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REACH: Improvement of guidance and methods for the identification and assessment of PMT/vPvM substances

by

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Abstract

There are substances with a specific combination of intrinsic substance properties that cause them to pose an inherent hazard to remote aquatic environments and the sources of our drinking water. These are substances that are very persistent in the environment and very mobile in the aquatic environment (vPvM); or, substances that are persistent in the environment, mobile in the aquatic environment and toxic (PMT). A review of substances detected in drinking water and groundwater found that 43% of them are REACH registered. Further, REACH registered substances were the most likely to be found at higher concentrations (above 0.1 µg/L). The German Environment Agency (UBA) has over several years, and most recently via this project, further discussed, developed, justified and decided upon the proposed criteria for identifying PMT and vPvM substances in the regulatory context of the EU REACH Regulation (EC) No 1907/2006 (Neumann and Schliebner, 2019). To assist implementation of these criteria, this report presents updated guidelines to prospectively or retrospectively use the REACH registration process to identify PMT/vPvM substances. Special considerations for data uncertainty are presented via the implementation of a "traffic light" system. The guidance was applied to all 15469 REACH registered substances as of May 2017. Of these, 260 met the PMT/vPvM criteria (Red), 224 met the PM criteria (Dark Yellow), 2377 had screening or low-quality data requiring further investigation (Yellow), 3665 did not meet the PMT/vPvM criteria (Green) and 3216 had insufficient data to make a conclusion (White). The list of PMT/vPvM substances is provided and discussed in terms of monitoring data, emission likelihood and current restrictions or regulations. Of the complete list, 122 chemical constituents are prioritized for further investigation to assess the need for introducing risk management measures. Without acting, the cost of clean-up and drinking water purification in Europe could be well into several billions of Euros.

Kurzbeschreibung

Es gibt Stoffe mit einer spezifischen Kombination von intrinsischen Stoffeigenschaften, die dazu führen, dass sie eine inhärente Gefahr für die entlegene aquatische Umwelt und die Quellen unserer Trinkwässer darstellen; dies sind Stoffe die in der Umwelt sehr persistent und in der aquatischen Umwelt sehr mobil sind (vPvM) oder die sowohl persistent, mobil und toxisch sind (PMT). Eine Auswertung der Literatur über im Trinkwasser und im Grundwasser nachgewiesene Stoffe ergab, dass 43% der nachgewiesenen Chemikalien unter REACH registrierte Stoffe sind. Unter denen, die bei höheren Konzentrationen (über 0,1 µg/L) nachgewiesen wurden, waren noch häufiger REACH-registrierte Stoffe. Das Umweltbundesamt (UBA) hat über viele Jahre und zuletzt mit Unterstützung durch dieses Vorhaben die im Rahmen der EU-Verordnung REACH (EG) Nr. 1907/2006 vorgeschlagenen Kriterien zur Identifizierung von PMT/vPvM-Stoffen weiter diskutiert, entwickelt, begründet und abgestimmt (Neumann and Schliebner, 2019). Zur Unterstützung der Anwendung der Kriterien werden durch diesen Bericht aktualisierte Leitlinien vorgestellt, um den REACH-Registrierungsprozess prospektiv oder retrospektiv zur Identifizierung von PMT/vPvM-Stoffen zu nutzen. Besondere Überlegungen zur Datenunsicherheit werden durch die Implementierung eines "Ampelsystems" angestellt. Die Leitlinien wurden angewendet auf alle 15469 bis Mai 2017 unter REACH registrierten Stoffe. Davon erfüllten 260 die PMT/vPvM-Kriterien (Rot), 224 die PM-Kriterien (Dunkelgelb), 2377 hatten nur Screeningdaten oder unsichere Daten, die einer weiteren Bewertung bedürfen (Gelb); 3665 erfüllten nicht die PMT/vPvM-Kriterien (Grün) und 3216 hatten unzureichende Daten, um eine Schlussfolgerung zu ziehen (Weiß). Die Liste der PMT/vPvM-Stoffe wird mit Bezug auf Monitoringdaten, Emissionswahrscheinlichkeit und vorliegenden Regulierungen präsentiert und diskutiert. Von der vollständigen Liste werden 122 Stoffe für eine weitergehende Bewertung priorisiert, um die Notwendigkeit der Einführung von Risikomanagementmaßnahmen zu beurteilen. Nicht-Handeln könnte in Europa zu Sanierungs- und Trinkwasseraufbereitungskosten in Höhe von mehreren Milliarden Euro führen.

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List of Abbreviations

CLP	Regulation 1272/2008/EC on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006
CMR	Carcinogenic, mutagenic, toxic for reproduction
DNEL	Derived no effect level
DT50	The half-life of a substance in soil
E-score	Emission-score
EC10	Concentration of a chemical that shows effects for 10% of the test animals
ECHA	European Chemicals Agency
InChI	International Chemical Identifiers
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 criterion
OECD	Organization for Economic Co-operation and Development
P	Persistent criterion
PBT	Persistent, bioaccumulative and toxic
NGI	Norwegian Geotechnical Institute
NOEC	No observed effect concentration
PM	Persistent and mobile in the aquatic environment
PMT	Persistent, mobile and toxic
PMT/vPvM	Persistent, mobile and toxic or very persistent, very mobile
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)
RMM	Risk management measures
SMILES	Simplified molecular-input line-entry system
STOT RE	Specific target organ toxicity - repeat exposure
T	Toxicity criterion
TPA	Tonnes per annum
UBA	The German Environment Agency (*Umweltbundesamt*)
UNEP	United Nations Environment Program
UC	Use Characteristic
UVCB	Substances of "Unknown or Variable composition, Complex reaction products or Biological material"
vP	Very persistent criterion
vM	Very mobile criterion
vPvB	Very persistent, very bioaccumulative
vPvM	Very persistent, very mobile

Summary

The German Environment Agency (UBA) has over several years, and most recently via the support of this project, further discussed, developed, justified and decided upon proposed criteria for identifying Persistent, Mobile and Toxic (PMT) substances and very Persistent, very Mobile (vPvM) substances in the regulatory context of the EU REACH Regulation (EC) No 1907/2006 (Neumann and Schliebner, 2019). PMT/vPvM substances are those which have the intrinsic substance properties that indicate they would pose a hazard to the sources of our drinking water if released into the environment. Herein the phrase "sources of our drinking water" refers to pristine and sometimes remote freshwater ecosystems, surface water reservoirs, water that undergoes bank filtration, groundwater aquifers or other aquatic environments that could potentially be used as a drinking water source. Using these criteria (Neumann & Schliebner, 2019), REACH registrants are able to assess, based on the intrinsic substance properties of their substances, whether they are PMT/vPvM. Depending on their uses and emissions, registrants could implement risk mitigation measures to precautionarily prevent pollution of PMT/vPvM substances. Proper management of PMT/vPvM substances and chemical safety over the complete life-cycle can be achieved by chemical stewardship programs. If necessary, authorities could implement regulatory measures to minimize emissions and to protect the valuable water resources for future generations.

This project addressed the following five working areas:

1) Compilation of monitoring data of chemicals detected in drinking water and groundwater
2) Scientific information for identifying and justifying the final M/vM criteria
3) Guidelines for conducting a PMT/vPvM assessment
4) A PMT/vPvM assessment of all substances registered under REACH (as of May 2017)
5) Impact assessment of implementing the PMT/vPvM criteria

The main outcomes of these five working areas are summarized below.

1) Compilation of monitoring data of chemicals detected in drinking water and groundwater

To demonstrate the need for developing PMT/vPvM criteria under REACH, a literature review was conducted to compile monitoring data of chemicals that have been detected in drinking water and groundwater. This review comprised of 25 studies, including many previous compilations, between 2000 and 2018. In total, 333 chemicals were identified, of which 246 were detected in drinking water and 187 were detected in groundwater, with 100 detected in both. This review can be considered a representative but by no means exhaustive list of all substances that have ever been detected in drinking water or groundwater. Of these 333 chemicals, 142 (43%) corresponded to substances that were registered under REACH (as of May 2017) of which 32 are also used as pharmaceuticals and 5 are also used as pesticides. The REACH registered substances comprise 113 (46%) of the 246 total drinking water contaminants and 75 (40%) of the 187 total groundwater contaminants. It can therefore be considered as a fact that a substantial portion of drinking water and groundwater contaminants are substances registered under REACH. This random collection of analytical data indicated that REACH registered substances are detected at higher concentrations. Only 40% (76 of 191) of the non-REACH registered substances exceed 0.1 µg/L, while 58% (83 of 142) of the detected REACH registered substances exceed this concentration level (Figure 2). These results clearly demonstrate the need for the

development of the PMT/vPvM criteria for substances registered under REACH, and for these criteria to be applied in order to protect the sources of our drinking water.

2) Scientific information identifying and justifying the final M/vM criteria

The PMT/vPvM criteria were developed through both scientific investigations and consultations at various meetings with experts and stakeholders (Neumann and Schliebner, 2019). A specific contribution from this project was to provide underlying scientific data and information that could be used to both identify and ultimately justify the final mobile criterion (M) and very mobile criterion (vM).

There has been consensus in the scientific literature since the 1980s that mobility of organic substances in the subsurface is driven by a combination of the intrinsic chemical properties of persistence and sorption to soil, the latter of which is generally best quantified by the organic carbon-water partition coefficient (K_{OC}) (Gustafson, 1989). From a practical point of view, K_{OC} is an intrinsic substance property that is readily available for many substances, or otherwise can be derived through standard laboratory methods, or monitoring and modelling simulations.

After the scientific investigations and consultations, the cut-off for vM was set to a log K_{OC} of less than 3.0 (Neumann and Schliebner, 2019). This is well supported in the scientific literature to be protective of groundwater (see section 6.1) and is currently utilized by the Groundwater Watch List coordinated by the EU Common Implementation Strategy Working Group Groundwater for identifying potential groundwater contaminants. The cut-off for M was set to a log K_{OC} of less than 4.0 (Neumann and Schliebner, 2019). This report demonstrates that such a high value of the M cut-off criteria is necessary to be protective of riverbank infiltration regarding P/vP substances. Both cut-off values are supported by empirical observations using the compilation of detected REACH-registered substances in drinking water and groundwater in this report, for which log K_{OC} data was available (n=88). Here all substances met the vM criterion except for 13% which met the M criterion, and 6% which were not mobile. The M/vM criteria are therefore considered to provide a reasonable level of protection of the sources of our drinking water.

When a K_{OC} value is not available, a screening cut-off of the lowest pH-dependent octanol-water partition coefficient, log D_{OW}, of less than 4.5 was set (Neumann and Schliebner, 2019). The log D_{OW} value of < 4.5 for the screening criteria for mobility (M) is justified based on correlations with log K_{OC}. It is also a practical parameter because of its integration with the screening criteria for bioaccumulation (B), as part of the PBT/vPvB assessment under REACH. For neutral molecules, the log D_{ow} value is equal to the log K_{ow} value. In this manner, P/vP substances having a log D_{ow} (or log K_{ow}) above 4.5 should be assessed for B, and those below should be assessed for M. Empirical justifications of these cut-offs are evident through the comparisons with the results of the literature review of REACH registered substances detected in drinking water and groundwater, and presented in Section 6.1 (Figure 6 and Figure 8).

3) Guidelines for conducting a PMT/vPvM assessment

Guidelines were developed for the P/vP, M/vM and T assessment. These guidelines are presented in a way that could be used prospectively for new substances or retrospectively for existing REACH registered substances. A central part of these guidelines is how to account for data quality, and the ability to assess, based on data quality, that there is sufficient weight of evidence to draw a conclusion related to the P, M or T assessment. Therefore, a "traffic light" colour scheme was introduced to account for data uncertainty with the following colour categories:

White – insufficient data for the PMT/vPvM assessment.

