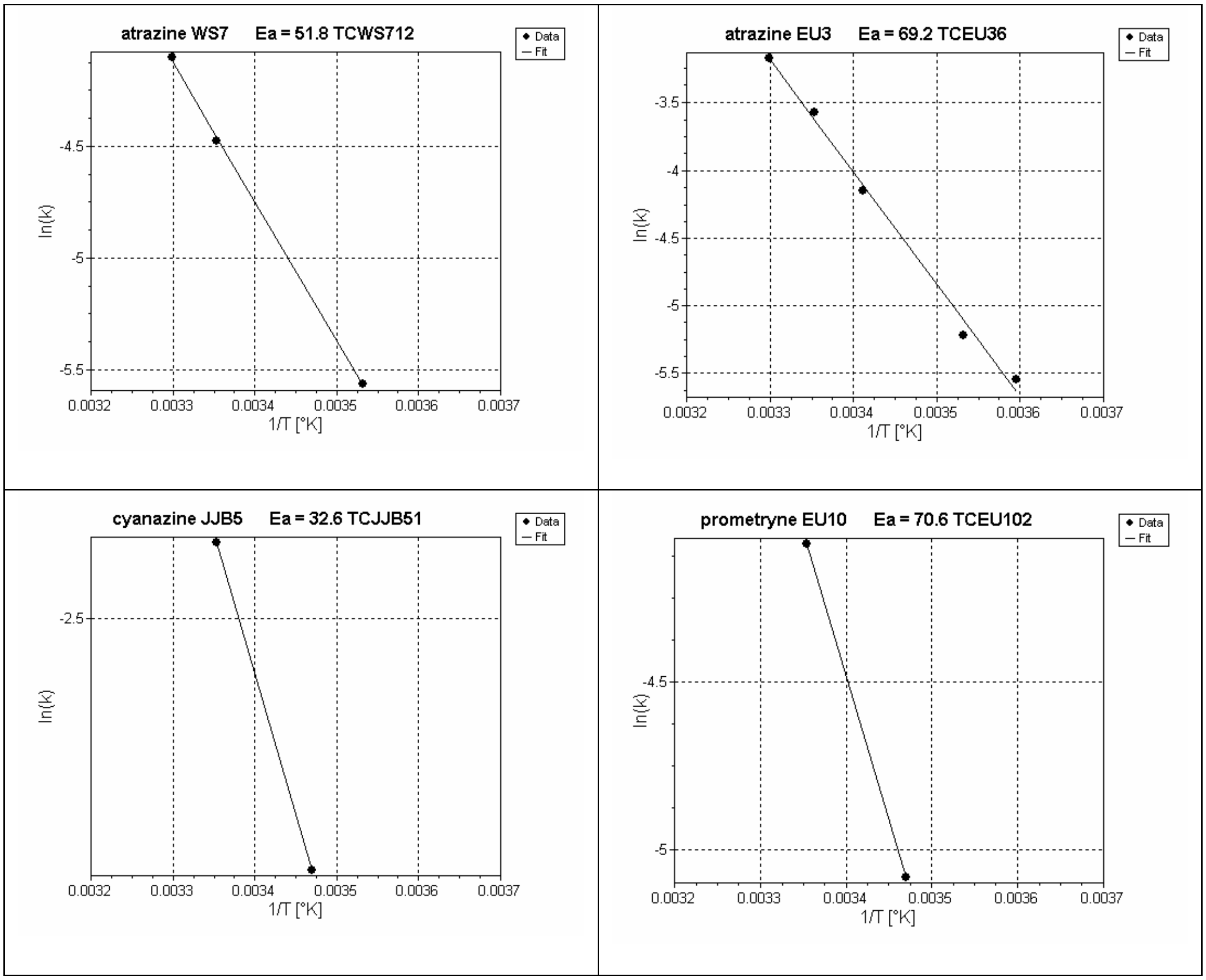

atrazine WS7 Ea = 33.7 TCWS73
Data
Fit
ln(k)
-4
-4.5
0.0032
0.0033
0.0034
0.0035
0.0036
0.0037
1/T [°K]


atrazine WS7 Ea = 37.8 TCWS76
Data
Fit
ln(k)
-3.5
-4
-4.5
0.0032
0.0033
0.0034
0.0035
0.0036
0.0037
1/T [°K]

