TEXTE
09/2018

Assessment of persistence, mobility and toxicity (PMT) of 167 REACH registered substances

2. Revised Edition

For our Environment

Umwelt Bundesamt

TEXTE 09/2018

Project No. 74925
Report No. (UBA-FB) 002595

Assessment of persistence, mobility and toxicity (PMT) of 167 REACH registered substances

2. Revised Edition

by

Urs Berger
Helmholtz Centre for Environmental Research - UFZ, Department of Analytical Chemistry, Leipzig

Norbert Ost
Helmholtz Centre for Environmental Research - UFZ, Department of Ecological Chemistry, Leipzig

Daniel Sättler, Ivo Schliebner
German Environment Agency (UBA), Section IV 2.3 Chemicals, Dessau-Roßlau

Ralph Kühne
Helmholtz Centre for Environmental Research - UFZ, Department of Ecological Chemistry, Leipzig

Gerrit Schüürmann
Helmholtz Centre for Environmental Research - UFZ, Department of Ecological Chemistry, Leipzig and Technical University Bergakadamie Freiberg, Freiberg

Michael Neumann
German Environment Agency (UBA), Section IV 2.3 Chemicals, Dessau-Roßlau

Thorsten Reemtsma
Helmholtz Centre for Environmental Research - UFZ, Department of Analytical Chemistry, Leipzig

On behalf of the German Environment Agency

Imprint

Publisher:
Umweltbundesamt
Wörlitzer Platz 1
06844 Dessau-Roßlau
Tel: +49 340-2103-0
Fax: +49 340-2103-2285
info@umweltbundesamt.de
Internet: www.umweltbundesamt.de

/umweltbundesamt.de
/umweltbundesamt

Study performed by:
Helmholtz Centre for Environmental Research - UFZ
Permoserstrasse 15
04318 Leipzig

Study completed in:
November 2017 (revised April 2018)

Edited by:
Section IV 2.3 Chemicals
Michael Neumann, Ivo Schliebner

Publication as pdf:
http://www.umweltbundesamt.de/publikationen

ISSN 1862-4804

Dessau-Roßlau, April 2018

Abstract

Chemicals that are persistent in the environment, mobile in the aquatic environment and toxic may be critical for the quality of raw waters. In the present study, a list of 167 REACH registered substances were assessed with respect to their intrinsic substance properties persistence in the aquatic environment (P_{aq}), mobility in the aquatic environment (M) and toxicity (T) using modified criteria earlier defined by Kalberlah et al. (2014). This was done by comprehensive manual research of all relevant information and data in all available data sources including mathematical models. Additionally, the substances were assessed and ranked with respect to their potential for environmental emissions based on the evaluation approach developed by Schulze et al. (2018).

The present study provides a consolidated list of substances assessed according to the above criteria, including 8 substances assessed as P_{aq}MT substances and 21 substances assessed as P_{aq}M substances with suspected T. Further 105 suspected P_{aq}MT substances were identified. Consequently, a total of 134 substances based on suspected P_{aq}MT properties combined with expected environmental emissions are recommended to the German Environment Agency (UBA) for further investigation and scientific and regulatory scrutiny. However, this result may not be suitable to indicate the need for regulatory measures. The study identified considerable data gaps (especially for experimental data) that in many cases hampered the assessment of the criteria, especially for M and T. Manufacturers, importers and downstream users of substances should strive to obtain and report data of better quality in order to carry out a more accurate assessment. Further, the results of this project will support the ongoing discussion to define PMT criteria under REACH.

Kurzbeschreibung

Stoffe, die persistent in der Umwelt, mobil im Wasserkreislauf und toxisch sind, könnten die Qualität der Rohwässer zur Trinkwassergewinnung gefährden. Im Rahmen des vorliegenden Vorhabens wurden 167 REACH-registrierte Stoffe mithilfe von modifizierten Bewertungskriterien von Kalberlah et al. (2014) hinsichtlich ihrer intrinsischen Stoffeigenschaften Persistenz in der aquatischen Umwelt (P_{aq}), Mobilität in der aquatischen Umwelt (M) und Toxizität (T) bewertet. Dies geschah durch eine aufwändige manuelle Recherche von allen relevanten Informationen und Daten in allen verfügbaren Datenbanken. Auch mathematische Modelle wurden zur Stoffbewertung herangezogen. Zusätzlich wurden die Stoffe anhand des Bewertungsschemas von Schulze et al. (2018) hinsichtlich erwarteter Umweltemissionen bewertet.

Im Ergebnis liegt eine konsolidierte Liste mit nach den o.g. Kriterien bewerteten P_{aq}MT-Stoffen (8 Substanzen), bewerteten P_{aq}M-Stoffen mit vermuteter Toxizität (21 Substanzen) und weiteren 105 vermuteten P_{aq}MT-Stoffen vor. Folglich werden insgesamt 134 Stoffe aufgrund vermuteter PMT-Eigenschaften in Kombination mit erwarteten Emissionen in die Umwelt dem Umweltbundesamt für weitere Untersuchungen und zur wissenschaftlichen und regulatorischen Überprüfung empfohlen. Jedoch ist dieses Ergebnis möglicherweise nicht geeignet, um auf die Notwendigkeit von Regulierungsmaßnahmen hinzuweisen. Das Vorhaben hat erhebliche Datenlücken (besonders von experimentellen Daten) aufgedeckt, die die Bewertung anhand der Kriterien, besonders für M und T, beeinträchtigten. Hersteller, Importeure und Anwender von Chemikalien sollten Daten von besserer Qualität zur Verfügung stellen, damit eine vollständigere Bewertung vorgenommen werden kann. Die Ergebnisse dieses Projekts unterstützen auch die laufende Diskussion zur Definition von PMT-Kriterien unter REACH.

Table of Contents

List of Figures

List of Tables

List of Abbreviations

CMR	Carcinogenic, mutagenic, toxic for reproduction
DNEL	Derived no effect level
DOC	Dissolved organic carbon
EC_{50}	Concentration of a chemical that shows effects for 50% of the test animals
ECHA	European Chemicals Agency
ErC_{50}	EC_{50} with respect to reduction of growth rate
H362	GHS (Globally Harmonized System of Classification) hazard statement: May cause harm to breast-fed children
LC_{50}	Concentration of a chemical that results in a mortality of 50% of the test animals
log K_{oc}	Soil sorption coefficient
LSER	Linear solvation energy relationship
M	Mobility or mobile in the aquatic environment
OECD	Organization for economic co-operation and development
P	Persistence or persistent in the environment
P_{aq}	Persistence or persistent in the aquatic environment
PBT	Persistent in the environment, bioaccumulative in biota and toxic
PM	Persistent in the environment and mobile in the aquatic environment
P_{aq}M	Persistent in the aquatic environment and mobile in the aquatic environment
PMT	Persistent in the environment, mobile in the aquatic environment and toxic
P_{aq}MT	Persistent in the aquatic environment, mobile in the aquatic environment and toxic
QSAR	Quantitative structure activity relationship
REACH	Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC
STOT RE	Specific target organ toxicity - repeat exposure
SW	Water solubility
T	Toxicity or toxic

1 Introduction and background

Polar organic chemicals exhibit a low tendency to sorb to surfaces or to organic matter in soils and sediment. These substances are therefore mobile in the aquatic environment. Mobile substances that are also persistent in the environment will most likely pass through wastewater treatment plants, be discharged into surface water and then penetrate into groundwater or bank filtrates. Eventually, these substances may reach the water resources for drinking water production (Reemtsma et al., 2016; Neumann, 2017). Substances that are persistent in the environment and mobile in the aquatic environment are abbreviated as PM substances. Most critical are PM substances that additionally exhibit toxic effects. These substances are referred to as PMT substances (Neumann, 2017).

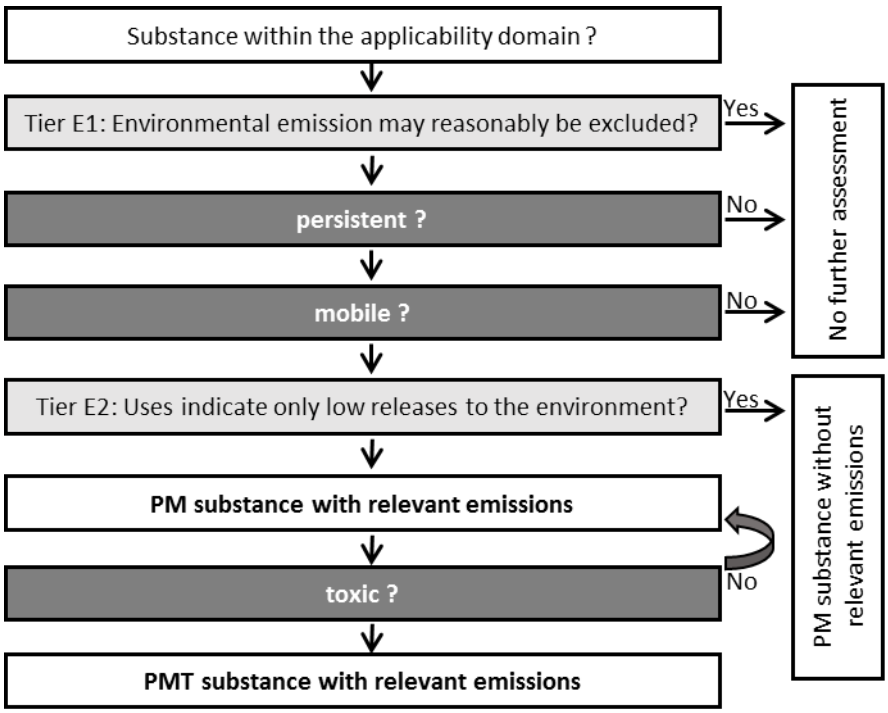
PM and or PMT substances are in the scope of current research. E.g., within the European research project PROMOTE (PROtecting water resources from MObile Trace chEmicals; www.promote-water.eu), REACH registered substances were prioritized with regard to their persistence in the aquatic environment, mobility in the aquatic environment (Arp et al., 2017) and expected environmental emissions (Schulze et al., 2018). This was done using mathematical models with primarily publicly available chemical property data as input. The result is a prioritization of REACH registered substances based on their modelled potential to occur in raw water used for the preparation of drinking water (Schulze et al., 2018). However, the mathematical modelling especially of highly polar (often ionic) substances is associated with considerable uncertainties (Arp et al., 2017). Additionally, PROMOTE did not consider toxicological or ecotoxicological effects of the substances.

Furthermore, in a recent project the German Environment Agency (UBA) developed a proposal for criteria and an assessment approach to identify PM and PMT substances among the substances registered under the EU chemical regulation REACH (Kalberlah et al., 2014). The criteria are defined by the REACH specific thresholds for half-life in the different environmental compartments (for P), physical-chemical property thresholds (for M) and various toxicity thresholds (for T), in the majority based on the specific criteria of Annex XIII of the REACH legislation. The proposed assessment concept builds on a stepwise assessment of environmental emissions during production and use of the substances and their intrinsic substance properties P, M and T (Figure 1). Kalberlah et al. (2014) proposed this stepwise procedure in order to reduce the assessment workload. The assessment approach accounts for the emission potential (step E1 and E2) of a substance and verifies if the proposed criteria for the intrinsic substance properties (P, M and T) are fulfilled. More recently, an updated proposal for PM and PMT criteria and an assessment approach focused on the intrinsic substance properties (P, M and T) was discussed within the competent authorities under REACH (Neumann and Schliebner, 2017).

2 Aim of the project

The aim of this project was to assess the intrinsic substance properties persistency in the aquatic environment (P_{aq}), mobility in the aquatic environment (M) and toxicity (T) of 167 substances registered under REACH using modified criteria proposed by Kalberlah et al. (2014). This was done to test the developed assessment approach and to check for the availability and consistency of data required for such an assessment. For this purpose, all relevant and available information and data (including validated mathematical Quantitative Structure Activity Relationship (QSAR) models) on the 167 substances have been manually searched, consolidated and used in a weight-of-evidence approach using expert judgement. Additionally, the potential for environmental emissions (E-score ranking) of the target substances should be assessed based on the approach developed within PROMOTE (Schulze et al., 2018).

Figure 1: Assessment concept developed by Kalberlah and co-workers (Kalberlah et al., 2014).



Source: own illustration

3 Methods

3.1 Selection of substances

The substances assessed in this project were selected from the research project PROMOTE (Arp et al., 2017; Schulze et al., 2018) and from a research project of the Germany Environment Agency (Kalberlah et al., 2014). All substances are registered under REACH. A total of 156 substances from the shortlist of PROMOTE for which the likelihood to occur in raw water was estimated to be high (modelled as persistent, mobile and with a high potential to be emitted into the environment) made up the main body of substances to be assessed. The remaining 11 substances were already considered as PM or PMT substances by Kalberlah et al. (2014). This resulted in a list of in total 167 substances to be assessed within this project.

3.2 Assessment criteria

The following criteria for the identification of persistent (in the aquatic environment), mobile (in the aquatic environment) and toxic substances were used in the assessment of the substances.

3.2.1 Persistence in the aquatic environment

A substance fulfils the 'persistence in the aquatic environment' criterion (P_{aq}) in any of the following situations:

a) the degradation half-life in marine water at pH 6–8 and 9°C is higher than 60 days;
b) the degradation half-life in fresh or estuarine water at pH 6–8 and 12°C is higher than 40 days.

These criteria for P_{aq} are identical with the water-based persistence criteria in Annex XIII of REACH (European Parliament, 2006) and the specification in the ECHA Guidance Document R.11 (European

Chemicals Agency, 2017). In case of lack of data on degradation in water (criteria a. and b.), the following criteria were within this project considered as indication for persistence in the aquatic environment:

c) the degradation half-life in marine sediment at pH 6–8 and 9°C is higher than 180 days;
d) the degradation half-life in fresh or estuarine water sediment at pH 6–8 and 12°C is higher than 120 days;
e) the degradation half-life in soil at pH 6–8 and 12°C is higher than 120 days.