Dark red or red – data indicate that the substance meets the PMT/vPvM criteria;

Dark yellow or yellow- data indicate that the substance is suspected of meeting the PMT/vPvM criteria;

Green – data indicate that the substance does not meet the PMT/vPvM criteria;

Seven different final conclusions from the PMT/vPvM assessment can result, depending on which criteria are met and their relative degree of certainty.

No conclusions possible – Either data for a P or M assessment at the screening level is lacking (White). Efforts should be made to obtain appropriate screening data.

PMT & vPvM - Indicates there is sufficient weight of evidence that the substance meets both the vP and vM criteria as well as the T criterion (Dark red).

vPvM - Indicates there is sufficient weight of evidence that the substance meets both the vP and vM criteria but not the T criterion (Dark red).

PMT - Indicates that there is sufficient weight of evidence that the substance meets the P, M and T criteria, but not both the vP and vM criteria (Red).

PM – Indicates there is sufficient weight of evidence that the substance meets both the P and M criteria but does not met the T criterion nor the vPvM criteria (Dark yellow). These comprise of PM, vPM and PvM substances, but not PMT/vPvM substances. Though these substances are not prioritized as a risk to the sources of our drinking water, these substances are recommended for further potential hazard investigation if they become widespread in the environment, such as in the case of high emissions or the formation of PMT/vPvM transformation products. New experimental data could change the status of these substances to PMT/ vPvM.

Potential PMT/vPvM – Indicates that only screening or low-quality data is available for P, M or both, and that either a conclusion of "Potential P/vP" and/or "Potential M/vM" was obtained. Such screening or low-quality data cannot rule out the conclusion of PM or vPvM (Yellow). Efforts should be made to obtain half-lives or K_{OC} data, or equivalent information.

Not PMT/vPvM – Indicates that either the criteria for "Not P" or "Not M" was met with sufficient weight of evidence (Green), the substance is therefore neither PMT nor vPvM.

4) A PMT/vPvM assessment of all substances registered under REACH (as of May 2017).

The guidelines were applied to all REACH registered substances as of May 2017. The ECHA database of REACH registered substances contained 15469 substances at the time queried, of which organic structures could be identified for 9742 substances. In summary there were 260 REACH registered substances that met the PMT/vPvM criteria (Red/Dark red), 224 met the PM criteria (Dark yellow), 2377 had screening data requiring further assessment (Yellow), 3505 did not meet the criteria (Green) and 3216 had insufficient data to make a conclusion (White).

In addition, the outcome for a subset of REACH registered substances which require a PBT/vPvB assessment was conducted. A PBT/vPvB assessment needs to be carried out for substances which are produced or imported in amounts more than 10 tonnes per year and are not used as an intermediate only (according to Article 14(1) of the REACH regulation). At the time of the PMT/vPvM assessment (May 2017), 3895 substances were registered for which a PBT/vPvB assessment should be conducted. Out of this subset of substances, 158 met the PMT/vPvM criteria (Red), 143 met the PM criteria (Dark yellow), 743 had screening or low-quality data requiring further assessment (Yellow); 2276 did not meet the criteria (Green) and 539 had insufficient data to make a conclusion (White).

In summary, from the full REACH registered list of 15469 substances (as of May 2017) there are 260 substances (1.7%) that met the PMT/vPvM criteria. From the subset requiring a PBT/vPvB assessment, there are only 158 substances (1.0%) that met the PMT/vPvM criteria. This is considered a

minor fraction. This percentage may change due to better data availability and data quality. Additional data for degradation half-lives could have a substantial effect. The inclusion of transformation products would increase this percentage.

A list of all PMT/vPvM substances identified in this project is provided in Annex 1.

Researchers, regulatory authorities and the water production sector could consider these PMT/vPvM substances in their risk assessments for drinking water quality and as part of their monitoring programs, particularly if there is a local industry that is known to use substances on the list. For some of the most mobile substances, these may be difficult to detect at trace levels using conventional analytical methods. This is described in the literature as the "analytical gap" (Reemtsma et al., 2016). To close this gap method development is encouraged to facilitate the detection of PMT/vPvM substances.

Researchers working with water treatment technology and contaminated land remediation should also consider if their technologies can remove/remediate the PMT/vPvM substances provided in the list in this report.

5) Impact assessment of implementing the PMT/vPvM criteria

The impact assessment performed in this project is not based on the specific, individual PMT/vPvM substances in Appendix 1, but is rather based on the number of PMT/vPvM substances and the general cost considerations caused by PMT/vPvM substances to society. Potential impacts the implementation of the PMT/vPvM criteria could have on the status quo of the chemical industry and drinking water sector in the EU is a topic of ongoing discussion. The outcome of this study addressed some questions related to this potential impact:

- How many of the PMT/vPvM substances are emitted, or could be emitted, into the environment in a way that pose a risk to contaminate the sources of our drinking water?

The list of PMT/vPvM substances were compared with monitoring data and emission likelihoods were estimated based on tonnage and use data from REACH registrations. Additional considerations such as use, volatility, and similarity of chemical constituents across substances were also considered. Ultimately it is concluded that 134 (0.9%) REACH registered substances (as of May 2017) likely pose a risk to contaminate the sources of our drinking water.

- How many of the PMT/vPvM substances are already subject to regulation?

15 substances of the prioritized 134 PMT/vPvM substance were either already identified as SVHC under REACH and partly subject to authorization (11 substances) or are regulated under other EU legislation (5 substances). These would not likely require further regulatory action because of a risk to drinking water quality (which is largely already known for these substances). However, further investigation is recommended for the other 122 (0.8%) of the REACH registered substances (as of May 2017) regarding the likelihood of risk to the sources of our drinking water.

- What are the potential costs and benefits of implementing the PMT/vPvM criteria?

For implementing the PMT/vPvM criteria, any costs verses benefits for introducing risk management measures (RMMs) or, if needed, regulation would have to be considered on a case-by-case basis. Some benchmarks to consider would be:

1) Cost of substituting to a non PMT/vPvM alternative
2) Cost of reducing emissions
3) Cost of monitoring and legislation compliance
4) Cost of contaminated site remediation and monitoring

5) Cost of upgrading water treatment infrastructure to reduce exposure
6) Cost of ecosystem services potentially compromised
7) Health costs or benefits of using a PMT/vPvM substance for an essential purpose compared to available non-PMT/vPvM alternatives
8) Etc.

It was estimated that costs between 0.8 – 1.5 billion €/year are required for only partial removal of vPvM substances in Germany alone (Neumann and Schliebner, 2019). Thus, it is not unreasonable when extrapolating from Germany to the whole of Europe and all existing PMT/vPvM substances that the clean-up and drinking water purification costs could be at the several billions of Euros level, and this is not even factoring in potential health-care costs or loss of ecosystem services. It is not always clear who should bear the costs of contamination, and with PMT/vPvM substances this can be especially difficult. These substances are mobile, and they transport far from the point of emissions, potentially obscuring the emission source. It can become legally and scientifically complicated as well as time-consuming to identify who covers the remediation, removal, health-effect and ecosystem-services costs. This could mean that in cases of unexplained contamination events, consumers of drinking water may have to burden the financial costs

It is anticipated that the greater the persistency and mobility of the substance, the more likely expensive remediation methods are needed for removal. The more mobile the substance implies the less effective activated carbon filtration or other filtration methods would be, as filtration ultimately relies on sorption. Even expensive, state-of-the-art methods, like reverse osmosis, are not completely effective for very mobile substances for drinking water production (Albergamo et al., 2019).

The list of PMT/vPvM substances presented in Annex 1 are considered a starting point for discussing the environment and economic benefits to society, through the avoidance, substitution and better management of PMT/vPvM substances. A potential follow-up with feedback from registrants and downstream users of substances on this list is needed to better understand their emission scenarios. Regulators could also consider if substances mentioned on the list require further attention. For some substances, it may be worth considering regulating according to Article 57 f of REACH based on “scientific evidence of probable serious effects to human health or the environment which give rise to an equivalent level of concern”.

Though a low portion of REACH registered substances meet the PMT/vPvM criteria, the potential environment and human health costs as well as the economic costs of not acting are substantial.

Zusammenfassung

Das Umweltbundesamt (UBA) hat über viele Jahre und zuletzt mit Unterstützung durch dieses Vorhaben die im Rahmen der EU-Verordnung REACH (EG) Nr. 1907/2006 vorgeschlagenen Kriterien zur Identifizierung von persistenten, mobilen und toxischen (PMT) Stoffen und sehr persistenten, sehr mobilen (vPvM) Stoffen die unter REACH (EG Nr. 1907/2006) registriert sind, weiter diskutiert, entwickelt, begründet und abgestimmt (Neumann and Schliebner, 2019). PMT/vPvM-Stoffe haben die intrinsischen Stoffeigenschaften, welche anzeigen, dass sich aus Emissionen in die Umwelt eine Gefahr für die Ressourcen unserer Trinkwässer ergeben könnte. In diesem Bericht bezieht sich der Ausdruck "Ressourcen unserer Trinkwässer" auf unberührte und manchmal abgelegene Süßwasserökosysteme, Oberflächenwasserspeicher, Wasser aus Uferfiltration, Grundwasserleiter oder andere aquatische Umweltkompartimente, die möglicherweise als Trinkwasserquelle genutzt werden könnten. Mit diesen Kriterien (Neumann and Schliebner, 2019) können REACH-Registranten die intrinsischen Stoffeigenschaften beurteilen und entscheiden, ob ihre Stoffe PMT/vPvM-Stoffe sind. Abhängig von den Verwendungen und den verursachten Emissionen sollten die Registranten Maßnahmen zur Risikominderung ergreifen bzw. empfehlen, um ein Kontamination durch PMT/vPvM-Stoffen vorsorglich zu verhindern. Ein ordnungsgemäßes Risikomanagement von PMT/vPvM-Stoffen und Chemikaliensicherheit über den gesamten Lebenszyklus kann durch Programme zur Unterstützung der Eigenverantwortung erreicht werden. Wenn notwendig, können die Behörden regulatorische Maßnahmen ergreifen, um Emissionen zu minimieren und die wertvollen Wasserressourcen für zukünftige Generationen zu schützen.

Dieses Projekt adressierte die folgenden fünf wissenschaftlichen Arbeitsbereiche:

1) Zusammenstellung von Monitoringdaten der im Trinkwasser und im Grundwasser nachgewiesenen Chemikalien
2) Wissenschaftliche Informationen zur Identifizierung und Begründung der finalen M/vM-Kriterien
3) Leitlinien für die Durchführung einer PMT/vPvM-Bewertung
4) PMT/vPvM-Bewertung aller unter REACH registrierter Stoffe (Stand Mai 2017)
5) Folgenabschätzung der Implementierung der PMT/vPvM-Kriterien

Die wichtigsten Ergebnisse dieser fünf Arbeitsbereiche werden im Folgenden zusammengefasst.

1) Zusammenstellung von Monitoringdaten der im Trinkwasser und Grundwasser nachgewiesenen Chemikalien

Um die Notwendigkeit der Entwicklung von PMT/vPvM-Kriterien im Rahmen von REACH nachzuweisen, wurde eine Literaturrecherche durchgeführt und Monitoringdaten der im Trinkwasser und Grundwasser nachgewiesenen Stoffe zusammen gestellt. Die Literaturrecherche umfasste 25 Studien zwischen 2000 und 2018, darunter viele frühere reviews. Insgesamt wurden 333 Chemikalien identifiziert, von denen 246 im Trinkwasser und 187 im Grundwasser nachgewiesen wurden, davon 100 in beiden Kompartimenten. Diese Zusammenstellung kann als repräsentativ angesehen werden, aber nicht als vollständige Liste aller Stoffe, die jemals in Trink- oder Grundwasser nachgewiesen wurden. Von diesen 333 Chemikalien sind 142 (43%) Stoffe, die unter REACH registriert wurden (Stand Mai 2017), von denen wiederum 32 auch als Arzneimittel- und 5 auch als Pflanzenschutzmittelwirkstoff verwendet werden. Unter REACH registrierte Stoffe machen 113 (46%) der 246 Trinkwasserkontaminanten und 75 (40%) der 187 Grundwasserkontaminanten aus. Es kann daher als eine Tatsache angesehen werden, dass ein erheblicher Teil der Trinkwasser- und Grundwasserkontaminanten Stoffe sind, die unter REACH registriert sind. Diese zufällige Sammlung von Analysedaten zeigt, dass REACH

registrierte Stoffe mit höheren Konzentrationen nachgewiesen werden. Nur 40% (76 von 191) der nicht-REACH registrierten Stoffe überschreiten 0,1 µg/L, während 58% (83 von 142) der erfassten REACH registrierten Stoffe diese Konzentration überschreiten (Abbildung 2). Die Ergebnisse zeigen deutlich, dass die Entwicklung der PMT/vPvM-Kriterien für unter REACH registrierte Stoffe notwendig ist und dass diese Kriterien zum Schutz der Ressourcen der Trinkwässer angewendet werden müssen.