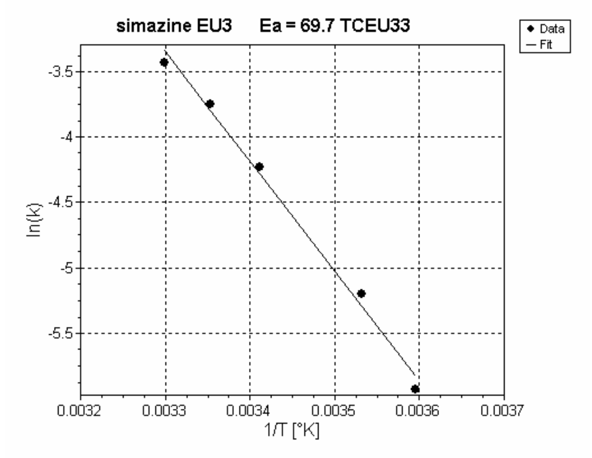

atrazine WS7 Ea = 43.8 TCWS79
Data
Fit
ln(k)
-4
-4.5
-5
0.0032
0.0033
0.0034
0.0035
0.0036
0.0037
1/T [°K]

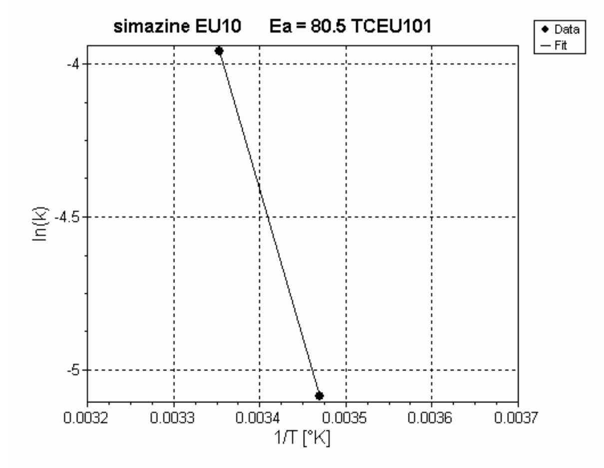

atrazine EU9 Ea = 46.1 TCEU92
Data
Fit
ln(k)
-4.5
-5
-5.5
0.0032
0.0033
0.0034
0.0035
0.0036
0.0037
1/T [°K]

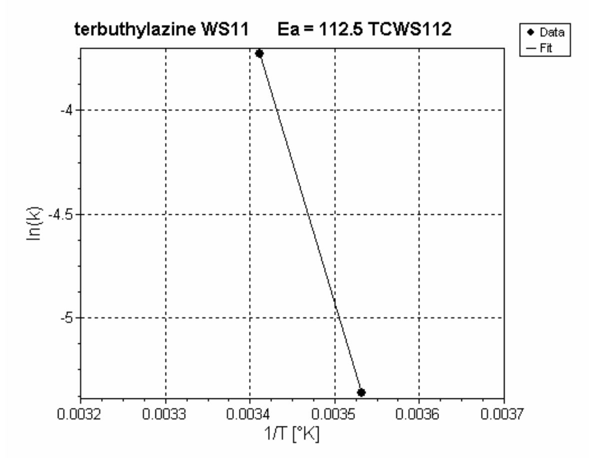
Triazines (contd.)



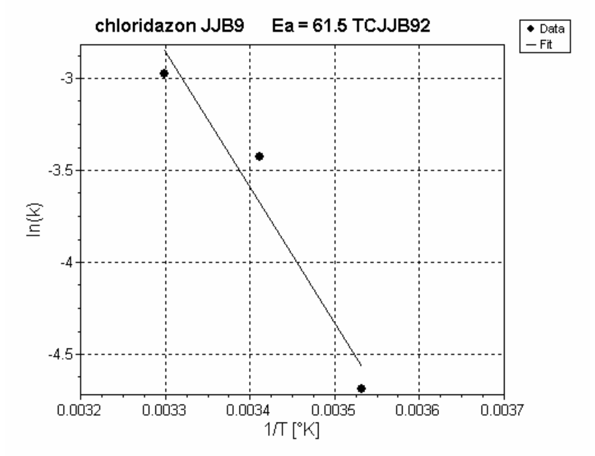
Triazines (contd.)