3.2.2 Mobility in the aquatic environment

A substance fulfils the 'mobility in the aquatic environment' criterion (M) in the following situation:

The water solubility (SW) at pH 6–8 and 12 °C is ≥150 µg/L and the log K_{oc} at pH 6–8 and 12 °C is ≤4.5.

This criterion is identical with the proposed mobility criterion (M) in Kalberlah et al. (2014).

3.2.3 Toxicity

A substance fulfils the toxicity criterion (T) in any of the following situations:

a) the long-term no-observed effect concentration (NOEC) or EC10 for marine or freshwater organisms is less than 0.01 mg/L;
b) the substance meets the criteria for classification as carcinogenic (category 1A, 1B or 2), germ cell mutagenic (category 1A, 1B or 2), or toxic for reproduction (category 1A, 1B or 2) according to Regulation EC No 1272/2008 (European Parliament, 2008);
c) there is other evidence of chronic toxicity, as identified by the substance meeting the criteria for specific target organ toxicity after repeated exposure (STOT RE category 1 or 2) according to Regulation EC No1272/2008;
d) the substance meets the criteria for classification as "additional category for effects on or via lactation" (H362), according to Regulation EC No1272/2008;
e) the derived no-adverse effect level (DNEL) is ≤9 µg/kg/d (oral, long term, general population).

The criteria a. and c. are identical with the criteria in Annex XIII of REACH. The criterion b. was basically also copied from Annex XIII of REACH. However, in our assessment substances which are classified as carcinogenic category 2 and germ cell mutagenic category 2 also fulfil the T criterion as proposed by Kalberlah et al. (2014). The criteria d. and e. were taken from Kalberlah et al. (2014).

3.3 Assessment approach and data sources

The assessment approach of the present project is shown in Figure 2. All intrinsic substance properties (P_{aq}, M, and T) were assessed for all 167 substances (Figure 2). This is in contrast to the stepwise assessment approach by Kalberlah et al. (2014), in which the assessment for a substance is stopped as soon as a criterion is not fulfilled (compare Figure 1 and Figure 2). Note that the criteria for P_{aq}, M and T in the present project differ in some respects from earlier criteria for P, M and T (Kalberlah et al., 2014; Neumann and Schliebner, 2017). Therewith, also the criteria for PM or PMT substances differ. In the present project, P_{aq}M substances or P_{aq}MT substances refer to substances that fulfil the criteria for P_{aq} and M or P_{aq}, M and T, respectively, according to the criteria given in section 3.2. In the present project, also the potential for environmental emissions was assessed for all 167 substances. The emission potential was used to prioritize identified P_{aq}M and P_{aq}MT substances.

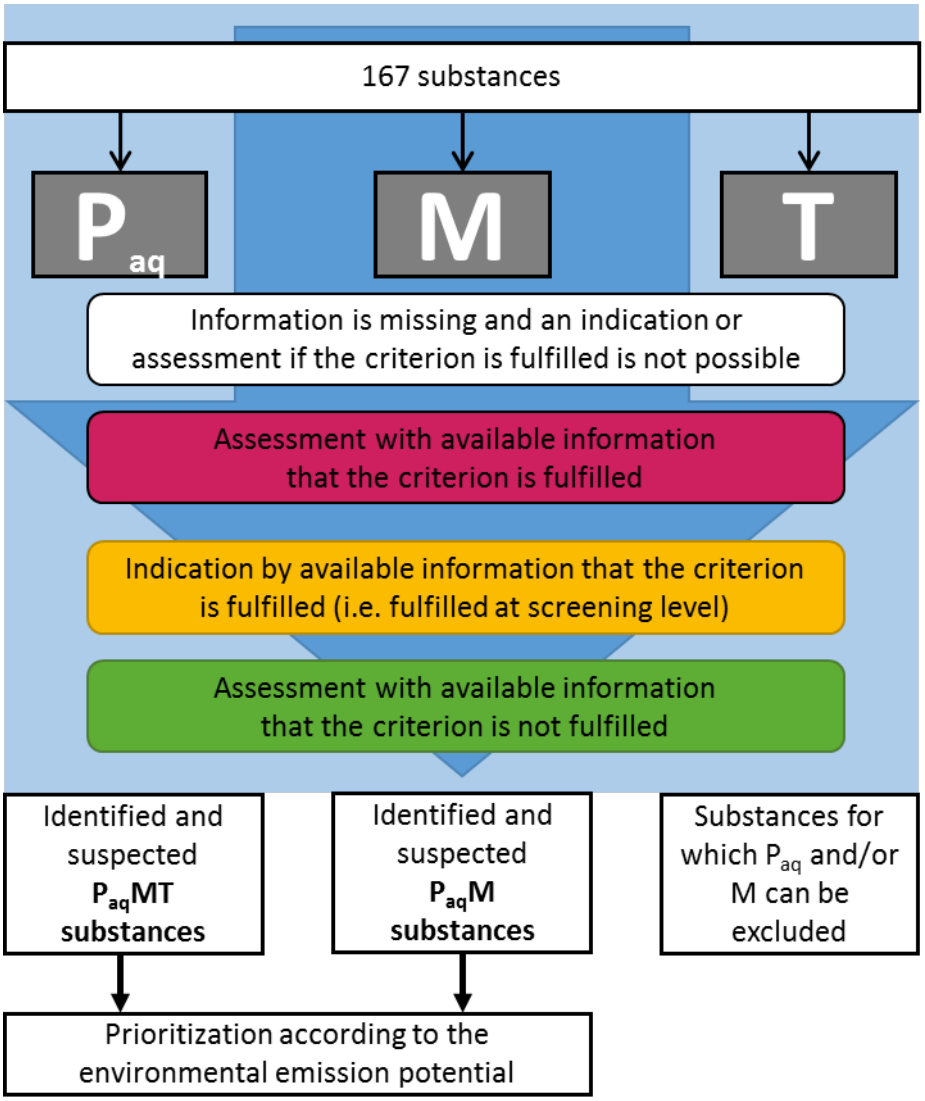
The following data sources were used in the present study:

- The public ECHA website with information from the registration dossiers
- The registration dossier-specific Chemical Safety Reports (CSR), accessed at the premises of the German Environment Agency

- Scientific literature
- QSARs (see sections 3.4 – 3.6 below). For all QSARs the chemical application domain was considered according to Kühne et al. (2009)

All available and relevant data and information were manually retrieved and the quality of the information was assessed. Depending on the quality, the information was used in the screening and assessment of the intrinsic substance properties P_{aq}, M and T, according to the criteria defined in section 3.2 using a weight-of-evidence approach. For illustration purposes, a traffic light colour scheme was used as shown in Figure 2 and detailed in subsequent sections 3.4 - 3.6.

Figure 2: Assessment approach of the present project applied to 167 preselected substances. All intrinsic substance properties (Paq, M, and T) were assessed for all 167 substances using the traffic light colour scheme (white, red, yellow and green) as defined in the figure. The relative ranking of the emission potential based on Schulze et al. (2018) was used to prioritize PaqM and PaqMT substances.



Source: own illustration

3.4 Indication and assessment of P_{aq} properties

The focus of the assessment within this project was on persistence in the aquatic environment (here denoted as P_{aq} in order to avoid confusion with the definition of persistence (P) within the PBT assessment). Nevertheless, if there was not enough data for persistence in the aquatic environment leading to a final decision with respect to criteria a. or b. (section 3.2.1), also tests and information on persistence in sediments and soil were considered (criteria c., d. and e. in section 3.2.1) in order to get to an indication of P_{aq}. This is in contrast to Annex XIII of REACH, where all criteria a.-e. are equally prioritized and a substance would be assessed as persistent if any of these criteria was fulfilled. This difference has no impact on substances assessed as P_{aq} ("red") in the present study, as these would also be assessed as persistent (P) according to Annex XIII of REACH. However, substances assessed as non-persistent (P_{aq} "green") or with indication for persistence (P_{aq} "yellow") based on criteria a. or b. (section 3.2.1) could still be assessed as persistent (P) according to the sediment- or soil-based criteria in Annex XIII of REACH.

The following test results, data and information were assembled for all substances if available:

- Screening tests on ready biodegradation OECD 301 A-F (OECD 301, 1992) and OECD 310 (OECD 310, 2006); Screening tests on inherent biodegradation OECD 302 B (OECD 302B, 1992) and C (OECD 302C, 2009)
- Simulation tests on biodegradation in different environmental media (OECD 307, 2002; OECD 308, 2002; OECD 309, 2004)
- Enhanced ready tests
- Non-OECD guidance tests
- PBT assessment, provided by the registrants as part of the registration dossiers; evaluated by the contractor in accordance with the corresponding ECHA guideline R.11 (European Chemicals Agency, 2017)
- Hydrolysis test OECD 111 (OECD 111, 2004)
- QSARs for persistence assessment EPIWIN 2, 3 and 6

In screening tests on biodegradation a substance with a degradation yield <20% was considered as persistent (no significant degradation).

The following rules were applied in the assessment approach with regard to the traffic light colour scheme:

Persistent in the aquatic environment (P_{aq} "red")

- Simulation tests, enhanced ready tests (longer than 40 d) and/or OECD 302 tests lead to the conclusion that the P_{aq} criterion is fulfilled (see 3.2.1) OR
- OECD 301 tests are available and do not show significant degradation and the substance is assessed as persistent in water in the PBT assessment OR
- the PBT assessment is the only available information and the substance is assessed as persistent in water.

Not persistent in the aquatic environment (P_{aq} "green")

- Simulation tests, enhanced ready tests (longer than 40 d) and/or OECD 302 tests lead to the conclusion that the P_{aq} criterion is not fulfilled (see 3.2.1) OR
- OECD 301 tests are available and show significant degradation above their threshold OR
- the substance is assessed as not persistent in water in the PBT assessment (however, not based on QSARs only).

Indication for persistence in the aquatic environment (P_{aq} "yellow")

The substance is not assessed as "red" or "green" according to the rules above AND

- simulation tests, enhanced ready tests (longer than 40 d) and/or OECD 302 tests show significant degradation but below their threshold OR
- OECD 301 tests are available and do not show significant degradation or show significant degradation but below their threshold OR
- the PBT assessment is inconclusive, non-reliable or indicates persistence but only based on QSARs OR
- non-OECD guidance tests show persistence OR
- QSARs are the only available information, the substance is within the applicability domain and the QSARs indicate persistence OR
- the substance hydrolyses but forms persistent hydrolysis products OR
- the substance is assessed as persistent in sediment or soil according to the criteria c., d. or e. in section 3.2.1.

If no information allowing an assessment as "red", "green" or "yellow" as detailed above was available then the assessment result was "white". However, on an individual basis, the assessment could deviate from the rules above. In these cases a specific justification is given in Table 3 in the Annex.

The present assessment of persistence deviated in the following points from the approach suggested by Kalberlah et al. (2014). 1) All tests and information relevant for an assessment of persistence were retrieved for all substances, even if the decision with regard to the colour scheme had already been made. This was done in order to reveal potential assessment discrepancies. 2) The EPISUITE QSAR (suggested by Kalberlah et al. (2014)) was not used for the assessment, since none of the substances was within the application domain of this QSAR. 3) Also non-OECD guidance tests were considered.

3.5 Indication and assessment of M properties

According to the definition by Kalberlah et al. (2014), assessment of mobility was based on the soil sorption coefficient (as log K_{oc}) and on the water solubility (SW) (see section 3.2.2). For both log K_{oc} and SW experimental values (including test guidelines OECD 106 (OECD 106, 2000) and OECD 121 (OECD 121, 2001) for log K_{oc} and OECD 105 (OECD 105, 1995) for SW) were preferably used. In case experimental values were not available, log K_{oc} values were calculated using experimental or calculated Linear Solvation Energy Relationship (LSER) descriptors (Poole and Poole, 1999; Endo et al., 2015) and the Molecular Connectivity Index method MCI of EPISUITE (US EPA, 2012). For this purpose an evaluation if a substance is ionic or ionisable in the pH range of 6-8 was made first. This was done using the ACD software (ACD Percepta, 2015) for the pH values 6, 7 and 8. If a substance was ionic or ionisable in the pH range 6-8 it was outside the application domain of the LSER-based QSAR and of the OECD 121 test. For calculation of SW the software EPISUITE was used no matter if the substance is within the application domain or not.

The following rules were applied in the assessment approach with regard to the traffic light colour scheme:

<u>Mobile in the aquatic environment (M "red")</u>

- log K_{oc} value determined by test OECD 106 and both log K_{oc} and SW fulfil the criterion for M (see 3.2.2) OR
- log K_{oc} value determined by test OECD 121 or by QSAR with the substance being within the application domain and both log K_{oc} and SW fulfil the criterion for M.

<u>Not mobile in the aquatic environment (M "green")</u>

- log K_{oc} value determined by test OECD 106 and either log K_{oc} or SW or both values do not fulfil the criterion for M OR
- log K_{oc} value determined by test OECD 121 or by QSAR with the substance being within the application domain and either log K_{oc} or SW or both values do not fulfil the criterion for M.

Indication for mobility in the aquatic environment (M "yellow")

- log K_{oc} value determined by test OECD 121 or by QSAR with the substance being outside the application domain and both log K_{oc} and SW fulfil the criterion for M.

If no information allowing an assessment as "red", "green" or "yellow" as detailed above was available then the assessment result was "white".

3.6 Indication and assessment of T properties

Toxicity was assessed according to the criteria defined in section 3.2.3. A conservative worst case consideration was made, i.e. the highest toxic effect determined the assessment of toxicity. In contrast to the approach suggested by Kalberlah et al. (2014), not only the official CMR or STOT RE classifications were considered, but also toxicity studies reported in the REACH registration dossiers (including the PBT assessment) or in the open scientific literature. For this purpose, a detailed analysis of scientific study results related to potential CMR properties (*in vitro* and *in vivo* genotoxicity, carcinogenicity, reproduction toxicity and teratogenicity) was made. Validated and reliable studies indicating CMR or STOT RE were considered equivalent to the official classification.