2) Wissenschaftliche Informationen zur Identifizierung und Begründung der finalen M/vM-Kriterien

Die PMT/vPvM-Kriterien wurden sowohl durch wissenschaftliche Untersuchungen als auch durch Konsultationen mit Experten und Stakeholdern entwickelt (Neumann and Schliebner, 2019).. Der Beitrag dieses Projekts bestand darin, grundlegende wissenschaftliche Daten und Informationen bereitzustellen, mit denen das endgültige Kriterium mobil (M) und das Kriterium sehr mobil (vM) identifiziert und letztendlich begründet werden konnten.

Seit den 1980er Jahren besteht in der wissenschaftlichen Literatur Konsens darüber, dass die Mobilität organischer Substanzen im Boden durch die Kombination der intrinsischen Stoffeigenschaften Persistenz und Sorption zum Boden beeinflusst wird. Letzteres wird im Allgemeinen am besten durch den Verteilungskoeffizient zwischen Wasser und organischer Substanz des Bodens (K_{OC}) quantifiziert wird (Gustafson, 1989). Aus praktischer Sicht ist der K_{OC} eine der intrinsischen Stoffeigenschaften die für viele Stoffe bereits verfügbar ist oder anderweitig durch Standardlaborverfahren oder Monitoring und Modellierungssimulationen abgeleitet werden kann.

Aufgrund der wissenschaftlichen Untersuchungen und dem Ergebnis der Konsultationen wurde als Kriterium für sehr mobil (vM) ein log K_{OC}-Wert von weniger als 3,0 festgelegt (Neumann and Schliebner, 2019). Dieses Kriterium wird in der wissenschaftlichen Literatur zum Schutz des Grundwassers unterstützt (siehe Abschnitt 6.1) und wird derzeit für die Grundwasserbeobachtungsliste genutzt, die von der EU-Arbeitsgruppe ”groundwater” zur Identifizierung potenzieller Grundwasserkontaminanten erstellt wird. Außerdem wurde der Kriterium für mobil (M) auf einen log K_{OC}-Wert von weniger als 4,0 festgelegt (Neumann and Schliebner, 2019). Die Ergebnisse dieses Forschungsbericht zeigen, dass ein so hoher Wert als M-Kriterium notwendig ist, um die Uferfiltration auch für emittierte P/vP-Stoffe zu schützen.

Beide Kriterien werden in diesem Bericht gestützt durch die empirischen Beobachtungen der nachgewiesenen REACH-registrierten Stoffe in Trinkwasser und Grundwasser, für die log K_{OC}-Werte verfügbar waren (n=88). Dabei erfüllten alle Stoffe das vM-Kriterium mit Ausnahme von 13%, die nur das M-Kriterium erfüllten, und nur weiteren 6%, die nicht mobil waren. Die M/vM-Kriterien können daher als ein angemessenes Schutzniveau für die Ressourcen unserer Trinkwässers gelten.

Wenn kein K_{OC}-Wert verfügbar ist, wird als Screeningkriterium für Mobilität der kleinste pH-abhängige Verteilungskoeffizient zwischen n-Oktanol und Wasser (log D_{OW}) von kleiner als 4,5 empfohlen (Neumann and Schliebner, 2019). Der log D_{OW}-Wert von < 4,5 als Screeningkriterium für Mobilität (M) ist begründet auf der Grundlage von Korrelationen mit log K_{OC}, sowie mit der Praktikabilität der Integration des Screeningkriteriums für Bioakkumulation (B), als Teil der PBT/vPvB Bewertung. Die wissenschaftliche Begründung ist, dass bei neutralen Molekülen der log D_{OW}-Wert gleich dem log K_{OW}-Wert ist. Dadurch sollten neutrale P/vP-Stoffe mit einem log D_{OW}-Wert (oder log K_{OW}-Wert) über 4,5 für B und die anderen für M bewertet werden. Eine empirische Begründung für diese Kriterien ergibt sich aus den Ergebnissen der Literaturrecherche über die in Trinkwasser und Grundwasser nachgewiesenen REACH-registrierten Stoffe, wie sie in Abschnitt 6.1 (Abbildung 6 und Abbildung 8) dargestellt sind.

3) Leitlinien für die Durchführung einer PMT/vPvM-Bewertung

Für die P/vP-, M/vM- und T-Bewertung wurden Leitlinien entwickelt. Diese Leitlinien werden so dargestellt, dass sie prospektiv für neue oder retrospektiv für bestehende REACH-registrierte Stoffe

angewendet werden können. Ein zentraler Bestandteil dieser Leitlinien ist die Frage, wie die Datenqualität zu berücksichtigen ist. Auf Grundlage der Datenqualität kann entschieden werden ob genügend „weight of evidence" vorhanden ist, um eine Schlussfolgerung bei der P/vP-, M/vM- oder T-Bewertung zu ziehen. Daher wird ein "Ampel"-Farbschema eingeführt, um der Datenunsicherheit Rechnung zu tragen, mit folgender Abstufung:

Weiß - unzureichende Daten für eine PMT/vPvM-Bewertung;

Dunkelrot oder Rot – Daten belegen, dass der Stoff die PMT/vPvM-Kriterien erfüllt;

Dunkelgelb oder Gelb - Daten belegen, dass der Stoff im Verdacht steht, die PMT/vPvM-Kriterien zu erfüllen;

Grün - Daten belegen, dass der Stoff die PMT/vPvM-Kriterien nicht erfüllt.

Je nachdem welche Kriterien erfüllt sind und wie sicher sie erfüllt sind, können sieben verschiedene abschließende Schlussfolgerungen aus der PMT/vPvM-Bewertung resultieren.

Keine Schlussfolgerungen möglich – Es fehlen entweder Daten für die P- oder für die M-Bewertung selbst auf Screening-Niveau (weiß). Es sollten Anstrengungen unternommen werden, um mindestens geeignete Screening-Daten zu erheben.

PMT & vPvM – Zeigt an, dass ausreichend weight of evidence vorliegt, dass der Stoff sowohl die vP- und vM-Kriterien als auch das T-Kriterium erfüllt.

vPvM – Zeigt an, dass ausreichend weight of evidence vorliegt, dass der Stoff die vP- und vM-Kriterien erfüllt, aber nicht das T-Kriterium.

PMT – Zeigt an, dass ausreichend weight of evidence vorliegt, dass der Stoff die P-, M- und T-Kriterien erfüllt, aber nicht die vP- und vM-Kriterien.

PM – Zeigt an, dass ausreichend weight of evidence vorliegt, dass der Stoff sowohl die P- als auch die M-Kriterien, aber weder das T-Kriterium noch die vPvM-Kriterien erfüllt. Diese umfassen PM-, vPM- und PvM-Stoffe, nicht aber PMT- oder vPvM-Stoffe. Obwohl diese Stoffe nicht prioritär als Bedrohung für die Ressourcen unseres Trinkwässers eingestuft werden, wird empfohlen, diese weiter auf mögliche gefährliche Stoffeigenschaften hin zu untersuchen, wenn sie sich in der Umwelt verbreiten, wie beispielsweise bei hohen Emissionen oder der Bildung von PMT/vPvM-Transformationsprodukten. Neue Testergebnisse könnten den Status dieser Stoffe in PMT oder vPvM ändern.

Potenziell PMT/vPvM – Zeigt an, dass nur Screening-Daten für P, M oder beide verfügbar sind und das deswegen die Schlussfolgerung "Potenziell P/vP" und/oder "Potenziell M/vM" getroffen wurde. Solche Screening-Daten können eine Bewertung als P oder M nicht mit ausreichend hoher Sicherheit ausschließen. Es sollten Anstrengungen unternommen werden, um z.B. Halbwertszeiten, K_{OC}-Daten oder gleichwertige Informationen zu erhalten.

Nicht PMT/vPvM – Es liegen Informationen vor, dass entweder das P- oder das M-Kriterium oder beide mit ausreichender Beweislast nicht erfüllt sind (grün). Der Stoff ist also weder PMT noch vPvM.

4) PMT/vPvM-Bewertung aller unter REACH registrierter Stoffe (Stand: Mai 2017).

Die Leitlinien wurden auf alle unter REACH registrierten Stoffe (Stand Mai 2017) angewendet. Die Datenbank der ECHA enthielt zu damaligen Zeitpunkt 15469 REACH-registrierte Stoffe , von denen organische Strukturen für 9742 Stoffe identifiziert werden konnten. Insgesamt gab es 260 REACH-registrierte Stoffe, die die PMT/vPvM-Kriterien erfüllen (rot), 224 erfüllen die PM-Kriterien (dunkelocker), für 2377 Stoffe lagen nur Screening-Daten vor, so dass für diese Stoffe eine weitere Bewertung

erforderlich ist (ocker), 3505 erfüllen nicht die Kriterien (grün) und 3216 hatten unzureichende Daten, um eine Schlussfolgerung zu ziehen (weiß).

Darüber hinaus wird das Ergebnis nur für solche REACH-registrierten Stoffe dargestellt, die eine PBT/vPvB-Bewertung erfordern. Eine PBT/vPvB-Bewertung muss für Stoffe durchgeführt werden, die in Mengen von mehr als 10 Tonnen pro Jahr hergestellt oder importiert werden und nicht nur als Zwischenprodukt verwendet werden (Artikel 14 Absatz 1 der REACH-Verordnung). Zum Zeitpunkt dieser PMT/vPvM-Bewertung (Mai 2017) waren 3895 Stoffe registriert, für die eine PBT/vPvB-Bewertung notwendig war. Aus dieser Untergruppe erfüllten 158 die PMT/vPvM-Kriterien (rot), 143 die PM-Kriterien (dunkelocker), für 743 lagen nur Screening-Daten vor, so dass für diese Stoffe eine weitere Bewertung erforderlich ist (ocker), 2276 erfüllten nicht die Kriterien (grün) und 539 hatten unzureichende Daten, um eine Schlussfolgerung zu ziehen (weiß).

Zusammenfassend ist festzuhalten, dass es aus der vollständigen REACH-registrierten Liste von 15469 Stoffen (Stand Mai 2017) 260 Stoffe (1,7%) gibt, die die PMT/vPvM-Kriterien erfüllen. Betrachtet man nur die Stoffe, die eine PBT/vPvB-Bewertung erfordern, gibt es nur 158 Stoffe (1,0%), die die PMT/vPvM-Kriterien erfüllen. Dies ist ein kleiner Anteil. Dieser Prozentsatz kann sich aufgrund einer besseren Datenverfügbarkeit und Datenqualität ändern. Zusätzliche Daten zu Abbau-Halbwertszeiten könnten einen signifikanten Effekt haben. Auch die Einbeziehung von Transformationsprodukten würde diesen Prozentsatz erhöhen. Eine Liste aller in diesem Projekt identifizierten PMT/vPvM-Stoffe ist in Anhang 1 enthalten.

Forscher, Überwachungsbehörden und die Wasserwirtschaft könnten diese PMT/vPvM-Stoffe in ihre Risikoanalysen und ihrem Monitoring zur Qualität der Trinkwässer berücksichtigen, insbesondere dann, wenn es in der Nähe Unternehmen gibt diese PMT/vPvM-Stoffe verwenden.