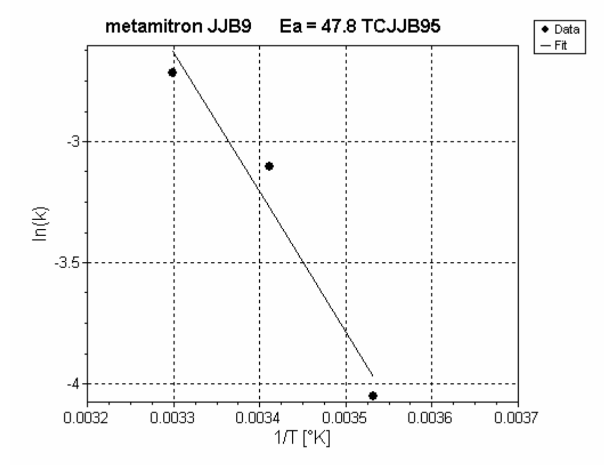


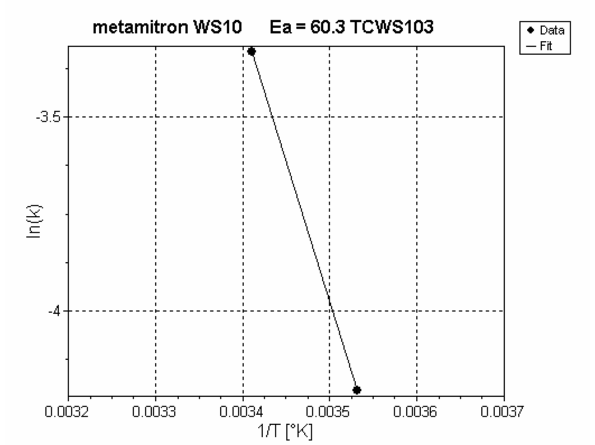


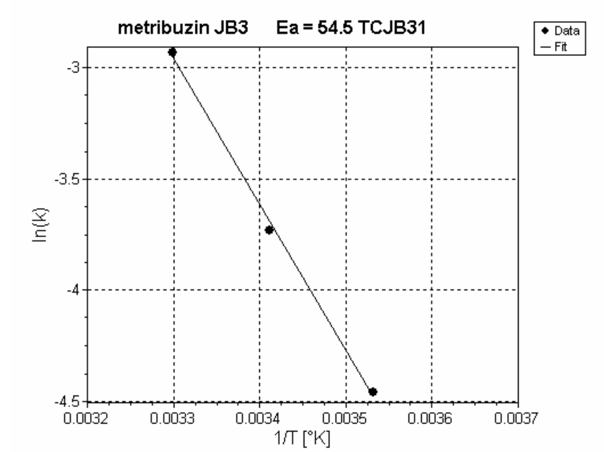


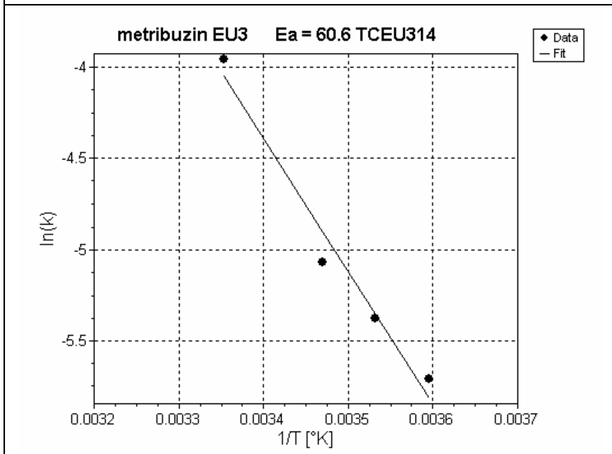
Triazinones



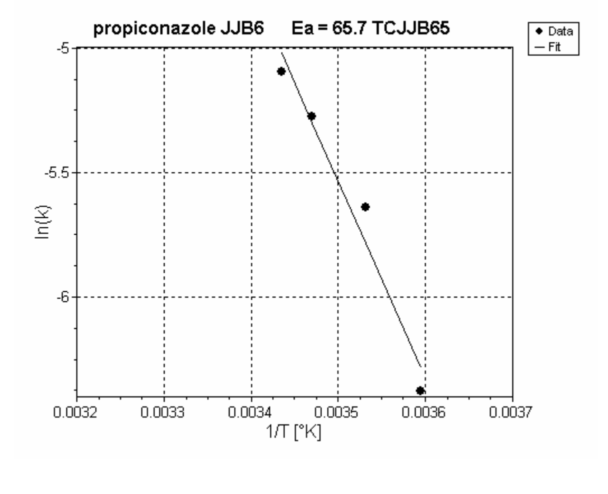