Ecotoxicity was assessed according to acute and chronic aquatic toxicity categories (hazard classes taken from dossiers). The classification detailed in Annex I of Regulation No. 1272/2008 on Classification, Labelling and Packaging of Chemicals (European Parliament, 2008) was considered. Aquatic toxicity values for algae, daphnia and fish were used.

Additionally, structural alerts for endocrine activity (implemented in a proprietary edition of ChemProp (UFZ, 2016)) were considered. As QSARs the rules by Benigni and co-workers on mutagenicity and carcinogenicity (Benigni and Bossa, 2008; Benigni et al., 2008 and 2009) and models on endocrine effects (UFZ, 2016) were used. Furthermore, the Cramer classification was used (Cramer et al., 1978).

The following rules were applied in the assessment approach with regard to the traffic light colour scheme:

Toxic (T "red")

- Any of the criteria a.-e. for toxicity listed in section 3.2.3 is fulfilled. For criterion a. it was sufficient if this criterion was fulfilled for one of the aquatic test species.

Indication for toxicity (T "yellow")

The substance is not assessed as "red" according to the rule above AND

- QSAR-based structural alerts (endocrine disruption or genotoxicity or carcinogenicity) indictate toxicity OR
- the substance is classified in Cramer class III OR
- the substance is classified in the aquatic toxicity category chronic I or acute I.

Not toxic (T "green")

The substance is not assessed as "red" or "yellow" according to the rules above AND

- the substance is classified in Cramer class I or II.

If no information allowing an assessment as "red", "yellow" or "green" as detailed above was available then the assessment result was "white".

3.7 Potential for environmental emissions

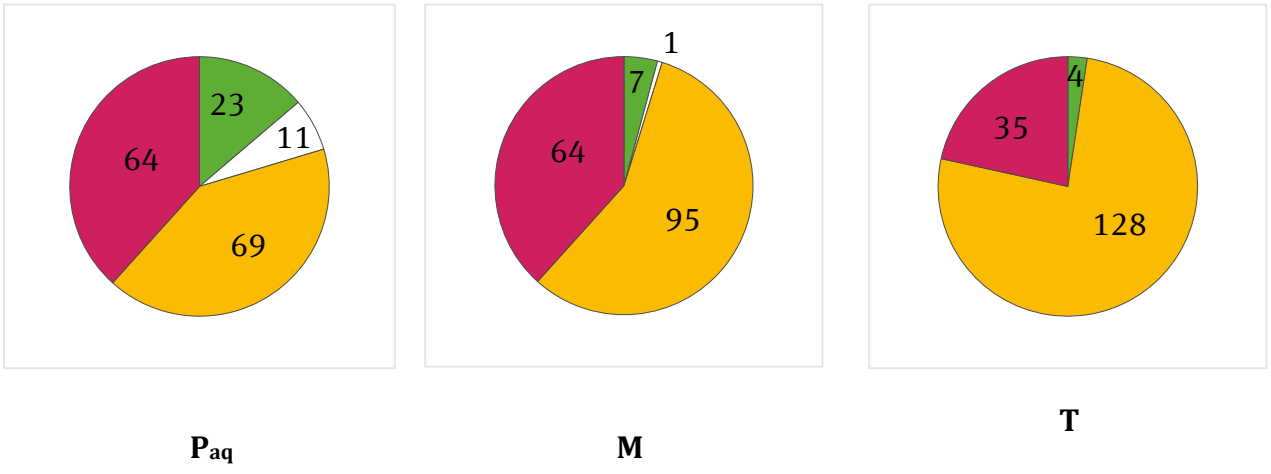
The potential for environmental emissions was assessed according to Schulze et al. (2018) using a model based on information under REACH on uses for each assessed substance. This information was combined with the annual tonnages of the substance marketed in Europe. The model allows an overall "yes"/"no"-decision (there is a potential/there is no potential for environmental emissions, respectively) based on the information on intended uses. The overall decision was "no" only in case the substance was exclusively registered as isolated intermediate according to REACH articles 17 or 18 and handled under strictly controlled conditions with high level containment techniques (Schulze et al., 2018). In all other cases the decision was "yes". Furthermore, for the substances possessing a potential for environmental emissions ("yes"-decision) the model results in a relative ranking of the substances with respect to their emission potential (E-score ranking). The E-score ranking is based on a scoring system for seven different use characteristics of the substances related to the probability of environmental emissions and the marketed tonnage of the substances. In the present study, the highest ranked substance (i.e. the substance with the highest potential for emissions according to the model) is given the E-score rank 1, the second highest the E-score rank 2 and so forth.

4 Results and discussion

4.1 Summary of the assessment results

The assessment results for all substances according to the criteria given in section 3.2 are summarized in Figure 3. Regarding persistence in the aquatic environment, of the 167 investigated substances 64 were assessed as persistent and 69 as suspected to be persistent (Figure 3). For 23 substances acceptable tests implied at least inherent biodegradability. These 23 substances were assessed not to be persistent in the aquatic environment mostly based on the judgement of results from screening tests. Eleven substances could not be assessed due to a lack of information. Generally, only QSARs were available to assess P_{aq} for these 11 substances, but the substances were all ionic or ionisable on the pH range 6-8 and thus outside the QSARs' application domain. For these 11 substances more data or data of better quality is needed in order to carry out a persistency assessment.

Figure 3: Summary of the assessment results for the 167 substances according to the inherent substance properties Paq, M and T. The number of substances in each assessment category (according to the traffic-light colour scheme) is given.



Source: own illustration

Regarding mobility in the aquatic environment, the majority of investigated substances were assessed as either being mobile in the aquatic environment (64) or as suspected to be mobile (95) and one substance could not be assessed based on the available data (Figure 3). Manufacturers, importers and downstream users should strive to obtain and report data of better quality in order to carry out a more accurate assessment. Only 7 of the 167 substances were assessed not to be mobile in the aquatic environment based on log K_{oc} and SW data.

A total of 35 substances were assessed to fulfil the criterion for toxicity (Figure 3). In most of these cases either the CMR and/or the STOT RE criterion was fulfilled (criteria b. and c. in section 3.2.3), whereas two substances were assessed as toxic based on the ecotoxicity criterion only (criterion a. in 3.2.3). Only 4 substances were assessed not to be toxic. The vast majority of 128 substances were assessed as suspected to be toxic. Of these 128 substances 87 were assessed as suspected to be toxic due to Cramer class III classification, in many cases in combination with structural alerts from other QSAR models. These results should be used with caution due to the severe shortcomings of the Cramer scheme leading to overestimation of toxicity for many substances. Additionally, also the structural alerts leading to suspected toxicity need to be interpreted cautiously, as in many cases the substances were outside the application domains of the QSARs in this screening assessment. For substances that are persistent in the environment and mobile in the aquatic environment, manufacturers, importers and downstream users should strive to obtain and report data that allow a full assessment of toxicity.

In Table 1 the assessment results for the 167 substances are summarized in a prioritized order of the inherent substance properties with the highest priority for P_{aq}, followed by M and T. As an example how to read Table 1, of the 64 substances assessed to be persistent in the aquatic environment, 29 were also assessed to be mobile in the aquatic environment ($P_{aq}M$ substances), while 31 substances were suspected to be mobile and 4 were assessed not to be mobile. Of the 29 $P_{aq}M$ substances, 8 were assessed to be toxic ($P_{aq}MT$ substances), while 21 were suspected to be toxic.

Table 1: Summary of the assessment results for the 167 substances prioritized in the order P_{aq}, M and T. The number of substances in each assessment category (according to the traffic-light colour scheme) is given.

P_{aq}	64						69							11	23				
M	29		31			4	28		37		1	3	11	7	16				
T	8	21	2	27	2	4	12	16	7	29	1	1	3	11	4	3	2	13	1

Source: own illustration

Almost all substances (164 out of 167) were evaluated to possess a potential to be emitted into the environment (Table 2). This is due to the fact that the assessment approach of PROMOTE (Schulze et al., 2018) was used in the present study. The vast majority of the assessed substances were from the shortlist of substances that have already been evaluated within PROMOTE to be emitted into the environment.

4.2 Details of the assessment results

The assessment results for each substance according to the criteria (section 3.2) are presented in Table 2. Each justification for the assessments according to the weight-of-evidence approach are summarized in the Annex in Tables 3, 4 and 5 for P_{aq}, M and T, respectively. Table 2 is firstly ranked based on the assessment result presented in the columns P_{aq}, M and T (identical to Table 1) and secondly regarding their emission potential in the column E-score ranking.

A total of 8 substances were assessed to be P_{aq}MT substances, i.e. to fulfil the criteria for P_{aq}, M and T (Table 2, ranking ID 1 to 8). All these 8 substances are neutral molecules in the pH range 6-8 (Table 4) and they are assessed as toxic based on CMR or STOT RE classification. All 8 substances are expected to be emitted into the environment with an E-score ranking between 1 and 137 of the 8 assessed P_{aq}MT substances (1,2-dichloroethane, trichloroethene and tetrachloroethene) are among the top ten of all assessed substances regarding their emission potential. 1,2-Dichloroethane and trichloroethene are used as intermediates for the production of other chemicals but have also many other applications such as usage as paint stripper, solvent degreasing agent, as extraction agent or as solvent, e.g. for asphalt and resins. Tetrachloroethene is used as solvent, as solvent degreasing agent and in other applications such as dry cleaning agents. Based on these usage patterns environmental emissions can be expected. Further assessed P_{aq}MT substances include 4-aminophenol, used as intermediate for the production of other chemicals, e.g. pharmaceuticals. However, from the registration dossiers intended uses of the types “wide dispersive use”, “industrial use” and “professional use” were identified. Therefore, emissions to the environment are expected also for this substance. 1,4-Dioxane is used as solvent and as stabilizer in the chemical industry, while 1,2,4-triazole is used as intermediate for the production of other chemicals, e.g. fungicides, but also as additive in fertilizer.

A total of 21 substances were assessed to be P_{aq}M substances with indication for toxicity (Table 2, ranking ID 9 to 29). This is mainly due to the high rate of screening T assessments by QSAR-based methods (especially Cramer class III), which would have to be confirmed by assessment information as discussed in section 4.1. All 21 substances are expected to be emitted into the environment with an E-score ranking between 2 and 163. In fact, all in Table 2 ranked top 29 substances (ID 1 to 29) assessed as P_{aq}M substances were either assessed to be toxic or at least fulfil the screening criterion.

A total of 105 substances are suspected P_{aq}MT substances, i.e. with indications that they fulfil the P_{aq}, M and T criteria or no information allowing an assessment (see Tables 1). For these substances neither P_{aq}, M nor T was assessed to be not fulfilled (“green”). They are ranked in Table 2 between ID 30 and ID 144, however the 10 substances with ID 59 to 64, ID 129 and ID 131 to 133 in Table 2 are not in this third prioritisation group. Further data and assessment is needed for these 105 substances to either confirm or disprove the suspected P_{aq}, M and T properties. The only three substances in this study assessed not to be emitted into the environment are within this group of 105 suspected P_{aq}MT substances. These are amantadine, 5-chloro-*o*-toluidine and 1H-pyrazole. They were shortlisted in the PROMOTE project due to chemical analytical studies identifying them as trace contaminants in environmental waters, which is an empirical proof for emissions. This apparent contradiction can be explained as follows: Schulze et al. (2018) modelled the potential for environmental emissions based on registration data under REACH, while the substances in question may have uses within other chemical regulatory frameworks as well. E.g., amantadine is registered under REACH solely as intermediate, while it is also used as antiviral and analgetic agent (De Clercq, 2004) as well as in the treatment of the Parkinson disease (Connolly and Lang, 2014). Nevertheless the E-score does not indicate emissions into the environment these three substances were included in this third prioritisation group due to the environmental findings.

Consequently, a total of 134 substances based on suspected P_{aq}MT properties combined with expected environmental emissions are recommended to the German Environment Agency (UBA) for further investigation and scientific and regulatory scrutiny. However, this result may not be suitable to indicate the need for regulatory measures. This study identified considerable data gaps (especially for experimental data) that in many cases hampered the assessment of the criteria, especially for M and T.

A total of 23 substances were assessed not to be persistent in the aquatic environment (Table 2, ranking ID 145 to 167). This may surprise at first, as the selection of substances to assess was made from shortlists of the PROMOTE project (Arp et al., 2017; Schulze et al., 2018) and from a research project of

the Germany Environment Agency (Kalberlah et al., 2014) (see section 3.1), which modelled or assessed these substances to be persistent in the environment. However, 22 of the 23 substances originated from PROMOTE with acknowledged considerable uncertainties in the persistence assessment, especially for ionic or ionisable chemicals (Arp et al., 2017). In the present study, 13 of these 22 substances were modelled to be ionic or ionisable in the pH range 6-8. The single one of the 23 substances originating from the shortlist by Kalberlah et al. (2014) was sodium cyanide, which was assessed in the present study not to fulfil the criterion for P_{aq} based on expert judgement. For the M assessment our assessment confirmed the results of the two other studies.

Table 2: List of all 167 substances and the results of the assessment according to the traffic-light colour scheme using the weight of evidence approach.