Bei einigen sehr mobilen Stoffen können diese mit den herkömmlichen Analysemethoden schwer oder gar nicht als Spurenstoff nachzuweisen sein.

Dies wurde in der Literatur als "analytische Lücke" für sehr mobile Stoffe beschrieben (Reemtsma et al., 2016). Um diese Lücke zu schließen, wird angeregt die analytischen Methoden anzupassen oder neu zu entwickeln, um dann auch einen Nachweis vom PMT/vPvM-Stoffen zu ermöglichen.

Forscher, die an Wasseraufbereitungstechnologien und Altlastensanierung arbeiten, sollten prüfen, ob ihre Technologien auch die in der Liste dieses Berichts aufgeführten PMT/vPvM-Stoffe entfernen können. Es wird erwartet, dass je höher die Persistenz und Mobilität ist, desto teurer die erforderliche Technologie ist.

5) Folgenabschätzung der Implementierung der PMT/vPvM-Kriterien.

Die in diesem Projekt durchgeführte Folgenabschätzung basiert nicht auf den spezifischen, einzelnen PMT/vPvM-Stoffen in Anhang 1, sondern auf der Anzahl der PMT/vPvM-Stoffe und allgemeinen Überlegungen zu Kosten, die durch PMT/vPvM-Stoffe für die Gesellschaft entstehen. Mögliche Auswirkungen der Implementierung der PMT/vPvM-Kriterien auf den Status quo der chemischen Industrie und der Trinkwasserwirtschaft werden derzeit in der EU diskutiert. Das Ergebnis dieses Vorhabens beantwortet einige Fragen im Zusammenhang mit den möglichen Auswirkungen:

- Wie viele PMT/vPvM-Stoffe werden oder könnten zurzeit in die Umwelt emittiert werden, so dass ein Risiko besteht, dass die Ressourcen unserer Trinkwässer kontaminiert werden?

Die Liste mit PMT/vPvM-Stoffen wurden mit Monitoringdaten verglichen und die Emissionswahrscheinlichkeiten wurden auf der Grundlage von Mengen- und Nutzungsdaten der REACH-Registrierungen geschätzt. Zusätzliche Überlegungen wurden auch in Bezug auf die Verwendung, Flüchtigkeit und Ähnlichkeit chemischer Bestandteile zwischen Stoffen angestellt. Letztendlich wird der Schluss gezogen, dass 134 (0,9%) REACH registrierte Stoffe (Stand Mai 2017) wahrscheinlich ein Risiko darstellen, die Quellen unserer Trinkwässer zu verunreinigen.

- Wie viele der PMT/vPvM-Stoffe unterliegen bereits einer Regulierung?

15 Stoffe befinden sich auf der Liste der priorisierten 134 PMT/vPvM-Stoffe, die entweder bereits unter REACH als SVHC identifiziert wurden und teilweise bereits zulassungspflichtig sind (11 Stoffe) oder unter anderen EU-Gesetzen reguliert sind (5 Stoffe). Für diese Stoffe sind vermutlich keine weiteren regulatorischen Maßnahmen in Bezug auf eine Gefährdung der Trinkwässer erforderlich. Für die restlichen 122 (0,8%) der unter REACH registrierten Stoffe (Stand Mai 2017) werden jedoch weitere Untersuchungen hinsichtlich des Risikos für die Ressourcen unsere Trinkwässer empfohlen.

- Welche potenziellen Kosten und Nutzen ergeben sich durch die Implementierung der PMT/vPvM-Kriterien?

Bei der Implementierung der PMT/vPvM-Kriterien müssten Kosten und Nutzen für die Einführung von Risikomanagementmaßnahmen (RMM) oder - falls erforderlich - Regulierungen im Einzelfall geprüft werden. Einige zu berücksichtigende Benchmarks wären:

1) Kosten für die Substitution durch eine Nicht-PMT/vPvM-Alternative

2) Kosten für die Minimierung der Emissionen

3) Kosten für Monitoring und gesetzmäßiges Handeln

4) Kosten für die Sanierung und Überwachung von Altlasten

5) Kosten für die Modernisierung der Wasseraufbereitungsinfrastruktur zur Verringerung der Exposition

6) Kosten der Ökosystemleistungen, die möglicherweise gefährdet sind

7) Gesundheitskosten beziehungsweise Kostenvorteile der Verwendung eines PMT/vPvM-Stoffs für einen essentiellen Zweck im Vergleich zu verfügbaren Nicht-PMT/vPvM-Alternativen.

8) Etc.

Schätzungen zufolge könnten für die nur teilweise Entfernung von PMT/vPvM-Stoffen allein in Deutschland Kosten zwischen 0,8 - 1,5 Milliarden €/Jahr erforderlich sein (Neumann and Schliebner, 2019).

Es erscheint angemessen, wenn man von Deutschland auf ganz Europa und auf alle vorhandenen PMT/vPvM-Stoffe extrapoliert, die Reinigungs- und Trinkwasserreinigungskosten weit in die Milliarden zu schätzen, und das ohne Berücksichtigung potenzieller Gesundheitskosten oder des Verlusts von Ökosystemleistungen.

Es ist nicht immer klar, wer die Unkosten durch eine Kontamination tragen müsste, und bei PMT/vPvM-Stoffen kann dies besonders schwierig sein. Da es sich um mobile Stoffe handelt, werden sie weit weg von dem Punkt der Emission transportiert. Dies kann unter Umständen die Emissionsquellen verschleiern. Es kann rechtlich und wissenschaftlich aufwendig und langwierig sein, festzustellen, wer die Kosten für die Sanierung, Reinigung, gesundheitliche Auswirkungen und ausgefallen Ökosystemdienstleistungen übernehmen sollte. Dies könnte bedeuten, dass im Falle einer unerklärlichen Kontamination die Verbraucher von Trinkwasser finanziell belastet werden.

Es kann erwartet werden, dass je größer die Persistenz und Mobilität eines Stoffes ist, desto wahrscheinlicher sind teure Sanierungsmethoden notwendig für die Beseitigung. Je mobiler der Stoff, desto weniger effektiv wäre ein Aktivkohlefilter oder andere Filtrationsmethoden, da diese letztlich auf Sorption beruht. Selbst teure, moderne Verfahren wie die Umkehrosmose sind bei sehr mobilen Substanzen zur Trinkwassergewinnung nicht vollständig wirksam (Albergamo et al., 2019).

Die im Anhang 1 enthaltene Liste mit PMT/vPvM-Stoffen kann als Ausgangspunkt fungieren für eine Diskussion über den ökologischen und wirtschaftlichen Nutzen für die Gesellschaft durch Vermeidung, Substitution und besseres Risikomanagement von PMT/vPvM-Stoffen. Registranten und nachgeschaltete Anwender von Stoffen dieser Liste könnten insbesondere die Emissionsszenarien ihrer Stoffe zu überprüfen. Regulierungsbehörden könnten prüfen, ob diese Stoffe weitere Aufmerksamkeit

erfordern. Für einige Stoffe könnte eine Regulierung nach Artikel 57 f REACH in Betracht gezogen werden und prüfen, ob ein Stoff „nach wissenschaftlichen Erkenntnissen wahrscheinlich schwerwiegende Wirkungen auf die menschliche Gesundheit oder auf die Umwelt hat, die ebenso besorgniserregend sind wie" ein PBT/vPvB-Stoff. Der Anteil der unter REACH registrierten Stoffe, die die PMT/vPvM-Kriterien erfüllen ist gering. Trotzdem sind aber die durch Nicht-Handeln verursachten Kosten für die Gesellschaft und die Wirtschaft hoch.

1 Introduction

Under REACH (Regulation (EC) No 1907/2006), industry must demonstrate in their registration dossier the safe use of substances over their entire life cycle. For substances with intrinsic substance properties that indicate severe hazards, scrutiny is needed during chemical risk assessment. Already prior to the establishment of REACH, there has long been consensus that certain intrinsic substance properties exclude a quantitative risk-based regulation. Substances with carcinogenic, mutagenic, reprotoxic, or endocrine disrupting properties, for which a threshold cannot be determined, or substances considered persistent, bioaccumulative and toxic (PBT) or very persistent and very bioaccumulative (vPvB) warrant *per se,* a minimisation of human and environmental exposure and therefore a qualitative, hazard-based regulation. REACH currently lacks similar criteria for intrinsic substance properties that indicate a potential drinking water contaminant. Consequently, there is a regulatory gap between the requirements of the drinking water directive and REACH to fulfil the precautionary protection of the sources of our drinking water. In order to close this gap, the German Environment Agency (UBA) deemed it necessary to scientifically and technically develop criteria under REACH for substances considered persistent, mobile and toxic (PMT) or very persistent and very mobile (vPvM) (Neumann and Schliebner, 2019).

Ensuring that the sources of our drinking water are secure from any threats caused by chemicals is of the utmost importance. The United Nations (UN, Resolution 64/292) and the World Health Organization (WHO, Guidelines for drinking-water quality) consider access to clean drinking water essential to the realisation of human rights and the protection of human health. Similarly, the European Union's (EU) drinking water directive (98/83/EC, amended 2015/1787) has the objective "*to protect human health from the adverse effects of any contamination of water [...] by ensuring that it is wholesome and clean*". The EU's groundwater directive (2006/118/EC) states, "*groundwater is a valuable natural resource and as such should be protected from [...] chemical pollution*". Moreover, the EU's water framework directive (2000/60/EC) states that "*member States shall ensure the necessary protection for the bodies of water identified with the aim of avoiding deterioration in their quality in order to reduce the level of purification treatment required in the production of drinking water*".

In consideration of this need to protect the sources of our drinking water from existing and emerging chemicals, the German Environment Agency (UBA) has funded research projects to develop PMT/vPvM criteria under REACH since 2010. These projects include: a review of existing prioritisation models (Kuhlmann et al., (2010) - FKZ 363 012 41); a study to identify relevant intrinsic substance properties (Skark et al., (2011) - FKZ 360 010 59); the initial development of an assessment concept tailor-made for REACH (Kalberlah et al., (2014) - FKZ 371 265 416); and an assessment of persistence, mobility and toxicity of 167 REACH registered substances (Berger et al. (2018) - Project No. 74925). This report presents the outcome of a research project (started in 2016) to support the implementation of the PMT/vPvM criteria, and to use these criteria to assess all REACH registered substances as of May 2017. The finalized PMT/vPvM criteria used herein is also introduced in a report by UBA (Neumann and Schliebner, 2019), which was published in tandem with this report.

This research project had five central working areas:

1. **Compilation of monitoring data of chemicals detected in drinking water and groundwater.** A review of monitoring data of substances detected in drinking water and groundwater was conducted, to obtain a better overview of their presence and intrinsic substance properties.

2. **Scientific information for identifying and justifying the final M/vM criteria.** The theoretical underpinnings about how the combination of persistence and mobility can

ultimately lead to substances entering the sources of our drinking water was reviewed and summarized, with a focus on a description of the parameters that can best be used to describe mobility. In the report the outcome of this scientific investigation is presented in the context of the finalized PMT/vPvM criteria (Neumann and Schliebner, 2019).

3. **Guidelines for conducting a PMT/vPvM assessment.** A practical guidance is presented for assessing if a substance is PMT/vPvM in relation to the final criteria. An approach to consider data quality and the available weight of evidence using a "traffic light" system is also presented.

4. **A PMT/vPvM assessment of all substances registered under REACH.** The guidelines were used retrospectively to identify a list of PMT/vPvM substances registered under REACH (as of May 2017).

5. **Impact assessment of implementing the PMT/vPvM criteria.** A brief assessment is presented to consider how many of the listed of PMT/vPvM substances are likely to be in the environment, and what type of costs and benefits occur for registrants and society when risk management measures for these substances are implemented.