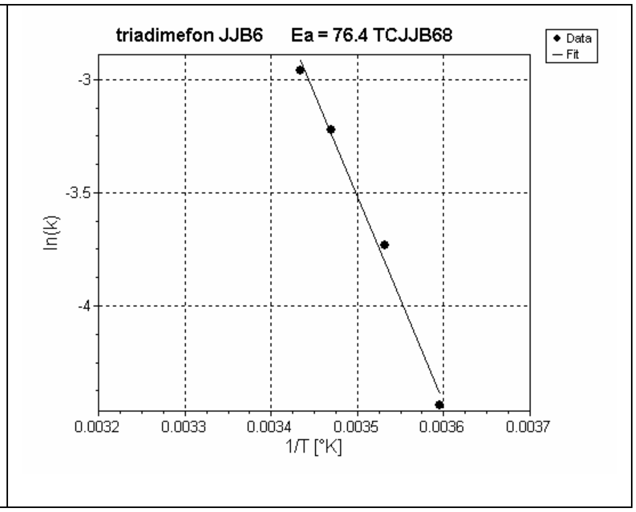


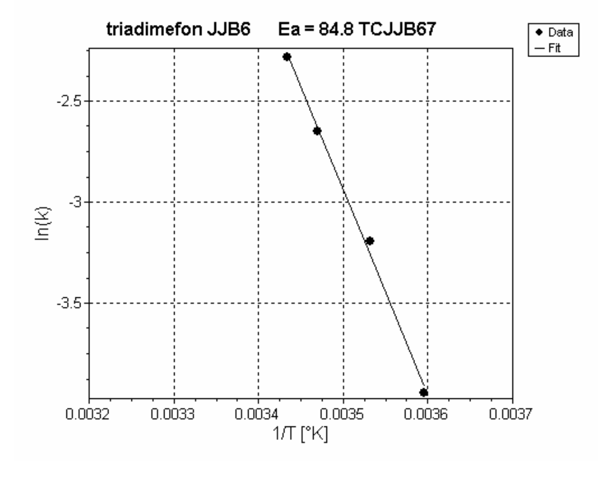




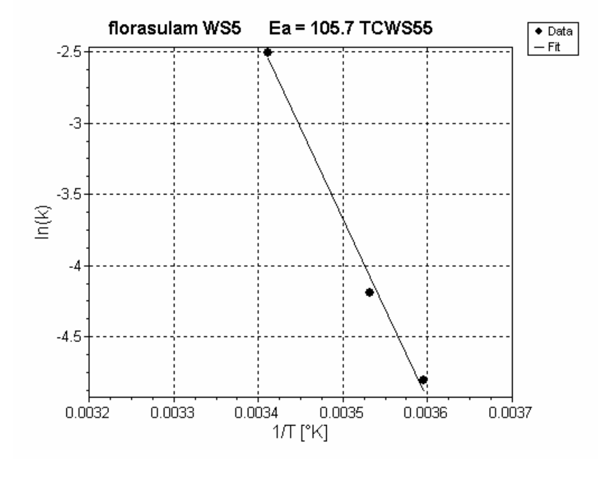
Triazoles


propiconazole JJB6 Ea = 65.7 TCJJB65
Data
Fit
ln(k)
1/T [°K]
-5
-5.5
-6
0.0032
0.0033
0.0034
0.0035
0.0036
0.0037