ID	CAS No.	EC No.	Substance name	Assessment			E-score ranking
				Paq	M	T	
1	107-06-2	203-458-1	1,2-Dichloroethan				1
2	127-18-4	204-825-9	Tetrachloroethene				4
3	79-01-6	201-167-4	Trichloroethene				10
4	123-30-8	204-616-2	4-Aminophenol				37
5	288-88-0	206-022-9	1,2,4-Triazole				51
6	123-91-1	204-661-8	1,4-Dioxane				52
7	1671-49-4	430-550-0	4-Mesyl-2-nitrotoluene				88
8	87-62-7	201-758-7	2,6-Dimethylaniline				137
9	2896-70-0	220-778-7	2,2,6,6-Tetramethyl-4-oxopiperidinooxy				145
10	108-78-1	203-615-4	1,3,5-Triazine-2,4,6-triamine				2
11	461-58-5	207-312-8	Cyanguanidine				19
12	4193-55-9	224-073-5	Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[[4-[bis(2-hydroxyethyl)amino]-6-(phenylamino)-1,3,5-triazin-2-yl]amino]-, disodium salt				22
13	13674-84-5	237-158-7	2-Propanol, 1-chloro-, phosphate (3:1)				25
14	91-76-9	202-095-6	1,3,5-Triazine-2,4-diamine, 6-phenyl-				26
15	63500-71-0	405-040-6	A mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol				44
16	126-86-3	204-809-1	2,4,7,9-Tetramethyldec-5-yne-4,7-diol				47
17	7529-22-8	231-391-8	4-Methylmorpholine 4-oxide monohydrate				66
18	2226-96-2	218-760-9	4-Hydroxy-2,2,6,6-tetramethylpiperidinoxyl				78
19	34730-59-1	252-173-9	Sodium 2-[(2-aminoethyl)amino]ethanesulphonate				90
20	80-08-0	201-248-4	Dapsone				92
21	12108-13-3	235-166-5	MMT				99
22	13472-08-7	236-740-8	2,2'-Azobis[2-methylbutyronitrile]				101
23	342573-75-5	460-100-9	1-Ethyl-3-methylimidazolium ethylsulfate				107
24	54686-97-4	402-950-5	1-(2,6-bis(4-Tolyl)-1,3-dioxano(5,4-d)-1,3-dioxan-4-yl)ethane-1,2-diol				120

ID	CAS No.	EC No.	Substance name	Assessment			E-score ranking
				Paq	M	T	
25	129909-90-6	603-373-3	4-Amino-N-(1,1-dimethylethyl)-4,5-dihydro-3-(1-methylethyl)-5-oxo-1H-1,2,4-triazole-1-carboxamide				146
26	141-98-0	205-517-7	O-Isopropyl ethylthiocarbamate				152
27	867-13-0	212-757-6	Triethylphosphonoacetate				154
28	542-02-9	208-796-3	6-Methyl-1,3,5-triazine-2,4-diyldiamine				157
29	88-19-7	201-808-8	Toluene-2-sulphonamide				162
30	62037-80-3	700-242-3	GenX				163
31	768-94-5	212-201-2	Amantadine				-
32	2855-13-2	220-666-8	Isophorondiamin				6
33	5281-04-9	226-109-5	2-Naphthalenecarboxylic acid, 3-hydroxy-4-[(4-methyl-2-sulfophenyl)azo]-, calcium salt (1:1)				8
34	140-31-8	205-411-0	1-Piperazineethanamine				13
35	84632-65-5	401-540-3	3,6-bis(4-Chlorophenyl)-2,5-dihydro-pyrrolo[3,4-c]pyrrol-1,4-dione				40
36	121-03-9	204-445-3	4-Nitrotoluol-2-sulfonsäure				41
37	201792-73-6	421-880-6	Disodium 4-amino-6-[[4-(N-(4-((E)-(2,4-diaminophenyl)diazenyl)phenyl)sulfamoyl)phenyl)diazenyl)-5-hydroxy-3-((E)-(4-nitrophenyl)diazenyl)naphthalene-2,7-disulfonate				45
38	36888-99-0	253-256-2	5,5'-(1H-Isoindole-1,3(2H)-diylidene)dibarbituric acid				54
39	3030-47-5	221-201-1	bis(2-Dimethylaminoethyl)(methyl)amine				64
40	3033-62-3	221-220-5	N,N,N',N'-Tetramethyl-2,2'-oxybis(ethylamine)				65
41	15214-89-8	239-268-0	1-Propanesulfonic acid, 2-methyl-2-[(1-oxo-2-propenyl)amino]-				68
42	55589-62-3	259-715-3	6-Methyl-1,2,3-oxathiazin-4(3H)-one 2,2-dioxide, potassium salt				77
43	52722-86-8	258-132-1	1-Piperidineethanol, 4-hydroxy-2,2,6,6-tetramethyl-				79
44	1704-62-7	216-940-1	2-[2-(Dimethylamino)ethoxy]ethanol				80
45	73037-34-0	277-242-0	Disodium oxybis[methylbenzenesulphonate]				87
46	1561-92-8	216-341-5	Sodium 2-methylprop-2-ene-1-sulphonate				91

ID	CAS No.	EC No.	Substance name	Assessment			E-score ranking
				Paq	M	T	
47	76199-85-4	278-388-8	2-Cyano-2-[2,3-dihydro-3-(tetrahydro-2,4,6-trioxo-5(2H)-pyrimidinylidene)-1H-isoindol-1-ylidene]-N-methylacetamide				97
48	83016-70-0	406-080-7	2-[(2-[2-(Dimethylamino)ethoxy]ethyl) methylamino]ethanol				108
49	4246-51-9	224-207-2	3,3'-Oxybis(ethyleneoxy)bis(propylamine)				111
50	92484-48-5	403-080-9	Sodium 3-(2H-benzotriazol-2-yl)-5-sec-butyl-4-hydroxybenzenesulfonate				116
51	4065-45-6	223-772-2	Sulisobenzone				118
52	7365-45-9	230-907-9	4-(2-Hydroxyethyl)piperazin-1-ylethanesulphonic acid				124
53	622-40-2	210-734-5	2-Morpholinoethanol				125
54	25956-17-6	247-368-0	Disodium 6-hydroxy-5-[(2-methoxy-4-sulphonato-m-tolyl)azo]naphthalene-2-sulphonate				132
55	1024699-81-7	688-159-8	N,N,N-Trimethyl-3-[(2-methylacryloyl)amino]propan-1-aminium 4-(C10-13-sec-alkyl)benzenesulfonate				142
56	561-41-1	209-218-2	4,4'-bis(Dimethylamino)-4''-(methylamino)trityl alcohol				150
57	46830-22-2	256-283-8	Benzenemethanaminium, N,N-dimethyl-N-[2-[(1-oxo-2-propenyl)oxy]ethyl]-, chloride				158
58	39148-16-8	444-960-2	Fosetyl Na				159
59	23386-52-9	245-629-3	Sodium 1,4-dicyclohexyl sulphonatosuccinate				84
60	3965-55-7	223-578-8	Sodium dimethyl 5-sulphonatoisophthalate				143
61	12239-87-1	235-476-0	Copper, [chloro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-				30
62	88122-99-0	402-070-1	Ethylhexyl triazone				105
63	74336-59-7	277-823-9	3-[(4-Chloro-2-nitrophenyl)azo]-2-methylpyrazolo[5,1-b]quinazolin-9(1H)-one				109
64	65113-55-5	265-449-9	[4-[p,p'-bis(Dimethylamino)benzhydrylidene]cyclohexa-2,5-dien-1-ylidene]dimethylammonium m-[[p-anilinophenyl]azo]benzenesulphonate				141
65	91-20-3	202-049-5	Naphthalene				5
66	2768-02-7	220-449-8	Silane, ethenyltrimethoxy-				17
67	101-77-9	202-974-4	4,4'- Diaminodiphenylmethane (MDA)				38
68	68479-98-1	270-877-4	Benzenediamine, ar,ar-diethyl-ar-methyl-				43

ID	CAS No.	EC No.	Substance name	Assessment			E-score ranking
				Paq	M	T	
69	1025-15-6	213-834-7	1,3,5-Triallyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione				81
70	55-63-0	200-240-8	1,2,3-Propanetriol, trinitrate				83
71	6610-29-3	229-563-2	4-Methylthiosemicarbazide				94
72	108-45-2	203-584-7	1,3-Benzenediamine				98
73	6362-79-4	228-845-2	Sodium hydrogen-5-sulphoisophthalate				123
74	834-12-8	212-634-7	1,3,5-Triazine-2,4-diamine, N-ethyl-N'-(1-methylethyl)-6-(methylthio)-				126
75	95-79-4	202-452-6	5-Chloro-o-toluidine				-
76	288-13-1	206-017-1	1H-Pyrazole				-
77	100-97-0	202-905-8	1,3,5,7-Tetraazatricyclo[3.3.1.13,7]decane				9
78	1477-55-0	216-032-5	1,3-Benzenedimethanamine				18
79	839-90-7	212-660-9	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(2-hydroxyethyl)-				21
80	102-06-7	203-002-1	1,3-Diphenylguanidin				23
81	115-21-9	204-072-6	Silane, trichloroethyl-				53
82	36483-57-5	253-057-0	2,2-Dimethylpropan-1-ol, tribromo derivative				59
83	505-65-7	208-015-6	1,3-Dioxepan				60
84	1071-93-8	213-999-5	Adipohydrazide				67
85	35948-25-5	252-813-7	6H-Dibenz[c,e][1,2]oxaphosphorin 6-oxide				70
86	106264-79-3	403-240-8	A mixture of: 3,5-dimethylthio-2,4-toluenediamine; 3,5-dimethylthio-2,6-toluenediamine				71
87	221667-31-8	485-320-2	Cyprosulfamide				72
88	615-50-9	210-431-8	2-Methyl-p-phenylenediamine sulfate				82
89	39236-46-9	254-372-6	N,N''-Methylenebis[N'-[3-(hydroxymethyl)-2,5-dioxoimidazolidin-4-yl]urea]				104
90	23847-08-7	245-910-0	1,1'-Dithiobis[hexahydro-2H-azepin-2-one]				117
91	68957-94-8	422-210-5	2,4,6-Tri-n-propyl-2,4,6-trioxo-1,3,5,2,4,6-trioxatriphosphorinane				151
92	1333-07-9	215-578-1	Toluenesulphonamide				161
93	101-72-4	202-969-7	1,4-Benzenediamine, N-(1-methylethyl)-N'-phenyl-				35
94	3380-34-5	222-182-2	2,4,4'-Trichloro-2'-hydroxy-diphenyl-ether; 5-chloro-2-(2,4-dichlorophenoxy)phenol (Triclosan)				62

ID	CAS No.	EC No.	Substance name	Assessment			E-score rank-ing
				Paq	M	T	
95	52556-42-0	258-004-5	Sodium 3-(allyloxy)-2-hydroxypropanesulpho-nate				63
96	56-93-9	200-300-3	Benzyltrimethylammonium chloride				89
97	61617-00-3	262-872-0	2-MMBI, zinc salt				95
98	107-66-4	203-509-8	Dibutyl hydrogen phosphate				110
99	70441-63-3	448-100-7	4-Fluoro-N-isopropylaniline				140
100	104-15-4	203-180-0	Benzenesulfonic acid, 4-methyl-				16
101	4098-71-9	223-861-6	Isophorondiisocyanat				20
102	2893-78-9	220-767-7	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3-dichloro-, sodium salt				24
103	90-72-2	202-013-9	2,4,6-Tris(dimethylaminomethyl)phenol				27
104	2008-39-1	217-915-8	2,4-D, DMA-Salz				31
105	16066-35-6	240-210-1	Benzenesulfonic acid, 4-(1-methylethyl)-				32
106	5165-97-9	225-948-4	1-Propanesulfonic acid, 2-methyl-2-[(1-oxo-2-propenyl)amino]-, monosodium salt				33
107	80-09-1	201-250-5	4,4'-Sulfonyldiphenol				42
108	121-57-3	204-482-5	Benzenesulfonic acid, 4-amino-				48
109	280-57-9	205-999-9	1,4-Diazabicyclooctane				49
110	6381-77-7	228-973-9	2,3-Didehydro-3-O-sodio-D-erythro-hexono-1,4-lactone				55
111	61260-55-7	262-679-1	1,2-bis((2,2,6,6-Tetramethyl-piperidin-4-yl)aminoethyl)ethane				58
112	3047-33-4	221-255-6	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, triso-dium salt				75
113	3039-83-6	221-242-5	Ethenesulfonic acid, sodium salt				76
114	42405-40-3	403-360-0	bis(3,5-bis(1,1-Dimethylethyl)-2-hydroxyben-zoato-O1,O2)zinc				85
115	3338-24-7	222-079-2	Sodium O,O-diethyl dithiophosphate				106
116	1493-13-6	216-087-5	Trifluoromethanesulphonic acid				114
117	97-39-2	202-577-6	1,3-Di-o-tolylguanidine				115
118	97042-18-7	479-880-7	BPS-MAE				119
119	45021-77-0	256-181-3	1-Propanaminium, N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-, chloride				121
120	121-47-1	204-473-6	3-Aminobenzenesulphonic acid				122