The outcome of the first working area (literature review) is presented in Chapter 2. The outcome of working areas two, three and four are presented side-by-side throughout Chapters 3 to 8; whereas the final working area is addressed in Chapter 9.

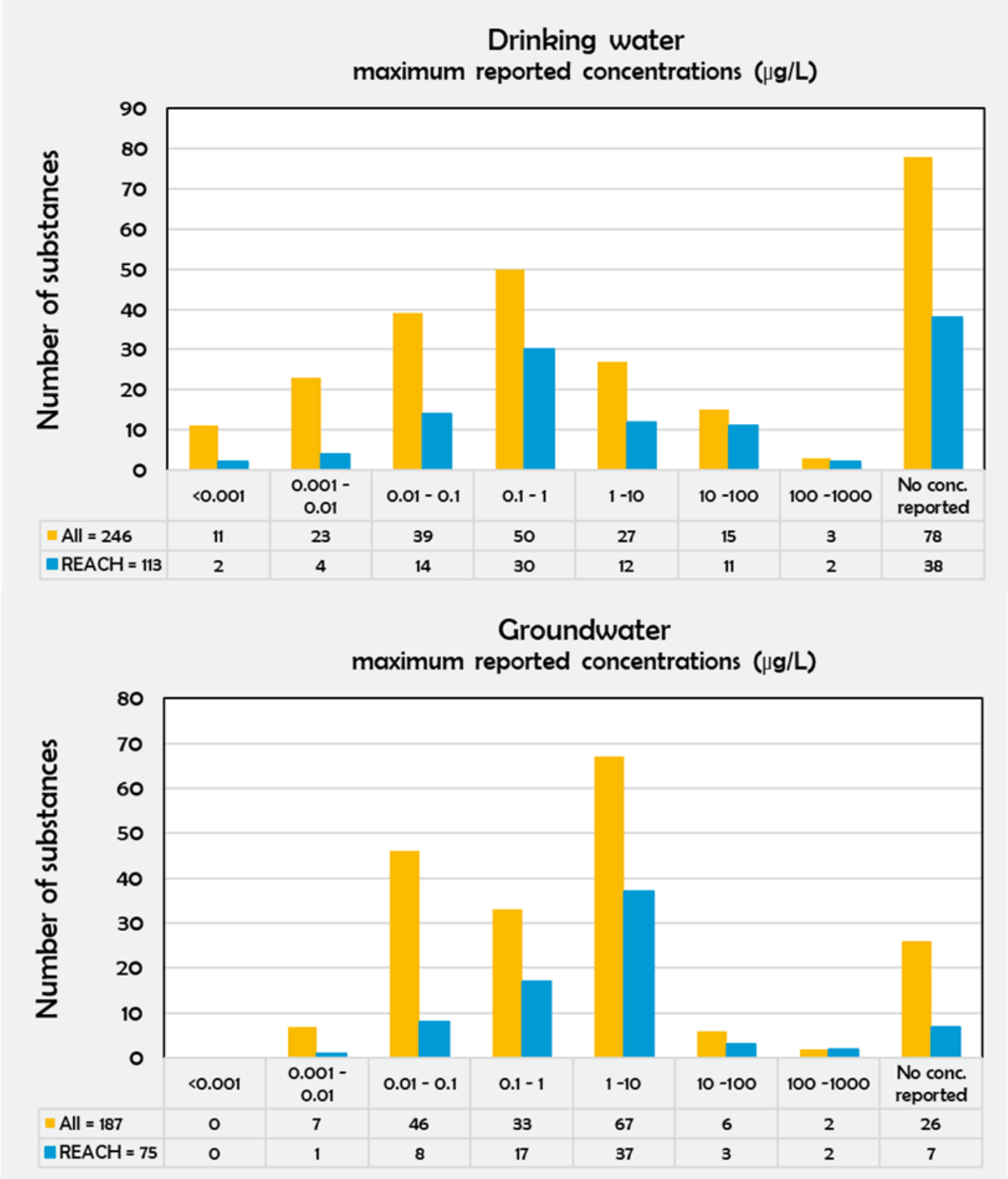
2 REACH registered substances in drinking water and groundwater

A literature review was conducted of organic substance monitoring studies that focussed on drinking water and groundwater. The purpose of this review was to evaluate the need for the existence of a PMT/vPvM criteria and in addition to empirically describe the suitability of the final criteria presented by UBA (Neumann and Schliebner, 2019). In total a literature review of 25 studies published between 2000 and 2018 was carried out. The list of 25 studies can be found in Annex 1. The studies reviewed usually targeted specific groups like pharmaceuticals, restricted chemicals, perfluoroalkyl and polyfluoroalkyl substances (PFAS), disinfection by-products and solvents. In total, 333 chemicals were identified, of which 246 were detected in drinking water and 187 were detected in groundwater, including 100 detected in both. This review can be considered a representative but by no means exhaustive list of all substances that have ever been detected in drinking water or groundwater. Of these 333 chemicals, 142 (43%) corresponded to substances that were registered under REACH (as of May 2017) of which 32 were also used as pharmaceuticals and 5 were also used as pesticides. These substances are presented in Annex Table A1, along with their PMT/vPvM evaluation. There were 191 chemicals not registered under REACH (as of May 2017), shown in Annex Table A3; the list of these substances contains several pharmaceuticals and their metabolites (74) as well as pesticides and their metabolites (62) and 55 chemicals belonging to other use categories. The REACH registered substances comprise 113 (46%) of the 246 total drinking water contaminants and 75 (40%) of the 187 total groundwater contaminants. It can therefore be considered as fact that a substantial portion of drinking water and groundwater contaminants are substances registered under REACH.

For many substances in this review, only whether they were detected or not was reported. Reasons for this include high limits of quantification, use of non-target analysis, missing quantification standards or absence of concentration data in the references. If available from the studies listed in Annex Table A2, the maximum concentration in drinking water and/or in groundwater is presented, as this was the most commonly reported parameter amongst these studies. The distribution of the maximum concentrations in drinking water and groundwater is visualized through two histograms in Figure 1, presenting data for all detected substances and of only the detected REACH registered substances.

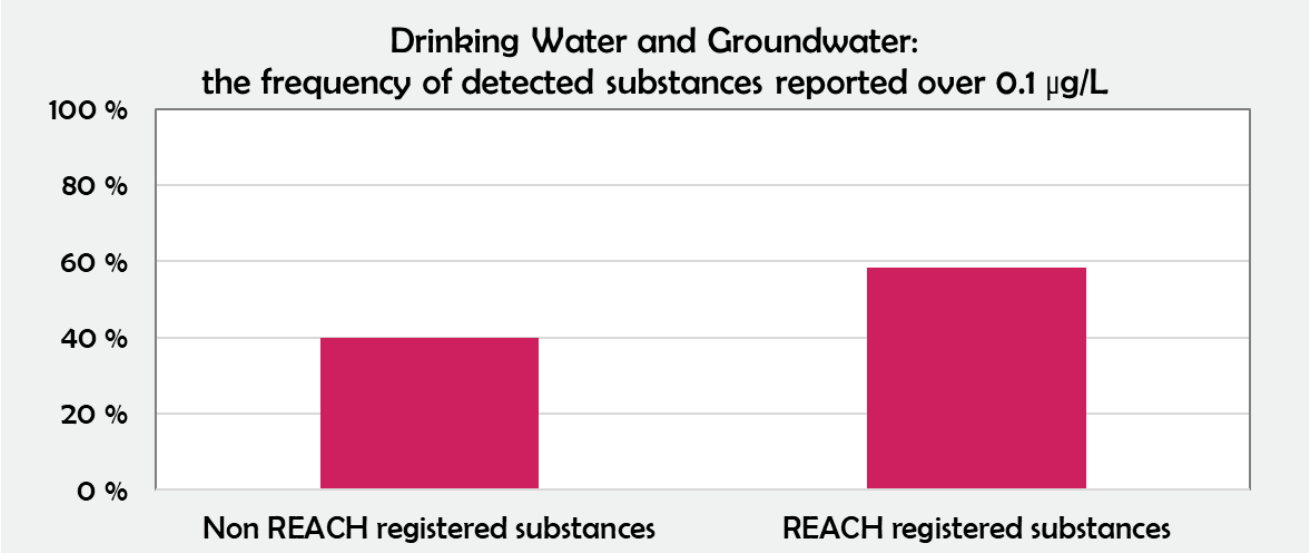
This collection of analytical monitoring data that was not specifically targeted at industrial substances indicates that REACH registered substance are in general detected at higher concentrations than other substances. While the REACH registered substances comprised 43% (142 of 333) of all the detected substances, this portion increased when considering only those substances exceeding 0.1 µg/L (i.e. the cut-off value of the drinking water directive (EU Regulation 98/83/EC) for pesticides). Figure 2 shows that only 40% (76 of 191) of the detected non REACH registered substances exceed 0.1 µg/L, while 58% (83 of 142) of the detected REACH registered substances exceed this concentration level.

Figure 1: Number of substances detected in drinking water (top panel) and groundwater (lower panel) in which the maximum reported concentration falls within one of the specified concentration ranges. The data are presented for all detected substances reported in the review of monitoring studies (yellow bars) and just for REACH registered substances as of May 2017 (blue bars).



Source: Original figure.

Figure 2: The percentage of substances that were reported in drinking water or groundwater with a maximum concentration over 0.1 µg/L for both non REACH registered substances and REACH registered substances.



Source: Original figure.

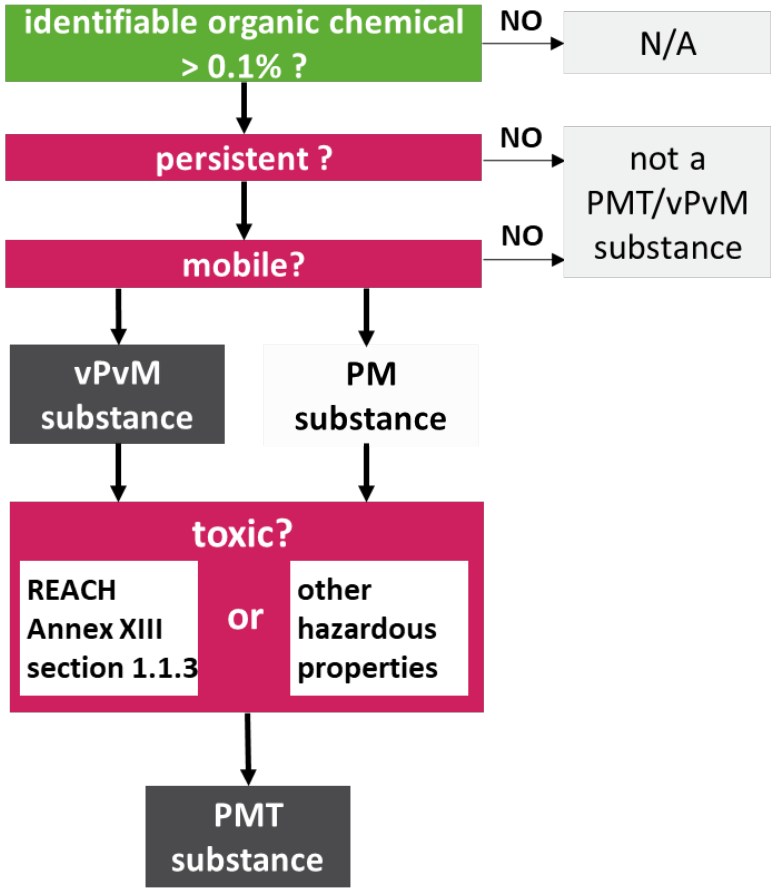
A substance may contaminate drinking water and groundwater when it is emitted into the environment and has the intrinsic substance properties of being persistent in the environment and mobile in the aquatic environment. Substances that contaminate drinking water and groundwater may cause a wide variety of problems, depending on their concentration and toxicity, including possible "cocktail effects" with other chemicals (Schriks et al., 2010). These problems can range from the tainting of flavour, such as the concern of sweetening agents like sucralose, to the concern of carcinogenic or endocrine disrupting substances that may exhibit adverse effects at low doses. For persistent and mobile substances, it is a concern that contamination can occur over long time scales, and therefore chronic effects, such as toxic effects from long term exposure, need to be considered. The outcome of this review of monitoring data is revisited in later chapters as part of the empirical justification for the developed PMT/vPvM criteria.