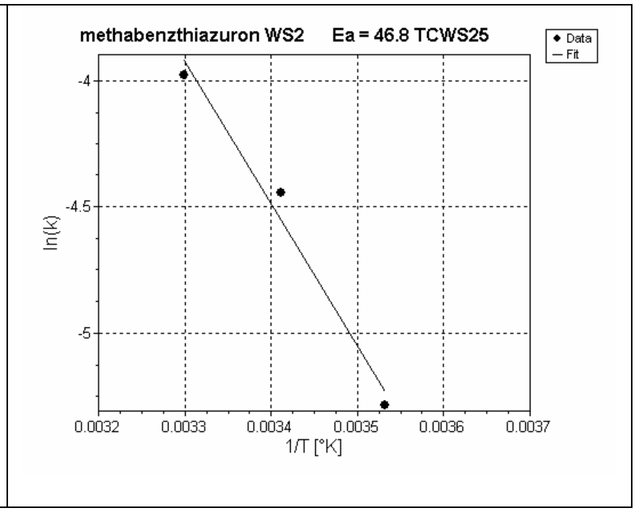

triadimefon JJB6 Ea = 76.4 TCJJB68
Data
Fit
ln(k)
1/T [°K]
-3
-3.5
-4
0.0032
0.0033
0.0034
0.0035
0.0036
0.0037


triadimefon JJB6 Ea = 84.8 TCJJB67
Data
Fit
ln(k)
1/T [°K]
-2.5
-3
-3.5
0.0032
0.0033
0.0034
0.0035
0.0036
0.0037

Triazolopyrimidine



Urea



Appendix 6

Documentation provided to EFSA

1. Letter from ECPA to EFSA, dated 8th December 2006, concerning the Q_{10} value describing the temperature dependence of degradation rates in soil. (ref. LE/06/PD/15818.
2. Comments by ECPA, dated 8th December 2006, on the Opinion by EFSA "Q_{10} value used to describe the temperature effect on transformation rates of pesticide in soil".
3. Wang M. & Winn N., 24th November 2006. Estimation of the Q_{10} value for deriving temperature dependence of degradation rates in soil. RIFON report nr. RA06069.

Appendix 7

Open-literature search by the PPR Unit in external data-bases

1. Background

The intention with the literature search was to collect additional information for determination of a Q_{10} value(s) as requested in the Terms of Reference on the 31st January 2007.

2. Performance of the EFSA search

The literature search was carried out by the EFSA PPR unit in external data-bases available to EFSA in the period from the 8th February till the 1st March 2007.

The search was done in the following databases using the search criteria:

Pesticide AND Soil AND Temperature AND (Degradation OR Transformation)

Title	Website
AGRICOLA (NAL Catalogue)	http://agricola.nal.usda.gov/
AGRIS (International Information System for the Agricultural Sciences and Technology)	http://www.fao.org/agris/search/search.do
CAB Abstracts	http://isi01.isiknowledge.com/ portal.cgi?DestApp=CABI&Func=Frame
FSTA	http://isi01.isiknowledge.com/portal.cgi? DestApp=FSTA&Func=Frame
Web of Science	http://isi01.isiknowledge.com/portal.cgi? DestApp=WOS&Func=Frame

Current contents	http://isi01.isiknowledge.com/portal.cgi? DestApp=CCC&Func=Frame
TOXNET	http://toxnet.nlm.nih.gov/index.html
Pubmed/Medline	http://www.ncbi.nlm.nih.gov/entrez/query.fcgi
OECD guidelines for the testing of chemicals	http://new.sourceoecd.org/rpsv/periodical/p15_about.htm?jnlissn=1607310X
Campden & Chorleywood Food Research Association (CCFRA)	http://www.campden.co.uk

Following each search, the titles and if relevant the abstracts were screened. References appearing to be relevant were ordered through the EFSA library for further evaluation by the Q_{10} Working Group.

References with no relevant content to the Q_{10} question were not ordered, and neither were other references already in the adopted Q_{10} opinion (EFSA, 2006) and provided to EFSA by ECPA (ECPA, 2006).

3. Result of the search

The complete search resulted in ordering of a total of 29 published papers for further evaluation by the working group.

4. Additional published papers provided by working group members

In addition to the EFSA literature search, working group members provided an additional 13 published papers for further evaluation by the working group.