ID	CAS No.	EC No.	Substance name	Assessment			E-score ranking
				Paq	M	T	
121	54553-90-1	259-224-4	Benzene-1,2,4,5-tetracarboxylic acid, compound with 4,5-dihydro-2-phenyl-1H-imidazole (1:1)				128
122	34335-10-9	696-577-7	Phosphonic acid, P-phenyl-, zinc salt				131
123	104-23-4	203-187-9	4'-Aminoazobenzene-4-sulphonic acid				144
124	7300-34-7	230-745-9	3,3'-[Butane-1,4-diylbis(oxy)]bispropanamine				147
125	85-73-4	201-627-4	Phthalylsulfathiazole				149
126	932-64-9	213-254-4	1,2-Dihydro-5-nitro-3H-1,2,4-triazol-3-one				156
127	77497-97-3	406-960-0	(S)-3-Benzyloxycarbonyl-1,2,3,4-tetrahydroisoquinolinium 4-methylbenzenesulfonate				160
128	6331-96-0	700-413-2	2-Amino-4,5-dichlorbenzolsulfonsäure				164
129	127-68-4	204-857-3	Sodium 3-nitrobenzenesulphonate				74
130	91273-04-0	401-280-0	1-(N,N-bis(2-Ethylhexyl)aminomethyl)-1,2,4-triazole				96
131	54660-00-3	402-400-4	3,6-Diphenyl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione				93
132	971-15-3	213-537-2	bis(Piperidinothiocarbonyl) hexasulphide				102
133	154702-15-5	421-450-8	UVASORB HEB				127
134	3160-86-9	700-230-8	Hexane-1,6-diaminium benzene-1,4-dicarboxylate (1:1):adipic acid, compound with hexane-1,6-diamine (1:1):sebacic acid, compound with hexane-1,6-diamine (1:1):dodecanedioic acid, compound with hexane-1,6-diamine (1:1)				3
135	13188-60-8	236-143-2	Dodecanedioic acid, compound with hexane-1,6-diamine (1:1)				7
136	2495-39-8	219-676-5	2-Propene-1-sulfonic acid, sodium salt				61
137	754186-36-2	700-272-7	(2S)-N-[(Diethylamino)methyl]-2-(2-oxopyrrolidin-1-yl)butanamide (2R,3R)-tartrate				73
138	69477-29-8	614-977-1	2,6-bis-(Diethanolamino)-4,8-dipiperidinopyrimido-(5,4-d)-pyrimidine, tosylat salt				113
139	130-26-7	204-984-4	Clioquinol				134
140	12225-21-7	235-428-9	Aluminium, 4,5-dihydro-5-oxo-1-(4-sulfophenyl)-4-[(4-sulfophenyl)azo]-1H-pyrazole-3-carboxylic acid complex				135
141	17636-10-1	241-620-3	Sodium 3-mercaptopropanesulphonate				136
142	81-07-2	201-321-0	1,2-Benzisothiazol-3(2H)-one 1,1-dioxide				139

ID	CAS No.	EC No.	Substance name	Assessment			E-score ranking
				Paq	M	T	
143	83-73-8	201-497-9	Diiodohydroxyquinoline				148
144	54981-42-9	805-128-8	Pyridine:sulphur trioxide--pyridine (1:1):2-acetamido-5-chlorobenzenesulfonic acid;pyridine				153
145	143-33-9	205-599-4	Sodium cyanide				11
146	88-12-0	201-800-4	1-Vinyl-2-pyrrolidon				15
147	4719-04-4	225-208-0	1,3,5-Triazine-1,3,5(2H,4H,6H)-triethanol				29
148	81646-13-1	279-791-1	Docosyltrimethylammonium methyl sulphate				57
149	100-20-9	202-829-5	1,4-Benzenedicarbonyl dichloride				56
150	5187-23-5	225-967-8	5-Ethyl-1,3-dioxane-5-methanol				69
151	497-18-7	207-837-2	Carbonohydrazide				138
152	108-74-7	203-612-8	1,3,5-Triazine, hexahydro-1,3,5-trimethyl-				39
153	38632-47-2	690-526-2	Methansulfonic acid (1,6-hexanediyl-diimino)bis[1-oxo, disodium salt				86
154	120-18-3	204-375-3	Naphthalenesulfonic acids				12
155	577-11-7	209-406-4	Butanedioic acid, sulfo-, 1,4-bis(2-ethylhexyl) ester, sodium salt				14
156	98-67-9	202-691-6	4-Hydroxybenzolsulfonsäure				34
157	25321-41-9	246-839-8	Benzenesulfonic acid, dimethyl-				36
158	103-83-3	203-149-1	Benzenemethanamine, N,N-dimethyl-				46
159	24634-61-5	246-376-1	Potassium (E,E)-hexa-2,4-dienoate				50
160	29923-31-7	249-958-3	Sodium hydrogen N-(1-oxododecyl)-L-glutamate				100
161	51410-72-1	257-182-1	(3-Methacrylamidopropyl)trimethylammonium chloride				103
162	928-70-1	213-180-2	Potassium isopentyl dithiocarbonate				112
163	112-33-4	203-960-0	2-[2-(3-Aminopropoxy)ethoxy]ethanol				129
164	2123-24-2	218-336-3	Hexahydro-2H-azepin-2-one, sodium salt				130
165	10595-49-0	234-204-8	Methyl trimethyl-3-[(1-oxododecyl)amino]propylammonium sulphate				133
166	299-27-4	206-074-2	D-Gluconic acid, monopotassium salt				155
167	1300-72-7	215-090-9	Benzenesulfonic acid, dimethyl-, sodium salt				28

5 Conclusions

For the first time a comprehensive list of 167 REACH registered substances were assessed with respect to their intrinsic substance properties persistence in the aquatic environment, mobility in the aquatic environment and toxicity using slightly modified criteria originally defined by Kalberlah et al. (2014). The results of this project will support the ongoing discussion to define PMT criteria under REACH based on the proposal by Neumann and Schliebner (2017). The present study provides a consolidated list of (in order of priority) assessed P_{aq}MT substances (8 substances), assessed P_{aq}M substances with suspected T (21 substances) and further 93 suspected P_{aq}MT substances. A total of 134 substances based on suspected P_{aq}MT properties combined with expected environmental emissions are recommended to the German Environment Agency (UBA) for further investigation and scientific and regulatory scrutiny. However, this result may not be suitable to indicate the need for regulatory measures.

The study has shown that there are considerable data gaps (especially for experimental data) that in many cases hampered the assessment whether or not a criterion was fulfilled. For the majority of M and T assessments as well as for a large number of P_{aq} assessments only indicative information was available. The assessment results presented in this study may therefore be used by registrants under REACH to identify and select substances that need data of better quality in order to carry out a more accurate PMT assessment. This may lead to a situation where registrants may want to considere safer alternatives or risk mitigation measures to minimize emissions into the environment of identified PMT substance.

It is known that substantial analytical challenge exists related to detection and quantification of polar (mobile) substances in water samples, as this has recently been described as the analytical and monitoring data gap (Reemtsma et al., 2016). Consequently the results of our project could also initiate the development of suitable analytic techniques for water monitoring.

Furthermore, as new substances continuously enter the market and production and/or use scenarios of substances are subject to changes, the present study needs to be repeated regularly in order to extend and update the results.

6 References

ACD Percepta (2015): Advanced Chemistry Development, Inc., Toronto, On, Canada, www.acdlabs.com.

Arp, H.P.H., Brown, T.N., Berger, U., Hale S.E. (2017): Ranking REACH registered neutral, ionizable and ionic organic chemicals based on their aquatic persistency and mobility. Environ. Sci. Process Impacts 19, 939-955.

Benigni, R., Bossa, C. (2008): Structure alerts for carcinogenicity, and the Salmonella assay system: A novel insight through the chemical relational databases technology. Mutat. Res.-Rev. Mutat. 659, 248-261.

Benigni, R., Bossa, C., Jeliazkova, N., Netzeva, T., Worth, A. (2008): The Benigni / Bossa rulebase for mutagenicity and carcinogenicity – a module of Toxtree.

Benigni, R., Bossa, C., Tcheremenskaia, O., Worth, A. (2009): Development of structural alerts for the in vivo micronucleus assay in rodents. EUR 23844 EN. Office for Official Publications of the European Communities, Luxembourg.

Connolly, B.S., Lang, A.E. (2014): Pharmacological treatment of Parkinson disease: a review. JAMA 311,1670-1683.

Cramer, G.M., Ford, R.A., Hall, R.L. (1978): Estimation of toxic hazard - A decision tree approach. Food and Cosmetics Toxicology 16, 255-276. Corrigendum: Food and Cosmetics Toxicology 16, 634.

De Clercq, E. (2004): Antiviral drugs in current clinical use. J. Clin. Virol. 30, 115-133.

Endo, S., Brown, T.N., Watanabe, N., Ulrich, N., Bronner, G., Abraham, M.H., Goss, K.-U. (2015) UFZ-LSER database v 3.1 [Internet], Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany. URL: http://www.ufz.de/lserd

European Chemicals Agency, ECHA (2017): Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.11: PBT/vPvB Assessment; version 3.0, June 2017.

European Parliament (2006) Regulation (EC) 1907/2006, OJ L 396 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC.

European Parliament (2008) Regulation (EC) 1272/2008, OJ L 353 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures - amending and repealing Directive 67/548/EEC and 1999/45/EC, and Regulation (EC) No 1907/2006, Official Journal of the European Union, 31.12.2008, L 353/1-35; Annex I, L 353/36-141.

Kalberlah, F., Oltmanns, J., Schwarz, M., Baumeister, J., Striffler, A. (2014): Guidance for the precautionary protection of raw water destined for drinking water extraction from contaminants regulated under REACH. Environmental Research of the Federal Ministry for the Environment, Nature Conservation, Building and Nuclear Safety. Project (UFOPLAN) FKZ 371265416. Umweltbundesamt, Dessau.

Kühne, R., Ebert, R.-U., Schüürmann, G. (2009): Chemical domain of QSAR models from atom-centered fragments. J. Chem. Inf. Model. 96, 2660-2669.

Neumann, M. (2017): Proposal for criteria and an assessment concept for the identification of Persistent, Mobile and Toxic (PMT) substances to protect raw water for the production of drinking water under the EU regulation REACH [in German]. Zbl. Geol. Paläont. Teil I, Jg. 2017, Heft 1, 91-101.

Neumann, M., Schliebner, I. (2017): Protecting the sources of our drinking water – A revised proposal for implementing criteria and an assessment procedure to identify Persistent, Mobile and Toxic (PMT) and very Persistent, very Mobile (vPvM) substances registered under REACH, Environmental Agency, ISSN 2363-8273, 16 pages, available from https://www.umweltbundesamt.de/publikationen/protecting-the-sources-of-our-drinking-water-from

OECD 105, 27 July 1995, available from http://www.oecd-ilibrary.org/environment/test-no-105-water-solubility_9789264069589-en

OECD 106, 21 January 2000, available from http://www.oecd-ilibrary.org/environment/test-no-106-adsorption-desorption-using-a-batch-equilibrium-method_9789264069602-en

OECD 111, 23 November 2004, available from http://www.oecd-ilibrary.org/environment/test-no-111-hydrolysis-as-a-function-of-ph_9789264069701-en

OECD 121, 22 January 2001, available from http://www.oecd-ilibrary.org/environment/test-no-121-estimation-of-the-adsorption-coefficient-koc-on-soil-and-on-sewage-sludge-using-high-performance-liquid-chromatography-hplc_9789264069909-en

OECD 301, 17 July 1992, available from http://www.oecd-ilibrary.org/environment/oecd-guidelines-for-the-testing-of-chemicals-section-3-degradation-and-accumulation_2074577x

OECD 302B, 17 July 1992, available from http://www.oecd-ilibrary.org/environment/oecd-guidelines-for-the-testing-of-chemicals-section-3-degradation-and-accumulation_2074577x

OECD 302C, 8 September 2009, available from http://www.oecd-ilibrary.org/environment/oecd-guidelines-for-the-testing-of-chemicals-section-3-degradation-and-accumulation_2074577x

OECD 307, 24 April 2002, available from http://www.oecd-ilibrary.org/environment/oecd-guidelines-for-the-testing-of-chemicals-section-3-degradation-and-accumulation_2074577x

OECD 308, 24 April 2002, available from http://www.oecd-ilibrary.org/environment/oecd-guidelines-for-the-testing-of-chemicals-section-3-degradation-and-accumulation_2074577x

OECD 309, 23 November 2004, available from http://www.oecd-ilibrary.org/environment/oecd-guidelines-for-the-testing-of-chemicals-section-3-degradation-and-accumulation_2074577x

OECD 310, 11 July 2006, available from http://www.oecd-ilibrary.org/environment/oecd-guidelines-for-the-testing-of-chemicals-section-3-degradation-and-accumulation_2074577x

Poole, S.K., Poole, C.F. (1999): Chromatographic models for the sorption of neutral organic substances by soil from water and air. J. Chromatogr. A 845, 381-400.

Reemtsma, T., Berger, U., Arp, H.P.H, Gallard, H., Knepper, T.P., Neumann, M., Quintana, J.B., de Voogt, P. (2016): Mind the gap: Persistent and mobile organic substances – water contaminants that slip through. Environ. Sci. Technol. 50, 10308-10315.

Schulze, S., Sättler, D., Neumann, M., Arp, H.P.H., Reemtsma, T., Berger, U. (2018): Prioritizing REACH registered organic chemicals that are persistent and mobile in groundwater based on their emission potential; Science of The Total Environment 625, 1122–1128.

UFZ (2016): ChemProp 6.5. Department of Ecological Chemistry. URL: http://www.ufz.de/ecochem/chemprop

US EPA (2012): Estimation Programs Interface Suite™ for Microsoft Windows. United States Environmental Protection Agency, Washington, DC, USA.

7 Annex

Table 3: Weight of evidence for persistence in the aquatic environment (P_{aq}) for all 167 substances. For the substance ID see Table 2. The color shows the result of the assessment according to the traffic-light color scheme.

ID	P_{aq}	Rationale
1		Due to lack of other information the substance was assessed by PBT assessment in water. Therefore this substance is assessed to be persistent in water.
2		No significant biodegradation in 301 C tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
3		No significant biodegradation in 301C and D tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
4		No significant biodegradation in 301C tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
5		All biodegradation results in 301A and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
6		No significant biodegradation in 301F test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
7		All biodegradation results in 301F and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
8		No significant biodegradation in 301F tests. 302B tests not reliable. Registrant evaluates this substance to be persistent. Therefore this substance is assessed to be persistent in water.
9		No significant biodegradation in 301F tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
10		All biodegradation results in 301C and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
11		No significant biodegradation in 301E tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
12		All biodegradation results in 301A and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
13		Biodegradation results in 301C and E tests <20% and persistence due to PBT assessment. Therefore this substance is assessed to be persistent in water.
14		No significant biodegradation in 301C and E tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
15		No significant biodegradation in 301B test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
16		All biodegradation results in 301B and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
17		All biodegradation results in 301A and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.