3 PMT/vPvM Assessment

3.1 Overview

An overview of the PMT/vPvM assessment as presented in Neumann and Schliebner (2019) is reproduced in Figure 3.

Figure 3: Overview of the assessment procedure to identify PMT/vPvM substances registered under REACH



Source: Neumann and Schliebner (2019).

The first two steps presented in Figure 3 are identical to the assessment of PBT/vPvB substances within REACH (ECHA, 2017a). First, the applicability of the PMT/vPvM assessment is determined. According to REACH Articles 14(1) and 14(2), the PBT/vPvB assessment is only mandated for non-intermediates, produced or imported at more than 10 tonnes/year, and contain organic and organometallic chemical constituent, including impurities, additives, and transformation products at greater than 0.1% abundance. General guidelines for carrying out this assessment are presented in the relevant PBT/vPvB guideline (ECHA, 2017a) as well as in Chapter 4 of this report for PMT/vPvM substances. Second, for applicable substances, the assessment of persistent (P) or very persistent (vP) is carried out, as described in Chapter 5 of this report. Substances that meet the P or vP criteria are further assessed for their mobility to see if they fulfil the mobile (M) or very mobile (M) criteria. These criteria are described in Chapter 6. If a substance does not contain any organic constituents that fulfil the criteria for P/vP or M/vM, no further action is required, and the substance is considered not a PMT/vPvM substance. If a substance fulfils both the criteria for vP and vM, it is considered a vPvM substance, otherwise it is considered a PM substance (which comprise substances fulfilling P and M, vP and M, or P

and vM). In either case, a PM or vPvM substance is assessed for toxic properties (T), as described in Chapter 7, to see if it is considered a PMT substance (which comprises substances fulfilling P and M and T, vP and M and T, P and vM and T, or vP and vM and T). Some substances can be considered both PMT and vPvM if they fulfil the necessary criteria. The method used to combine the P, M and T assessments to make the final PMT/vPvM assessment is presented in Chapter 8.

3.2 Data Quality

A key challenge when conducting reliable PMT/vPvM assessments is dealing with missing data as well as the varying quality of existing data. Data quality ultimately has a key role on the weight-of-evidence behind individual P, M or T conclusions. In Table 1, a strategy is presented for dealing with missing data or data of varying quality; whereby the PMT/vPvM assessment conclusions are ultimately ranked using a "traffic light" colour scheme.

Table 1: Traffic light colour scheme representing whether P, M or T criteria are met and the corresponding level of data quality

Colour	Criteria Met	Data Quality
White	Unknown	Data missing or data quality too poor/inconsistent to make a screening level assessment
Dark red	vP, vM or vPvM	High quality data indicating that vP, vM or vPvM are met.
Red	P, M, T or PMT	High quality data indicating that P, M, T or PMT are met. There may be some evidence that vP, vM or vPvM may be met.
Dark yellow	"Potential P/vP++" or PM	"Potential P/vP++" indicates there is sufficient weight of evidence that P or vP is met, but it is unclear which. "Potential P/vP++" is differentiated from the term "Potential P/vP" which is used to indicate that available screening or low-quality data makes it ambiguous to decide whether the substance meets the Not P, P or vP criteria. Dark yellow is also used when the PM criteria is met but not PMT/vPvM criteria.
Yellow	Potential P/vP, Potential M/vM, Potential T, Potential PMT or Potential vPvM	Screening data or low-quality data indicates the substance could potentially be P (or vP), M (or vM), T, or PMT/vPvM, but it is ambiguous which. More data is needed to decide.
Green	Not P, Not M, Not T, Not PMT or Not vPvM	High quality data or sufficient weight of evidence that P, M or T criteria are not met, and therefore the substance is not a PMT/vPvM substance.

Part of the advantage of the "traffic light" colour system is that it can help to make visual summaries in the form of charts or lists that are very clear and easy to disseminate. In summary, dark red, red, and green categories are reserved for final assessments of vPvM, PM or not P/not M, respectively. Yellow indicates that the screening criteria is met, but there is not enough data for a final assessment. Dark yellow indicates that there is sufficient data and P or PM is met, but it is unclear if vP, vPM or vPvM is met. White indicates that either no, or only preliminary and conflicting data is available. More details about how this traffic light system is applied to each step of the P, M, T and PMT/vPvM assessment is presented in the subsequent chapters.

4 PMT/vPvM assessment of REACH registered substances

4.1 REACH registered substances within the domain of the PMT/vPvM assessment

The first step of the PMT/vPvM assessment is identical to the assessment of PBT/vPvB substances within REACH (ECHA, 2017a). In brief, the PBT/vPvB assessment is only mandated for substances manufactured and imported in amounts of 10 or more tonnes per year (according to Article 14(1) of the REACH regulation), unless they are exempted based on Article 14(2), e.g. for constituents present at less than 0.1%, on-site or transported isolated intermediates, or substances used for product and process-oriented research and development. Further, regarding substance composition, the guideline for PBT/vPvB assessments states that "*Regardless of whether full substance identification is possible or not for the whole composition, the registrant should make efforts for carrying out a PBT/vPvB assessment for all constituents, impurities and additives present in concentrations above 0.1% (w/w)*" (ECHA, 2017a). For UVCB substances, which may have many constituents <0.1% (w/w), structurally similar constituents should be grouped together if applicable concentrations are above 0.1% (w/w), for instance using representative "proxy substances" for the group. Further recommendations and details are presented in the PBT/vPvB guideline (ECHA, 2017a). To reduce workload for registrants the same is proposed for the PMT/vPvM assessment (Neumann & Schliebner, 2019)

4.2 REACH registered substance constituent and chemical structure information

In order to conduct the PMT/vPvM assessment for REACH registered substances (as of May 2017), all entries, regardless of whether they would be exempt from the PBT/vPvB assessment according to Article 14 of the REACH regulation, were considered. However, those PMT/vPvM substances that would be exempt were noted, and this is considered throughout this report. Further, due to logistical and time challenges, only the most dominant organic constituent in each substance by weight were considered, rather than considering all organic constituents present above 0.1%. Impurities and transformation products were also not considered as part of this current report. Strategies for including such substances have been presented earlier (Arp et al., 2017; Schulze et al., 2018).

Obtaining structural information for substances under REACH is not always a straight-forward process. Sometimes this information is provided, other times one must rely on existing databases or computational QSARs that convert names to structures. However, computational methods and even databases are prone to errors, particularly with heteroaromatics, tautomeric structures or ionic substances. Various efforts were used to obtain as much constituent and chemical structural information as possible for the 15469 REACH registered substances registered as of May 2017. Information was sought in terms of chemical structural information represented by SMILES codes or International Chemical Identifiers (InChI). An analysis of REACH registered SMILES and InChI obtained by the IUCLID 6 database (https://iuclid6.echa.europa.eu/de/reach-study-results, accessed on April 10, 2017) only found chemical structure data for 5510 unique substance entries, after removing a substantial amount of false entries (i.e. incorrectly formatted SMILES or InChI information). An earlier acquisition to obtain structural information based on CAS numbers for the REACH registered substances was also utilized (Arp et al., 2017), which contained structural information for 7313 unique CAS numbers belonging to REACH registered substances. A database of structures from QSAR toolbox (https://qsar-toolbox.org/, accessed November 2017) was also used, which contained structural information for 4997 substances. These databases collectively gave structural data for 8809 individual REACH registered substances. For the remaining substances, the "Name to Structure" algorithm of the commercial software Chemaxon (https://chemaxon.com/) was used to convert IUPAC and common names to structural information. The molecular structures obtained were quality controlled by comparison across databases when they were identified to differ, and by checking for charge neutrality to ensure

the counterions were provided in the structure as presented in the substance name (Arp et al., 2017). In total structural information was obtained for 10745 of the 15469 REACH registered substances.

Most of the substances for which structural information could be obtained were mono-constituent substances or were represented by a single chemical structure (8200 substances). For the remaining multi-constituent and UVCB substances, the number of identified constituents within an individual substance (being either permanent ions, mixtures of neutral compounds, or a combination) varied between 2 and 51 (with the latter being for wood tar, CAS 91722-33-7). The identified organic chemical structures were categorized as "pure organic", "organoborate", "organosilicone", "pseudorganic" and "organometallic", with everything else being "inorganic", based on the definitions in Table 2.

Table 2: Definitions of organic constituents used in this study

Constituent type	Column heading	Number of substances with the dominant organic constituent of this type*
Pure organic	structures containing a C-H or C-C bond, or 2 carbons along with any combination of the elements H, C, O, N, Si, P, S, F, Cl, and Br	9197
Organoborate	meets the definition of "organic" and has at least one "B" atom	35
Organosilicone	meets the definition of "organic" and has at least one "Si" atom	217
Pseudoorganic	structures containing a single C in combination with one or more of the elements H, O, N, Si, P, S, F, Cl, Br and I	178
Organometallic	meets the definition of "organic" or "pseudoorganic", but with any other element than "B" or "Si" present	115

*Example, if a substance has a weight ratio of 60:30:10 pure organic:organoborate:inorganic, the substance would be considered "pure organic" rather than "organoborate" or "inorganic". Source of definitions: (Arp et al., 2017)

Of the 10745 substances where structural information was available, 9742 substances contained an organic constituent greater than 0.1%, while the other 1004 substances did not contain any organic constituents. The dominant (by weight) organic constituent of the 9742 substances were subdivided into the organic constituent categories, presented in Table 2. The vast majority were pure organic (94%).

5 Persistency

The PMT/vPvM criteria for persistent (P) and very persistent (vP) are consistent with those in Annex XIII of REACH for the PBT/vPvB assessment (Neumann and Schliebner, 2019). These criteria are reproduced in Box 1.

Box 1. P/vP criteria

A substance fulfils the persistent criterion (P) in any of the following situations:

(a) the degradation half-life in marine water at 9 °C is higher than 60 days;
(b) the degradation half-life in fresh or estuarine water at 12 °C and pH 4-9 is higher than 40 days;
(c) the degradation half-life in marine sediment at 9 °C is higher than 180 days;
(d) the degradation half-life in fresh or estuarine water sediment at 12 °C and pH 4-9 is higher than 120 days;
(e) the degradation half-life in soil at 12 °C and pH 4-9 is higher than 120 days.

A substance fulfils the "very persistent" criterion (vP) in any of the following situations:

(a) the degradation half-life in marine (9 °C), fresh or estuarine water (12 °C and pH 4-9) is higher than 60 days;
(b) the degradation half-life in marine (9 °C) fresh or estuarine water sediment (12 °C and pH 4-9) is higher than 180 days;
(c) the degradation half-life in soil (12 °C and pH 4-9) is higher than is higher than 180 days.

Source: Annex XIII of REACH as presented in Neumann and Schliebner (2019)

5.1 Justification of the P and vP criteria

The persistent criterion (P) and very persistent criterion (vP) are taken directly from Annex XIII of REACH. This greatly facilitates PMT/vPvM assessments, because existing regulatory definitions of P and vP are used, and existing conclusions of P and vP for the PBT/vPvB assessment, if available, can be directly used for the PMT/vPvM assessment.

The P/vP criteria are based on various half-life cut-off values for substances in freshwater, freshwater sediments, marine water, marine water sediments, and soil. For subsurface water transport, such as through aquifers, river banks and lake banks, the most relevant half-life would be those for soil and freshwater sediments. For surface water transport, the freshwater half-life would be the most relevant. It has been argued during consultations within this project, that the marine water and marine water sediment half-lives are irrelevant for the PMT/vPvM criteria, as the focus of the assessment is on freshwater systems. However, no exception is proposed here to eliminate these criteria because marine water data is considered as a suitable proxy for freshwater data, particularly when no freshwater data exists. In addition, marine water half-life studies are quite rare compared to freshwater studies based on previous experience and are rarely used in persistency assessments.

In order to assess whether the half-life cut-off values themselves provide the appropriate level of precaution to protect the sources of our drinking water, the time taken for a substance to travel from its point of emission to the sources of our drinking water should be considered as a measure for persistence. If a substance is not persistent enough to survive this travel time, it would not pose a hazard. An extreme case here is when emissions are occurring directly into a source of drinking water, where there is no barrier and negligible travel times occur; here the P criterion would be irrelevant. A more realistic situation in for most of Europe is that water first passes through the banks of a river or lake, a process referred to as bank filtration, before reaching a source of drinking water. In Germany and the

Netherlands, bank filtration travel times are typically in the range of 5 days or longer (Tufenkji et al., 2002; Schmidt et al., 2003). The most mobile substances sorb negligibly to soil and can travel up to the same speed as water through the bank of a river or lake. A substance that meets the P criterion of 120 days in soil and travels through soil/sediment at, or near, the speed of water would easily break-through bank filtration barriers with short travel distances (e.g. 5 days). Regarding remote aquatic ecosystems, one can consider typical flow velocities in groundwater, such as 0.15 to 15 m/day for sandy to gravelly aquifers, respectively (Harter, 2003). During the vP half-life for soil of 180 days this would correspond to travel distances from 27 to 2700 m. Considering that 50% of a chemical remains in the environment after at the time of half-life, heavily emitted, highly mobile substances with a half-life of 180 days could be transported hundreds of kilometres before degrading to negligible concentrations. In river water, where flow velocities are orders of magnitude faster than in groundwater, transport distances over the freshwater P half-life time of 40 days can theoretically be thousands of kilometres. As an example, consider the river Rhine which has a length of 1230 km and a flow rate of 86 km/day (Blaser et al., 2008). Assuming this flow rate, a substance would be carried along the entire Rhine river in 14 days if sorption and degradation processes were not operating. Therefore, highly mobile substances meeting the P criterion can contaminate the sources of our drinking water as well as remote aquatic ecosystems and accumulate in urban "wastewater to drinking water" cycles.

Anaerobic conditions may be considered within the persistency assessment as part of the weight-of-evidence in the P/vP assessment. Volatilization is not considered, as this process is only relevant for surface water transport and not for groundwater and bank filtration transport. However, it is worth remembering that highly volatile substances are likely removed during water treatment through aeration; however, this is not applicable for untreated groundwater. Therefore, such considerations are not used as part of the P/vP assessment, but more for considering emission scenarios and risk reduction measures for substances that meet the PMT/vPvM criteria (see Chapter 9).

5.2 Guidelines for the P and vP assessment

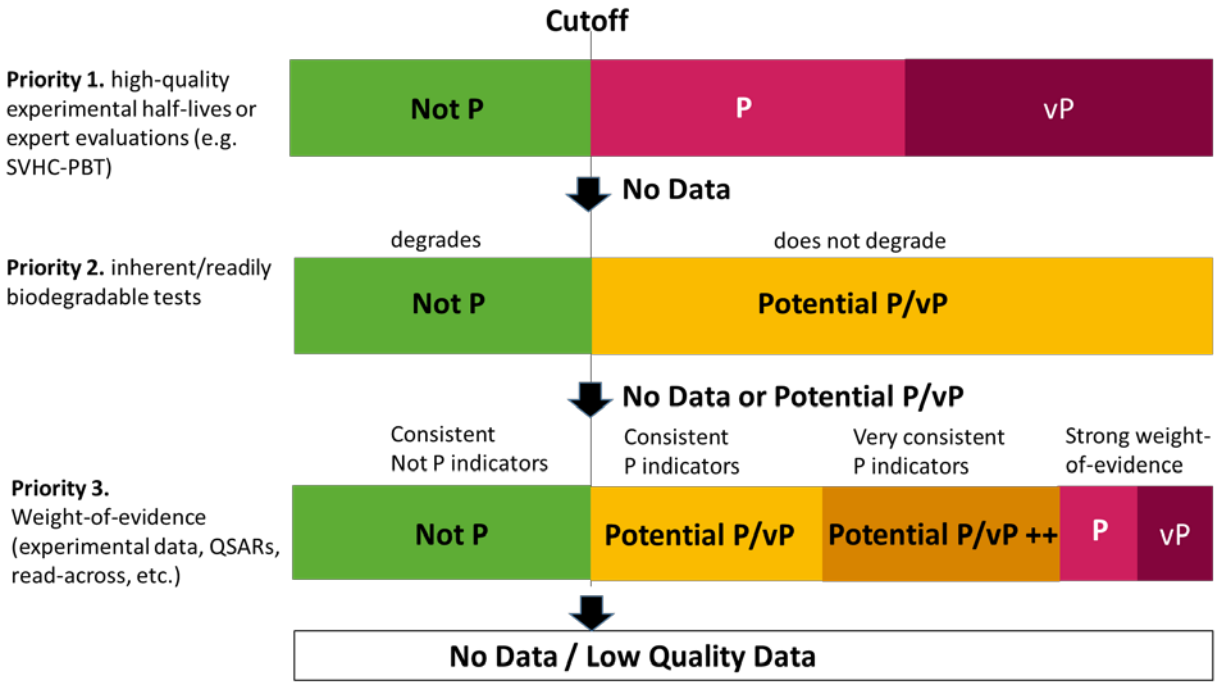
Half-lives for the P and vP assessment can be quantified using standardized methods such as OECD 307 (soil), OECD 308 (sediment) and OECD 309 (water). ECHA's PBT/vPvB guidelines state that OECD 309 (water test) is considered the most relevant, except in cases where soil and sediment are relevant exposure media (ECHA, 2017a). For PMT/vPvM assessment, soil and sediment are considered relevant exposure media, as subsurface mobility is a key concern. Determining half-lives to see if a substance fulfils the P criteria is both expensive and difficult. Therefore, and unfortunately, experimental data is very rare (Goldenman et al., 2017). A 2013 UNEP report found that only 220 out of 95,000 chemicals used by industry have experimentally determined biodegradation half-lives (UNEP, 2013). To try to alleviate this problem, ECHA has recommended low-cost ways of demonstrating non-persistence, to prioritize which substances warrant half-life determinations (ECHA, 2017a). In brief, first a ready biodegradation test (e.g. OECD 301; OECD 310) should be conducted; if the conclusion is clearly and consistently not persistent, then no further tests are needed. Other approaches can also be used to check for non-persistency or potential persistency, such as the inherent biodegradation test (e.g. OECD 302b; OECD 302c), enhanced screening tests, the application of QSARs, pure culture data, evidence of anaerobic degradation, abiotic degradation data, field studies and monitoring data. Such data can be used collectively to amass a conclusion of P, vP or not P based on weight of evidence, or if the outcome is not clear to conclude that experimental half-life data from a simulation study is needed (ECHA, 2017a).

In principle, one could obtain P conclusions directly from the registration dossiers for substances were a PBT/vPvB evaluation was conducted. However, in practice when considering the entire REACH database, this approach was met with difficulties in certain cases. Firstly, when using advanced data searches via IUCLID 6, inconsistent P/vP conclusions across multiple dossiers were common (for example at the time of writing, for cyclohexane, six PBT assessments can be found, five with "not P" and one reporting "P"). Second, P assessments are not available for all REACH registered substances, e.g.

intermediates and those produced at low tonnages, and the initial aim of this assessment was to consider all REACH registered substances as of May 2017.

Therefore, the approach presented in Figure 4 was used to prioritize relevant information to evaluate P independently. Instead of simply relying on the P conclusions in the dossiers, this approach summarizes the P/vP data that is currently and readily available and conducts the P/vP assessment anew based on this data. The approach in Figure 4 is effectively the opposite in sequence to the approach in the PBT guideline (ECHA, 2017a) for evaluating new substances that are to be registered in REACH. Instead of prospectively looking at low-cost screening data first for the P/vP assessments to see if high-quality experimental simulation half-life data are needed, here available high-quality simulation experimental half-life data are consulted first, and if this is not available, screening information is consulted retrospectively. However, checking for consistency between simulation and screening data is recommended, and this was conducted herein, before final conclusions are made.

Figure 4: Schematic representation of the approach used to evaluate P and vP based on the best quality data available.



Source: Original figure

Figure 4 utilizes the "traffic light" system for data quality presented in Table 1. As Figure 4 shows, **Priority 1** is to look at high-quality P/vP data such as experimental half-lives. This includes reported results for OECD 307, 308 and 309 tests at the relevant temperature presented in Box 1. In addition, the candidate list of substances of very high concern (SVHC) that meet PBT/vPvB criteria or the Stockholm Convention's list of Persistent Organic Pollutants (i.e. present on Annex I of the Regulation EC 850/200), or other reports of high quality that demonstrate P/vP, are considered as Priority 1 data. In cases where no Priority 1 data are available, **Priority 2** data is consulted. This includes the results of inherent / readily biodegradable screening tests. If the results are consistently "readily biodegradable" or "inherently biodegradable", a conclusion of "not P" is made, otherwise if "not readily biodegradable" or "not inherently biodegradable" a "Potential P/vP" decision is made. If there is no Priority 2 data or the conclusion of Priority 2 is "Potential P/vP", then more data is assessed, such as QSARs, field and monitoring data, etc, as part of **Priority 3**, to see if a weight of evidence conclusion related to P can be made. There are, theoretically several ways to conduct a Priority 3 P-assessment, and at this level it

may be that different researchers come to different conclusions when looking at the same data. The approach used here at the Priority 3 level is presented in Annex 2 as a suggested guideline. The potential conclusions from the Priority 3 assessment are:

Not P - there is some evidence that can be used to assess “not persistent” with confidence, such as extremely short QSAR half-lives, hydrolysis data, read-across from similar structures, etc.;"

Potential P/vP – there is only screening level data from Priority 2 or QSAR data that indicate potential persistency;

Potential P/vP++ - the weight-of-evidence suggests it is quite likely the P criterion is met, due to all lines of evidence indicating persistency, though half-lives are not available;

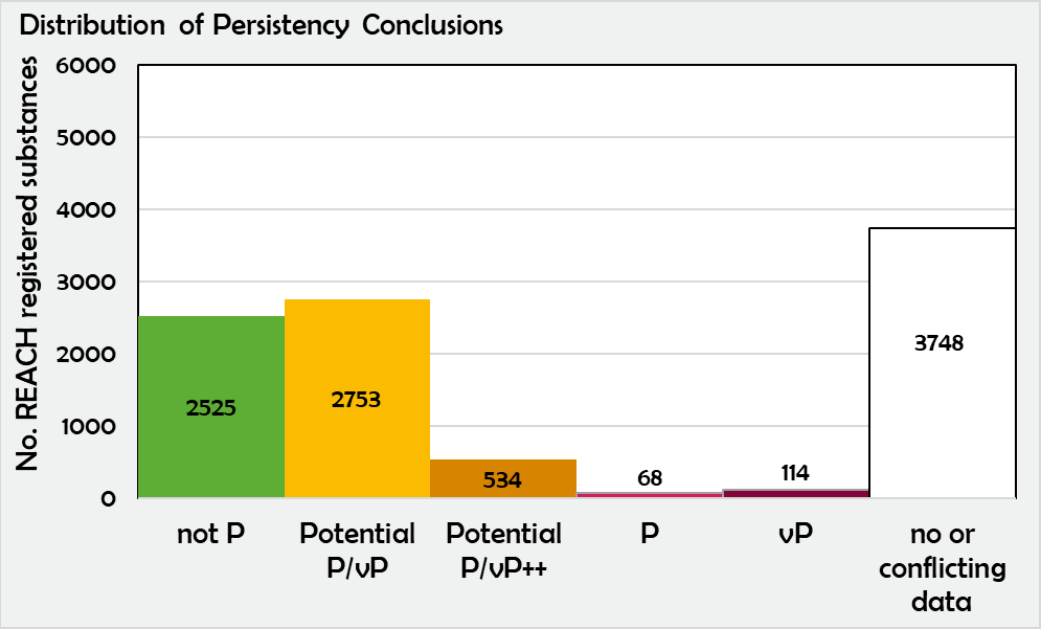
P or vP– there is very strong evidence for a conclusion of P or vP, despite no experimental half-life data, such consistent screening data that shows no biodegradation in combination with extremely long predicted half-lives, read-across from very similar chemical structures with a P or vP conclusion, or several reports of environmental persistence from monitoring data despite low or modest emissions.