ID	P_{aq}	Rationale
18		No significant biodegradation in 301A tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
19		All biodegradation results in 301E and 302C tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
20		No significant biodegradation in 301D tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
21		No significant biodegradation in 301D tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
22		No significant biodegradation in 301D test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
23		All biodegradation results in 301B and 302C imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
24		No significant biodegradation in 301D and C tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
25		Due to lack of other information the substance was assessed by PBT assessment in water. Therefore this substance is assessed to be persistent in water.
26		No significant biodegradation in 301D test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
27		All biodegradation results in 301B and 302B imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
28		No significant biodegradation in an enhanced 301E test. PBT assessment evaluates this substance to be persistent. Therefore this substance is assessed to be persistent in water.
29		No significant biodegradation in 301C test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
30		All biodegradation results in 301B and 302C imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
31		No significant biodegradation in 302B tests. Therefore this substance is assessed to be persistent in water.
32		No significant biodegradation in 301A tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
33		Biodegradation results in 301 C test <20% and persistence due to PBT assessment. Therefore this substance is assessed to be persistent in water.
34		All biodegradation results in 301D and F and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
35		No significant biodegradation in 301B tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
36		No significant biodegradation in 301E and C tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.

ID	P_{aq}	Rationale
37		No significant biodegradation in 302B test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
38		Due to lack of other information the substance was assessed by PBT assessment in water. Therefore this substance is assessed to be persistent in water.
39		All biodegradation results in 301C and E and 302B imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
40		All biodegradation results in 301F and 302B imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
41		Due to lack of other information the substance was evaluated by PBT assessment in water. Therefore this substance is assessed to be persistent in water.
42		All biodegradation results in 301A and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
43		No significant biodegradation in 301B tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
44		All biodegradation results in 301F and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
45		No significant biodegradation in 301F and C tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
46		No significant biodegradation in a 301A analogue test with preadaption. Due to lack of other information the substance was assessed by PBT assessment. Therefore this substance is assessed to be persistent in water.
47		No significant biodegradation in 301F test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
48		No significant biodegradation in 301D tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
49		No significant biodegradation in enhanced OECD 301B (<10% in 60 d). This is considered to be sufficient to evaluate this substance as persistent. Therefore this substance is assessed to be persistent in water.
50		No significant biodegradation in 301A test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
51		All biodegradation results in 301F and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
52		No significant biodegradation in 301D tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
53		No significant biodegradation in 302B test. Therefore this substance is assessed to be persistent in water.
54		Due to lack of other information the substance was assessed by PBT assessment in water. Therefore this substance is assessed to be persistent in water.

ID	P_{aq}	Rationale
55		No significant biodegradation in 301D tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
56		Due to lack of other information the substance was assessed by PBT assessment in water. Therefore this substance is assessed to be persistent in water.
57		Due to lack of other information the substance was assessed by PBT assessment in water. Therefore this substance is assessed to be persistent in water.
58		No significant biodegradation in 301D test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
59		All biodegradation results in 301B, D and E and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
60		All biodegradation results in 301C and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water.
61		No significant biodegradation in 301C and F tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
62		No significant biodegradation in 301C and E tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
63		Due to lack of other information the substance was assessed by PBT assessment in water. Therefore this substance is assessed to be persistent in water.
64		No significant biodegradation in 301F and C tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water.
65		OECD 301 C implies fast degradation while 302C does not imply any. Due to these contradicting results this substance is assessed with screening P_{aq}.
66		The substance is assessed to hydrolyze quickly. No significant biodegradation in 301F test but in 301B. The PBT assessment (including hydrolysis products) is ambiguous. Therefore this substance is assessed with a screening P_{aq}.
67		OECD 301B test implies significant biodegradation below threshold (46% in 28d) by radio chemical measurement; in addition to that several older studies are available implying either nearly no biodegradation or ready biodegradation; furthermore in soil this substance in considered to be persistent but not in freshwater. This substance is thus assessed screening P_{aq} due to ambiguous results and different degradation behavior in soil and water.
68		No significant biodegradation in 301D test. The PBT assessment is not reliable. Therefore the substance is assessed with screening P_{aq}.
69		No significant biodegradation in 301C test. The PBT assessment evaluates the substance to be persistent in worst case. Thefore the substance is assessed screening P_{aq}.
70		No significant biodegradation in 301B test. Results for non-OECD guidance tests probably obtained with adapted inoculum. The PBT assessment is thus not reliable. Therefore the substance is assessed with screening P_{aq}.
71		No significant biodegradation in 301B test, the PBT assessment (including hydrolysis products) is ambiguous. Therefore this substance is assessed with a screening P_{aq}.

ID	P_{aq}	Rationale
72		No significant biodegradation in 301D test, the PBT assessment is ambiguous. Therefore this substance is assessed with a screening P_{aq}.
73		No significant biodegradation in 301B test. The PBT assessment was ambiguous. Therefore the substance is assessed screening P_{aq}.
74		Only a non-OECD guideline test implying no significant biodegradation was available. Reliability of available PBT assessment is not clear. Therefore the substance is assessed screening P_{aq}.
75		OECD 302 B test implies significant biodegradation below threshold (30% in 10 d, 68% in 28 d, 95% in 55 d). Therefore the substance is assessed screening P_{aq}.
76		No significant biodegradation in 301A test, but no additional information. Therefore the substance is assessed screening P_{aq}.
77		Several studies with ambiguous results and/or unclear design and thus questionable results. Therefore the substance is assessed worst case screening P_{aq}.
78		Biodegradation result in 301B test is 49%, but in 302C only 22%; i.e. some significant biodegradation but below the threshold. Therefore this substance is evaluated with screening P_{aq}.
79		No significant biodegradation in 301A and F and 302B tests, incomlete documentated OECD 308 study implying a half-life <30 d (cannot be validated). Therefore this substance is assessed with a screening P_{aq}.
80		Several 301 tests imply high degradation rates for this substance but the documentation of theses studies is not sufficient. Therefore this substance is assessed with a worst case screening P_{aq}.
81		No significant biodegradation in 310 test, the PBT assessment (including hydrolysis products) is ambiguous. Therefore this substance is assessed with a screening P_{aq}.
82		OECD 302 B test implies significant biodegradation below threshold (77% in 36 d). Therefore the substance is assessed screening P_{aq}.
83		No significant biodegradation in 301F test, but no additional information. Therefore the substance is assessed screening P_{aq}.
84		Reliable 301C test implying no significant biodegradation; OECD 301E test failed slightly the threshold with 62% DOC removal, 301F implies ready biodegradation. Due to these ambiguous results this substance is assessed worst case screening P_{aq}.
85		No significant biodegradation in 301B tests. The PBT assessment was ambiguous. Therefore the substance is assessed screening P_{aq}.
86		No significant biodegradation in 301D test, but no additional information. Therefore the substance is assessed screening P_{aq}.
87		OECD 301F test implies significant biodegradation below threshold (30% in 28 d). Several OECD 307 tests do not imply persistence in soil. Extrapolation from aerobic soil to water is questionable. Therefore the PBT assessment is questionable and the substance is assessed screening P_{aq}.
88		No significant biodegradation in 301D test, the PBT assessment (including hydrolysis products) is ambiguous. Therefore this substance is assessed with a screening P_{aq}.

ID	P_{aq}	Rationale
89		The substance is not hydrolytically stable. OECD 301B test for its main transformation product implies significant biodegradation below threshold (43% in 25 d). This is not sufficient to conclude an inherent biodegradability, i.e. the PBT assessment is questionable. Furthermore, specific PBT guidance criteria have not been proved. Therefore this substance is assessed with screening P_{aq}.
90		OECD 301B and F tests imply significant biodegradation below threshold (35% and 57% in 28 d). Furthermore 302C showed 58% degradation in 28 d. The PBT assessment is questionable and the substance is assessed screening P_{aq}.
91		Only a non-OECD guideline test implying no significant biodegradation was available. Reliability of PBT assessment is not clear. Therefore the substance is assessed screening P_{aq}.
92		Due to lack of other information the substance was assessed by worst case PBT assessment as screening P_{aq}.
93		The substance itself is hydrolysable. No significant biodegradation has been found in 301 B, C and D tests. The PBT assessment also evaluates at least one transformation product to be persistent. Therefore this substance is evaluated with screening P_{aq}.
94		No significant biodegradation in OECD 301B and C tests. 302B test implies nerly full degradation but adaption is not specified. Further tests implying good biodegradation are not suitable for evaluation. Therefore this substance is assessed with a screening P_{aq}.
95		No significant biodegradation in 301C tests. The PBT assessment was ambiguous. Therefore this substance is assessed screening P_{aq}.
96		No significant biodegradation in 301A and C tests, but no additional reliable information. Therefore the substance is assessed with screening P_{aq}.
97		No significant biodegradation in 301B and F tests. The PBT assessment is not reliable. Therefore the substance is assessed with screening P_{aq}.
98		No significant biodegradation in 301C and D tests. Results for 302B (98% in 28 d) obtained with adapted inoculum. The PBT assessment is not reliable due to assumed non-adaption in 302B test. Therefore the substance is assessed with screening P_{aq}.
99		No significant biodegradation in 301E test, but no additional information. Therefore the substance is assessed screening P_{aq}.
100		No significant biodegradation in 301D tests. The PBT assessment was ambiguous. Therefore the substance is assessed screening P_{aq}.
101		No significant biodegradation in 301C tests. The PBT assessment was ambiguous. Therefore the substance is assessed screening P_{aq}.
102		No significant biodegradation in 301D test, but no additional information. Therefore the substance is assessed screening P_{aq}.
103		OECD 301A test implies significant biodegradation below threshold (40-50% in 28 d). Furthermore PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed screening P_{aq}.
104		OECD 301E test implies significant biodegradation below threshold (38% in 28 d). The PBT assessment is questionable and the compound is assessed screening P_{aq}.

ID	P_{aq}	Rationale
105		OECD 301A test implies significant biodegradation below threshold (54% in 28 d). For an additional test impying full degradation in 5 d preadaption cannot be excluded. The PBT assessment is thus questionable and the substance is assessed screening P_{aq}.
106		No significant biodegradation in 301C test, but no additional information. Therefore the substance is assessed screening P_{aq}.
107		Applicability of applied QSAR unclear, PBT assessment questionable. Therfore this substance is assessed worst case screening P_{aq}.
108		No significant biodegradation in 301B test, the PBT assessment (including hydrolysis products) is ambiguous. Therefore this substance is assessed with a screening P_{aq}.
109		Applied QSAR questionable. No other reliable information. Therefore the substance is assessed screening P_{aq}.
110		No significant biodegradation in 306 test, the PBT assessment is ambiguous. Therefore this substance is assessed with a screening P_{aq}.
111		No significant biodegradation in 301D test, but no additional information. Therefore the substance is assessed screening P_{aq}.
112		No significant biodegradation in 301F test. The PBT assessment was ambiguous. Therefore the substance is assessed screening P_{aq}.
113		No significant biodegradation in 301D tests. The PBT assessment was ambiguous. Therefore the substance is assessed screening P_{aq}.
114		No significant biodegradation in 301C tests. The PBT assessment was ambiguous. Therefore the substance is assessed screening P_{aq}.
115		No significant biodegradation in 301D test, but no additional information. Therefore the substance is assessed screening P_{aq}.
116		OECD 301A test implies significant biodegradation below threshold (40-50% in 28 d). Furthermore PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed screening P_{aq}.
117		OECD 301E test implies significant biodegradation below threshold (38% in 28 d). The PBT assessment is questionable and the compount is assessed screening P_{aq}.
118		OECD 301A test implies significant biodegradation below threshold (54% in 28 d). For an additional test impying full degradation in 5 d preadaption cannot be excluded. The PBT assessment is thus questionable and the substance is assessed screening P_{aq}.
119		No significant biodegradation in 301C test, but no additional information. Therefore the substance is assessed screening P_{aq}.
120		Applicability of applied QSAR unclear, PBT assessment questionable. Therfore this substance is assessed worst case screening P_{aq}.
121		No significant biodegradation in 301B test, the PBT assessment (including hydrolysis products) is ambiguous. Therefore this substance is assessed with a screening P_{aq}.
122		Applied QSAR questionable. No other reliable information. Therefore the substance is assessed screening P_{aq}.

ID	P_{aq}	Rationale
123		No significant biodegradation in 306 test, the PBT assessment is ambiguous. Therefore this substance is assessed with a screening P_{aq}.
124		No significant biodegradation in 301D test, but no additional information. Therefore the substance is assessed screening P_{aq}.
125		No significant biodegradation in 301F test. The PBT assessment was ambiguous. Therefore the substance is assessed screening P_{aq}.
126		No significant biodegradation in 301D tests. The PBT assessment was ambiguous. Therefore the substance is assessed screening P_{aq}.
127		No significant biodegradation in 301C tests. The PBT assessment was ambiguous. Therefore the substance is assessed screening P_{aq}.
128		No significant biodegradation in 301D test, but no additional information. Therefore the substance is assessed screening P_{aq}.
129		No significant biodegradation in 301C tests. Two older 302B tests (without preadaption) imply >70% DOC removal in 5 d. Due to their poor documentation level the substance is assessed with a worst case screening P_{aq}.
130		One OECD 301B test implies significant biodegradation below threshold (40-50% in 28 d), several other observe no significant biodegradation, one study expects >80% DOC removal in 28 d, but this result is questionable. The PBT assessment is questionable and the compound is assessed screening P_{aq}.
131		No significant biodegradation in 301B and D tests, but no additional information. Therefore the substance is assessed screening P_{aq}.
132		No significant biodegradation in 301F test, the PBT assessment is ambiguous. Therefore this substance is assessed with a screening P_{aq}.
133		No significant biodegradation in 301B test, the PBT assessment (including hydrolysis products) is ambiguous. Therefore this substance is assessed with a screening P_{aq}.
134		Data gap due to registration as TII (Art. 18).
135		Data gap due to registration as OSII (Art. 17).
136		ISO 7827 (301A) implies fast biodegradation, but the documentation is poor. No other information available.
137		Data gap due to registration as TII (Art. 18).
138		Data gap due to no active registration.
139		Used QSAR not applicable - substance is out of its application domain. No further information.
140		Used QSAR not applicable - substance is out of its application domain. No further information.
141		Used QSAR not applicable - substance is out of its application domain. No further information.
142		Used QSAR not applicable - substance is out of its application domain. No further information.

ID	P_{aq}	Rationale
143		Used QSAR not applicable - substance is out of its application domain. No further information.
144		Data gap due to registration as OSII (Art. 17).
145		Despite no reliable tests are available, this substance is assessed to be not persistent according to expert judgement.
146		The substance is assessed to be not persistent due to positive 301A and 302B tests.
147		The substance is assessed to be not persistent due to positive 301A and D tests.
148		OECD tests (301B and D) for surrogate imply no persistence. Therefore the substance is assessed not to be persistent.
149		The substance hydrolyzes fast in water. Main hydrolysis product (EC No. 202-830-0) is readily biodegradable. Therefore this substance is assessed to be not persistent.
150		The substance is assessed to be not persistent due to positive 301A test.
151		The substance shows significant biodegradation above the threshold in a OECD 306 sea water test. The threhold is reached in an early stage of the test, therefore it can be expected that the substance would also degrade in freshwater. Used QSAR not applicable - substance is out of its application domain. Therefore the substance is assessed not to be persistent.
152		The substance shows significant biodegradation above the threshold in a OECD 306 sea water test. The threhold is reached in an early stage of the test, therefore it can be expected that the substance also would be degraded in freshwater. Used QSAR not applicable - substance is out of its application domain. Therefore the substance is assessed not to be persistent.
153		The substance is assessed to be not persistent due to positive 301F test.
154		OECD tests (301B and E) for surrogate imply no persistence. Therefore the substance is assessed not to be persistent.
155		Several OECD 301 studies imply this substance not to be persistent. Therefore the substance is assessed not to be persistent.
156		Several read-across studies including 301B and 301D tests imply no persistence. Therefore the substance is assessed not to be persistent.
157		Several read-across studies including 301B and D tests imply no persistence. Therefore the substance is assessed not to be persistent.
158		No significant biodegradation in 301C and D tests, but nearly complete biodegradation in 302B test. Therefore the substance is assessed not to be persistent.
159		The substance is assessed to be not persistent due to positive 301D test.
160		The substance is assessed to be not persistent due to positive 301E and D tests.
161		Results from enhanced ready test enable the conclusion that the substance is not persistent in water.
162		This substance hydrolyses depending on pH (slowly in acidic, fast in alcaline conditions). The main hydrolysis products (CS2 and isopropyl alcohol) are both readily biodegradable. Hy-

ID	P_{aq}	Rationale
		drolysis tests with applied surrogates are reasonable despite both hydrolysis and biodegradation will be slower for this substance than for the applied surrogates. Applied 301A test with unspecified adaption is documented well. Main biotransformation products are similar for those of hydrolysis. 302B Tests with surrogates and non adaption implying fast degradation are also reasonable, despite inoculum from industry. For these reasons this substance is assessed to be not persistent.
163		Results from enhanced ready test enable the conclusion that the substance is not persistent.
164		The substance is assessed to be not persistent due to positive 301C test.
165		The substance is assessed to be not persistent due to positive 301B tests.
166		The substance is assessed to be not persistent due to positive 301D and 302B tests.
167		Several 301 tests imply no persistence. Therefore the substance is assessed not to be persistent.

Table 4: Weight of evidence for mobility in the aquatic environment (M) for all 167 substances. For the substance ID see Table 2. The color shows the result of the assessment according to the traffic-light color scheme.

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
1		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	1.61	LSER exp. parameter		7900	
2		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.46	LSER exp. parameter		150	
3		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.08	LSER exp. parameter		1100	
4		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	0.55	OECD 121		650	esti-mated from wt%
5		log Koc (exp) <4.5 OECD 106 and SW (exp) >0.15 mg/l	in	no	2.00	OECD 106		700000	
6		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	0.8	LSER exp. parameter		1000000	
7		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.3	OECD 121		370	
8		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.14	LSER exp. parameter		8240	
9		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	1.53	LSER calc. parameter		216000	
10		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	0.72	LSER calc. parameter		3160	
11		log Koc (calc) <4,5 and SW (handbook data) >0,15 mg/l	in	no	0.38	LSER exp. parameter		32000	hand-book data
12		log Koc (exp) <4,5 OECD 106 and SW (exp) >0,15 mg/l	in	yes	4	OECD 106		48200	
13		log Koc (exp) <4,5 OECD 106 and SW (exp) >0,15 mg/l	in	no	2.24	OECD 106	read across grouping approach	1080	

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
14		log Koc (exp) <4,5 OECD 121 and SW (exp) >0,15 mg/l	in	no	1.40	OECD 121		300	
15		log Koc (exp) <4,5 OECD 121 and SW (exp) >0,15 mg/l	in	no	1.4	OECD 121		23653	
16		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	2.85	LSER calc. parameter		1700	
17		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	0.82	LSER calc. parameter		335000	
18		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	1.19	LSER calc. parameter		629300	
19		log Koc (exp) <4,5 OECD 106 and SW (calc) >0,15 mg/l	in	yes	-1.3	OECD 106		1000000	
20		log Koc (exp) <4,5 OECD 121 and SW (exp) >0,15 mg/l	in	no	1.76	OECD 121		380	
21		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	3.4	OECD 121		10	
22		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	2.53	LSER calc. parameter		392	average value
23		log Koc (exp) <4,5 OECD 121 and SW (exp) >0,15 mg/l	in	no	2.2	OECD 121	average value	1000000	or higher
24		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	3.09	LSER calc. parameter		1.1	average
25		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	2.1	LSER calc. parameter		4600	
26		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	1.72	LSER calc. parameter		277500	
27		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	1.25	OECD 121	or lower value	1000000	set value, the sub-stance is miscible

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
									with water in all proportions
28		log Koc (calc) <4,5 and SW (handbook data) >0,15 mg/l	in	no	1.06	LSER calc. parameter		11200	handbook data
29		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	in	no	1.68	LSER exp. parameter		1600	
30		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	1.09	OECD 121		739000	
31		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	2.23	LSER exp. parameter		175	
32		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	1.92	LSER calc. parameter		492000	or higher
33		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	3.47	LSER calc. parameter parent structure		1.3	
34		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	0.51	LSER calc. parameter		100000	or higher
35		log Koc <or >4,5, depending on estimating method and SW (exp) >0,15 mg/l	in	no	5.29	LSER calc. parameter	log Koc in dossier 4,1356 (calculated with MCI)	10	or lower
36		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	1.66	LSER calc. parameter		667000	
37		log Koc (exp) <4,5 OECD 121 and SW (exp) >0,15 mg/l	out	yes	0.07	OECD 121	read across with EC 286-384-2	270000	
38		log Koc (calc) <4,5 and SW (exp) <or >0,15	out	yes	1.98	LSER calc. parameter		0.0029	calc value: 206700

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
		mg/l depending on estimated or experimental SW							
39		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	1.41	LSER calc. parameter		1000000	set value, the substance is miscible with water in all proportions
40		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	1.16	LSER calc. parameter		1000000	set value, the substance is miscible with water in all proportions
41		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	0.99	LSER calc. parameter		500000	or higher
42		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	0.86	LSER calc. parameter parent structure		237000	
43		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	1.23	LSER calc. parameter		27800	
44		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	0.67	LSER calc. parameter		1000000	set value, the substance is miscible with water in all proportions
45		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	1.99	LSER calc. parameter		242000	

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
						parent structure			
46		log Koc (exp) <4,5 OECD 121 and SW (exp) >0,15 mg/l	out	yes	1.26	OECD 121		523000	
47		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	1.78	LSER calc. parameter		10000	or lower
48		log Koc (exp) <4,5 OECD 121 and SW (exp) >0,15 mg/l	out	yes	4.07	OECD 121	average value	570000	or higher
49		log Koc (exp) <4,5 OECD 121 and SW (exp) >0,15 mg/l	out	yes	1.8	OECD 121	mean of 25% and 75% peak	1000000	set value, the substance is miscible with water in all proportions
50		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	3.66	LSER calc. parameter parent structure		9800	
51		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	2.27	LSER calc. parameter		313700	
52		log Koc (exp) <4,5 OECD 121 and SW (exp) >0,15 mg/l	out	yes	1.32	OECD 121	or lower value	703600	
53		log Koc (exp) <4,5 OECD 121 and SW (exp) >0,15 mg/l	out	yes	1.25	OECD 121	or lower value; at PH7 log Koc in domain	1000000	or higher
54		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	3.69	LSER calc. parameter parent structure		4200	

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
55		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	no info.	2.01	MCI		300	
56		log Koc <or >4,5, depending on estimating method and SW (exp) >0,15 mg/l	in	no	4.76	LSER calc. parameter	log Koc dossier 4,1359 (MCI)	90	
57		log Koc (calc) <4,5 and SW (calc) >0,15 mg/l	out	no	2.78	MCI		280000	
58		log Koc (calc) <4,5 and SW (exp) >0,15 mg/l	out	yes	3.36	LSER calc. parameter		770000	
59		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.19	LSER calc. parameter parent structure		74150	
60		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.6	LSER calc. parameter parent structure		32000	
61		log Koc (calc) >4.5 and SW (exp) <0.15 mg/l	in	no	6.23	LSER calc. parameter parent structure		0.0065	average database value read-across and WOE
62		log Koc (exp) >4.5 OECD 121 and SW (exp) <0.15 mg/l	in	no	5.63	OECD 121	or higher	0.005	
63		log Koc <or >4.5. depending on estimating method and SW (exp) <0.15 mg/l	out	yes	5.36	LSER calc. parameter		0.01	or lower
64		log Koc (calc) >4.5 and SW (exp) <0.15 mg/l	out	no	4.7	Dossier value		0.01	or lower
65		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	3.07	LSER exp. parameter		31.7	
66		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	1.44	LSER exp. parameter		20000	

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
67		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.63	LSER exp. parameter		1000	
68		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.82	LSER calc. parameter		2300	esti-mated from wt%
69		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.58	LSER calc. parameter		3500	
70		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	1.87	LSER exp. parameter		1500	
71		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	1.09	LSER calc. parameter		40200	
72		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	1.39	LSER exp. parameter		429000	
73		log Koc (exp) <4.5 OECD 106 and SW (exp) >0.15 mg/l	in	yes	2.63	OECD 106		345000	
74		log Koc (exp) <4.5 OECD 106 and SW (exp) >0.15 mg/l	in	no	2.29	OECD 106		204	
75		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.37	LSER exp. parameter		1200	
76		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	0.8	LSER exp. parameter		1000000	or higher
77		log Koc (calc) <4.5 and SW (handbook data) >0.15 mg/l	in	no	-1.4	LSER calc. parameter		813000	hand-book data
78		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	1.85	LSER calc. parameter		1000000	set value, the sub-stance is miscible with wa-ter in all propor-tions
79		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	0.47	LSER calc. parameter		572000	

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
80		log Koc (exp) <4.5 OECD 106 and SW (exp) >0.15 mg/l	in	yes	2.86	OECD 106	average value	325	
81		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.33	LSER calc. parameter		1000000	
82		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.74	LSER calc. parameter		1930	
83		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	0.96	LSER exp. parameter		263000	
84		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	0.74	LSER calc. parameter		102000	
85		log Koc (exp) <4.5 OECD 121 and SW (exp) >0.15 mg/l	in	no	1.56	OECD 121		3574	
86		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	3.35	LSER calc. parameter		230	average data
87		log Koc (exp) <4.5 OECD 106 and SW (exp) >0.15 mg/l	in	yes	0.90	OECD 106		1090	
88		log Koc (exp) <4.5 OECD 121 and SW (exp) >0.15 mg/l	in	no	1.24	OECD 121		5030	
89		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	-2.1	LSER calc. parameter		1000000	or higher
90		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.99	LSER calc. parameter		1400	
91		log Koc (calc) <4.5 and SW (calc) >0.15 mg/l	in	no	0.74	LSER calc. parameter		3693	
92		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	1.68	LSER exp. parameter		5100	
93		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	4.12	LSER calc. parameter		15	
94		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.92	OECD 121	at PH7 log Koc in domain	12	

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
95		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	0.09	LSER calc. parameter parent structure		781100	
96		log Koc (calc) <4.5 and SW (calc) >0.15 mg/l	out	no	2.95	Dossier value		190300	
97		log Koc (exp) <4.5 OECD 121 and SW (exp) >0.15 mg/l	out	yes	1.19	OECD 121		32	
98		log Koc (exp) <4.5 OECD 121 and SW (exp) >0.15 mg/l	out	yes	0.5	OECD 121		17195	
99		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.74	LSER calc. parameter	at PH7 log Koc in domain	1100	
100		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1	LSER exp. parameter		1154000	
101		log Koc <or >4.5. de-pending on estimating method and SW (exp) >0.15 mg/l	in	no	2.05	LSER calc. parameter	log Koc from dos-sier 4,562 (no method specified)	15	
102		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.94	LSER calc. parameter parent structure		242500	average of exper-iments
103		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.34	LSER calc. parameter		850000	or higher
104		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.34	LSER exp. parameter parent structure		750000	
105		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.85	LSER calc. parameter		821000	
106		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	0.99	LSER calc. parameter		1000000	

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
						parent structure			
107		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.29	LSER calc. parameter	at PH7 log Koc in domain	1774	
108		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	0.5	LSER exp. parameter		12510	
109		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.6	LSER calc. parameter		610000	
110		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	-0.0	LSER calc. parameter parent structure		146000	
111		log Koc <or >4.5. depending on estimating method and SW (exp) >0.15 mg/l	out	yes	5.18	LSER calc. parameter		1760	
112		log Koc (calc) <4.5 and SW (calc) >0.15 mg/l	out	yes	0.37	LSER calc. parameter parent structure		1000000	
113		log Koc (exp) <4.5 OECD 121 and SW (exp) >0.15 mg/l	out	yes	1.41	OECD 121		1000000	set value, the substance is miscible with water in all proportions
114		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	3.56	LSER calc. parameter parent structure		187.7	
115		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.53	LSER calc. parameter parent structure		1000000	or higher

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
116		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	-0.0	LSER calc. parameter		1604000	or higher
117		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.91	LSER calc. parameter		70	
118		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	3.12	LSER calc. parameter	at PH7 log Koc in domain	5.95	
119		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	no	1.48	MCI		800000	or higher (soluable at least 80% with water)
120		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.03	LSER calc. parameter		15000	
121		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	0.44	Dossier value		3000	
122		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	0.72	LSER calc. parameter parent structure		7.7	
123		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.77	LSER calc. parameter		513	
124		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	0.71	LSER calc. parameter		1000000	set value, the sub-stance is miscible with wa-ter in all propor-tions
125		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	3.36	LSER calc. parameter		143.33	
126		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	0.82	LSER calc. parameter		17200	
127		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	3.12	LSER calc. parameter		4040	

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
						parent structure			
128		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.69	LSER calc. parameter		1900	
129		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.42	LSER calc. parameter parent structure		336000	
130		log Koc (exp) >4.5 OECD 121 and SW (calc) >0.15 mg/l	out	yes	5.5	OECD 121	at PH7 log Koc in domain	1.2	
131		log Koc (exp) <4.5 OECD 106 and SW (exp) <0.15 mg/l	in	no	3.39	OECD 106		0.008	or lower
132		log Koc (calc) >4.5 and SW (exp) <0.15 mg/l	in	no	5.44	LSER calc. parameter		0.01048	
133		log Koc (exp) >4.5 OECD 121 and SW (exp) <0.15 mg/l	in	no	5.63	OECD 121	or higher	0.005	
134		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	-0.2	LSER exp. parameter		3900	
135		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	4.38	LSER exp. parameter		1000	
136		log Koc (calc) <4.5 and SW (calc) >0.15 mg/l	out	yes	1.2	LSER calc. parameter parent structure		11600	read across from parent structure
137		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	-0.2	LSER exp. parameter		3900	
138		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	4.38	LSER exp. parameter		1000	
139		log Koc (calc) <4.5 and SW (calc) >0.15 mg/l	out	yes	1.2	LSER calc. parameter parent structure		11600	read across from parent structure

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
140		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	-0.2	LSER exp. parameter		3900	
141		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	4.38	LSER exp. parameter		1000	
142		log Koc (calc) <4.5 and SW (calc) >0.15 mg/l	out	yes	1.2	LSER calc. parameter parent structure		11600	read across from parent structure
143		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	-0.2	LSER exp. parameter		3900	
144		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	4.38	LSER exp. parameter		1000	
145		log Koc (calc) <4.5 and SW (handbook data) >0.15 mg/l	in	no	0.62	LSER exp. parameter parent structure		370000	hand-book data
146		log Koc (calc) <4.5 and SW (calc) >0.15 mg/l	in	no	0.92	LSER calc. parameter		52100	
147		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	0.13	LSER calc. parameter		1000000	or higher
148		log Koc (exp) <4.5 OECD 106 and SW (exp) >0.15 mg/l	in	no	3	OECD 106	read across grouping approach	7	
149		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	2.56	LSER calc. parameter		19	
150		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	in	no	1.5	LSER calc. parameter		1000000	or higher
151		log Koc (exp) <4.5 OECD 121 and SW (exp) >0.15 mg/l	in	no	1.25	OECD 121		234000	
152		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.12	LSER calc. parameter	at PH7 log Koc in domain	320000	

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
153		log Koc (exp) <4.5 OECD 121 and SW (exp) >0.15 mg/l	out	yes	3.6	OECD 121		424000	
154		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.33	LSER calc. parameter		354000	
155		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	3.64	LSER calc. parameter parent structure		8170	
156		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	0.9	LSER calc. parameter		1154000	
157		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.66	LSER calc. parameter		1156000	
158		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.01	LSER exp. parameter		12000	
159		log Koc (exp) <4.5 OECD 121 and SW (exp) >0.15 mg/l	out	yes	-1.8	OECD 121		5390	
160		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.32	LSER calc. parameter parent structure		1110.2	
161		log Koc (calc) <4.5 and SW (calc) >0.15 mg/l	out	no	1.68	Dossier value		1059000	
162		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	2.26	LSER calc. parameter parent structure		350000	
163		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	0.23	LSER calc. parameter		1000000	set value, the substance is miscible with water in all proportions

ID	M	Rationale	Domain log Koc (in/out)	ionic/ionizable pH 6-8 (yes/no)	log Koc	log Koc method	log Koc re-marks	SW [mg/l]	SW remarks
164		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.26	LSER calc. parameter parent structure		866899	read across value from CAS: 105-60-2
165		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	no	3.49	MCI		400000	or higher
166		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	no info.	-0.2	LSER calc. parameter parent structure		1000	set value, due to very high solubility in water
167		log Koc (calc) <4.5 and SW (exp) >0.15 mg/l	out	yes	1.66	LSER calc. parameter parent structure		664000	

Table 5: Weight of evidence for toxicity (T) for all 167 substances. For the substance ID see Table 2. The color shows the result of the assessment according to the traffic-light color scheme.

ID	T	Rationale
1		carcinogenicity category 1B
2		carcinogenicity category 2
3		carcinogenicity category 1B
4		mutagenicity category 2 and reproduction toxicity category 2
5		reproduction toxicity category 2
6		carcinogenicity category 2
7		reproduction toxicity category 2
8		carcinogenicity category 1B
9		Cramer class III
10		structural alert thyroid, estrogenic/androgenic, mutagenicity and carcinogenicity
11		Cramer class III
12		structural alert thyroid, estrogenic/androgenic, mutagenicity and carcinogenicity (out of domain)
13		structural alert thyroid, mutagenicity and carcinogenicity
14		structural alert thyroid, estrogenic/androgenic and mutagenicity and carcinogenicity
15		Cramer class III and structural alert androgenic (out of domain)
16		Cramer class III and structural alert thyroid, estrogenic (out of domain) and androgenic (out of domain)
17		Cramer class III
18		Cramer class III
19		structural alert mutagenicity and Cramer class III
20		structural alert mutagenicity and carcinogenicity
21		significant hints on reproduction toxicity (maternal toxicity) in detailed dossier analysis (cut-off value failed)
22		significant hints on reproduction toxicity (maternal toxicity) in detailed dossier analysis (cut-off value failed)
23		Cramer class III
24		Cramer class III and structural alert estrogenic (out of domain), mutagenicity (out of domain)
25		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
26		Cramer class III and structural alert estrogenic/androgenic (partly out of domain), mutagenicity and carcinogenicity (out of domain)
27		Cramer class III and structural alert carcinogenicity and mutagenicity (out of domain)

ID	T	Rationale
28		structural alert thyroid, estrogenic/androgenic and mutagenicity and carcinogenicity
29		structural alert carcinogenicity and Cramer class III
30		STOT RE category 2
31		reproduction toxicity category 2
32		Cramer class III
33		structural alert thyroid, estrogenic/androgenic and mutagenicity and carcinogenicity
34		structural alert mutagenicity and Cramer class III
35		structural alert mutagenicity and Cramer class III
36		structural alert androgenic, carcinogenicity and mutagenicity
37		structural alert mutagenicity and carcinogenicity
38		structural alert thyroid and androgenic (out of domain) and Cramer class III
39		structural alert miconucleus assay and Cramer class III
40		structural alert miconucleus assay and Cramer class III
41		Cramer class III
42		structural alert mutagenicity and carcinogenicity (out of domain) and Cramer class III
43		structural alert mutagenicity and Cramer class III
44		structural alert mutagenicity and Cramer class III
45		structural alert androgenic (out of domain), carcinogenicity and mutagenicity
46		Cramer class III
47		structural alert thyroid and androgenic (out of domain)
48		structural alert mutagenicity and Cramer class III
49		structural alert mutagenicity and Cramer class III
50		Cramer class III and structural alert estrogenic/androgenic (partly out of domain) and mutagenicity (out of domain)
51		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
52		Cramer class III and structural alert mutagenicity (out of domain)
53		structural alert mutagenicity and Cramer class III
54		structural alert thyroid, estrogenic/androgenic and mutagenicity and carcinogenicity
55		structural alert mutagenicity and carcinogenicity
56		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
57		Cramer class III
58		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
59		Cramer class II, no aquatic toxicity class

ID	T	Rationale
60		Cramer class I despite a structural alert androgenic (out of domain), no aquatic toxicity class
61		structural alert thyroid and Cramer class III
62		structural alert thyroid and carcinogenicity
63		structural alert carcinogenicity, mutagenicity (out of domain) and Cramer class III
64		structural alert androgenic (out of domain), carcinogenicity and mutagenicity (out of domain) and Cramer class III
65		carcinogenicity category 2
66		STOT RE category 2
67		carcinogenicity category 1B, mutagenicity category 2, STOT RE category 2
68		STOT RE category 2
69		STOT RE category 2
70		STOT RE category 2
71		STOT RE category 1
72		mutagenicity category 2
73		mutagenicity category 2
74		toxicity in PBT assessment based on ecotoxicity criterion
75		carcinogenicity category 2
76		STOT RE category 1
77		Cramer class III
78		structural alert mutagenicity and carcinogenicity
79		structural alert thyroid, mutagenicity and Cramer class III
80		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
81		Cramer class III
82		structural alert estrogenic (out of domain), carcinogenicity and mutagenicity (out of domain) and Cramer class III
83		significant hints on reproduction toxicity (maternal toxicity) in detailed dossier analysis (cut-off value failed)
84		structural alert mutagenicity and carcinogenicity (out of domain) and Cramer class III
85		Cramer class III and structural alert carcinogenicity (out of domain)
86		structural alert androgenic (out of domain), mutagenicity and Cramer class III
87		Cramer class III and structural alert carcinogenicity (out of domain)
88		structural alert androgenic, mutagenicity and carcinogenicity
89		structural alert thyroid, mutagenicity and carcinogenicity (out of domain)

ID	T	Rationale
90		Cramer class III and structural alert mutagenicity (out of domain)
91		Cramer class III
92		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
93		read-across NOEC fish meeting T criterion chronic aquatic ecotoxicity of cat. 1
94		evidence of endocrine effects and structural alerts for estrogenic, androgenic and thyroid as well as for carcinogenicity and mutagenicity
95		reproduction toxicity category 2
96		mutagenicity category 2
97		reproduction toxicity category 2 and STOT RE category 2
98		carcinogenicity category 2
99		mutagenicity category 2
100		Cramer class III
101		structural alert estrogenic (out of domain), mutagenicity and Cramer class III
102		structural alert thyroid and Cramer class III
103		structural alert estrogenic/androgenic
104		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
105		Cramer class III
106		structural alert mutagenicity and carcinogenicity (out of domain) and Cramer class III
107		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
108		Cramer class III
109		structural alert miconucleus assay and Cramer class III
110		structural alert mutagenicity (out of domain) and Cramer class III
111		Cramer class III
112		Cramer class III
113		Cramer class III
114		Cramer class III
115		structural alert thyroid and Cramer class III
116		Cramer class III
117		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
118		structural alert estrogenic/androgenic (partly out of domain) and Cramer class III
119		structural alert mutagenicity and carcinogenicity
120		Cramer class III
121		Cramer class III

ID	T	Rationale
122		Cramer class III
123		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
124		Cramer class III
125		significant hints on reproduction toxicity in detailed dossier analysis (cut-off value failed)
126		structural alert mutagenicity and Cramer class III
127		endocrine structural alert (androgenic) (out of application domain) and Cramer class III
128		endocrine structural alert (androgenic) and Cramer class III
129		Cramer class I, no aquatic toxicity class
130		Cramer class III
131		Cramer class III
132		structural alert carcinogenicity (out of domain) and Cramer class III
133		structural alert carcinogenicity and Cramer class III
134		Cramer class III
135		Cramer class III
136		Cramer class III
137		structural alert mutagenicity
138		Cramer class III
139		structural alert thyroid and estrogenic/androgenic
140		Cramer class III
141		Cramer class III
142		structural alert carcinogenicity (out of domain) and Cramer class III
143		structural alert thyroid and estrogenic/androgenic
144		Cramer class III
145		STOT RE category 1
146		carcinogenicity category 2, STOT RE category 2
147		STOT RE category 2
148		STOT RE category 2
149		structural alert mutagenicity and carcinogenicity
150		Cramer class III
151		structural alert mutagenicity and carcinogenicity (out of domain) and Cramer class III
152		STOT RE category 2
153		reproduction toxicity category 1B

ID	T	Rationale
154		structural alert thyroid and androgenic
155		Cramer class III and structural alert carcinogenicity (out of domain)
156		structural alert estrogenic/androgenic
157		structural alert androgenic and carcinogenicity
158		Cramer class III
159		Cramer class III
160		structural alert mutagenicity and Cramer class III
161		structural alert mutagenicity and carcinogenicity
162		Cramer class III
163		structural alert mutagenicity and Cramer class III
164		Cramer class III
165		Cramer class III
166		structural alert mutagenicity and Cramer class III
167		Cramer class I, no aquatic toxicity class