If a satisfactory Priority 3 assessment cannot be made due to lack of data i.e. in cases where no or only inconsistent QSAR data are available, a conclusion of "**no or conflicting data**" is assigned.

5.3 Conclusion of the P and vP assessment

A breakdown of the P conclusions of the 9742 REACH registered substances (as of May 2017) that had a known organic constituent at greater than 0.1% is presented in Figure 5. The basis for these conclusions is presented in Annex 2, where a detailed description of the experimental data sources, QSAR data sources, their uncertainty and the weight of evidence procedure to make a final P conclusion is provided.

Figure 5: Distribution of persistency conclusions for REACH registered substances (as of May 2017) containing a known organic constituent greater than 0.1%.



Source: Original figure

For nearly 40% of the substances (3748 substances), no or conflicting outcomes resulted from the P assessment because of insufficient or low-quality data; typically for these substances there was either no data or just QSAR data, wherein the QSAR data was considered inconsistent across multiple models or too uncertain to make any conclusion (see Annex 2). A substantial fraction of substances (2525) were considered "Not P"; and in the majority of cases this was based on the results from experimental screening assays for biodegradation at the Priority 2 level (1705 substances), or on weight of evidence from consistent QSAR predictions at the Priority 3 level. A conclusion of P or vP was only drawn for a small minority of substances: 68 met the P criterion and an additional 114 the vP criterion. This is due to the high and strict data requirements required to make P and vP assessments. 2753 substances were considered "Potential P/vP" and 534 substances "Potential v/vP++".

As detailed in chapter 4.2, this assessment was conducted on the largest organic constituent per substance, and not all constituents, impurities or transformation products. If these substances had been included, then the number of substances with P and vP conclusions would increase.

6 Mobility

The mobile criterion (M) and very mobile criterion (vM) are unique to the PMT/vPvM assessment (Neumann and Schliebner, 2019) and are given in Box 2.

Box 2. M/vM criteria

A substance fulfils the mobile criterion (M) in the following situation:

(a) the lowest organic carbon-water coefficient log K_{OC} over the pH range of 4-9 is less than 4.0

A substance fulfils the "very mobile" criterion (vM) in the following situation:

(b) the lowest organic carbon-water coefficient log K_{OC} over the pH range of 4-9 is less than 3.0.

Source: Neumann and Schliebner (2019)

If no K_{OC} data is available, screening for mobility is recommended. The UBA has recommended to screen for mobility using either the octanol-water partition coefficient (K_{OW}) or the pH-dependant octanol-water coefficient for ionisable substances (D_{OW}), as shown in Box 3.

Box 3. M/vM screening

(a) For ionisable substances, the lowest pH dependent octanol-water distribution coefficient (D_{ow}) experimentally determined between pH 4-9 in accordance with Section 7.8 of Annex VII of REACH or estimated by (Q)SAR models in accordance with Section 1.3 of Annex XI of REACH.

(b) For other substances, the octanol-water partition coefficient (K_{ow}) experimentally determined in accordance with Section 7.8 of Annex VII of REACH or estimated by (Q)SAR models in accordance with Section 1.3 of Annex XI of REACH.

(c) Other information provided that its suitability and reliability can be reasonably demonstrated.

Source: Neumann and Schliebner (2019)

6.1 Justification of the M and vM criteria

REACH in Annex II section 12.4 defines mobility in soil as: "*the potential of the substance or the components of a mixture, if released to the environment, to move under natural forces to the groundwater or to a distance from the site of release. The potential for mobility in soil shall be given where available. Information on mobility in soil can be determined from relevant mobility data such as adsorption studies or leaching studies, known or predicted distribution to environmental compartments, or surface tension. For example, K_{oc} values can be predicted from octanol/water partition coefficients (K_{ow}). Leaching and mobility can be predicted from models. This information shall be given where available and appropriate, for each individual substance in the mixture which is required to be listed in Section 3 of the safety data sheet. Where experimental data is available, that data shall, in general, take precedence over models and predictions*".

REACH itself points to the use of the organic carbon-water coefficient, K_{oc}, as a central intrinsic substance property to describe mobility, alongside K_{OW}. The use of this parameter is firmly rooted in scientific literature with a long history. Since the 1980s persistence and K_{oc} in combination have been used to describe mobility (Gustafson, 1989). More recently, a modelling exercise by Kalberlah et al.,

(2014) demonstrated that K_{oc} was the parameter that correlated best with modelled amounts of breakthrough fractions from wastewater treatment for persistent substances,. The use of the lowest log K_{oc} over the pH range of 4-9 as the assessment parameter to describe mobility has been widely supported in the expert consultations that occurred throughout this project; though there were some discussions on the role of clays and minerals in reducing soil mobility. In specific situations, particularly for ionic substances in clay rich soils and sediments, the clays and minerals can measurably reduce mobility (Droge and Goss, 2013). However, these specific cases are difficult to generalize. Clays and minerals with different soils and sediments can have widely differing available surface areas and capacities for ion-exchange. This makes their influence on mobility extremely substance and site specific. Therefore, it is conceptually challenging to include a generic parameter to account for clay and mineral sorption as part of a hazard criterion.

The pH range of 4 to 9 is included in the mobility criteria, which is considered slightly broader than the ranges of pH typically found in the environment. The reason why this is included is that pH can affect the charges of ionisable substances, as well as the sorption properties of soil, and therefore can influence the K_{oc} value. Examples of ionizable substances are organic bases which become more cationic with decreasing pH, or organic acids which become anionic with increasing pH. Because soils are generally anionically charged, typically the greater the proportion of the cationic form of a substance, the larger its K_{oc} value. Most acids and bases are most mobile (have the lowest K_{oc}) at high pH because acids are more anionic and bases less cationic; however, for some soil types, such as those with metal oxides, which can have a large anionic exchange capacity, this general rule of thumb may not apply.

Initially, there was some uncertainty regarding where to set the threshold log K_{oc} value. Before the initiative of UBA was commenced, there had been an apparent consensus within the scientific community that a log K_{oc} cut-off of approximately 3.0 was a suitable cut-off for the protection of groundwater from persistent substances, regardless of clay and mineral content. For instance, in the late 1980's the "Groundwater ubiquity score", GUS (Gustafson, 1989) was developed based on the following metric to assess subsurface mobility:

$$GUS = \log DT_{50soil} (4 - \log K_{oc}) \quad (1)$$

Where DT_{50soil} is the half-life in soil. Based on comparisons with empirical observations of different organic compounds, a GUS value of 2.8 or greater was considered a "soil leacher" that has the potential to reach well water (i.e. it is mobile), below 1.8 a "non-leacher" (i.e. it is not mobile), and those in between in the "transition zone" and capable of leaching (i.e. it is potentially mobile). Considering the vPvM criteria proposed by UBA, a vP soil half-life (DT_{50soil}) of 180 days and a vM log K_{oc} value of 3.0 would correspond to a GUS of 2.25. This is in the middle of the transition zone between "leacher" and "non-leacher", and therefore according to this metric, a value that can be considered protective of groundwater.

The cut-off value of the assessment criterion for vM (log K_{oc} value less than 3.0) is harmonised with the Groundwater Watch List coordinated by the EU Common Implementation Strategy Working Group Groundwater (EC, 2016), which uses this cut-off value to identify groundwater relevant substances (EC, 2016; Kozel and Wolter, 2019).

The cut-off value of the assessment criterion for M (log K_{oc} value less than 4.0) is scientifically justified for the protection against bank filtration breakthrough of substances emitted in high volumes or in close proximity to the sources of our drinking water. This can be demonstrated theoretically by considering that the breakthrough time of a substance in bank filtrate $t_{substance}$ compared to that of water, t_{water} is:

$$t_{substance} = t_{water} (1 + (\rho/\Theta) K_{oc} f_{oc}) \quad (2)$$

which includes the fraction of organic carbon (f_{oc}), soil bulk density, ρ, and porosity, Θ, where the latter two are typically 1.7 kg/L and 0.4 in Europe, respectively (ECHA, 2016b). The f_{oc} for an agricultural soil is typically 0.02 (ECHA, 2016b) and in less organic rich environments such as sandy soils it is 0.002 (Hale et al., 2017). Setting these parameters as constants, the retention of substances relative to water

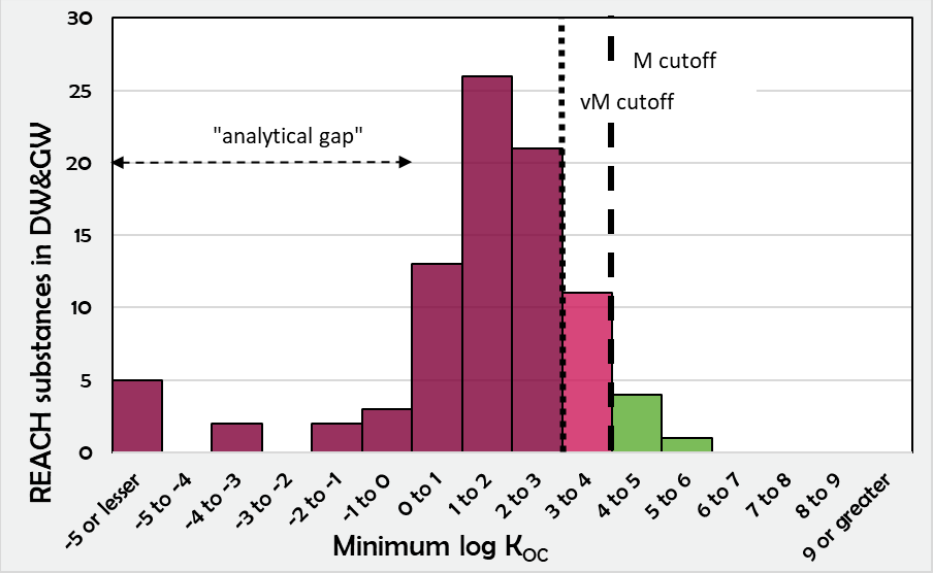
during bank filtration becomes a function of K_{oc}, where extremely small K_{oc} values result in $t_{substance}$ values being only slightly larger or the same as t_{water} values. For instance, if we consider an agricultural soil (f_{oc} = 0.02) and a substance with a log K_{oc} of 1, then $t_{substance}$ would only be approximately only twice that of t_{water} (i.e. $t_{substance}$ = 1.85 t_{water}); for a sandy soil (f_{oc} = 0.002) the difference would be negligible (i.e. $t_{substance}$ = 1.085 t_{water}). For the M assessment criteria of log K_{oc} of 4.0, it is useful to consider the case of rapid bank filtration, such as when t_{water} is 5 days. Here it would take 430 days for a substance with a log K_{oc} of 4.0 to breakthrough a sandy soil. This breakthrough time is larger than the P criteria for soil of 120 days; however, considering the general equation for exponential decay as a function of the soil half-life (equation 3), some substance will still remain after breakthrough of 430 days:

$$\text{fraction of substance remaining} = 0.5^{\,\text{time / DT50}} \qquad (3)$$

In the example above, 8% of a substance with a half-life of 120 days and a log K_{oc} of 4.0 would reach the recipient with a t_{water} of 5 days in a sandy river bank. Therefore, log K_{oc} of 4.0 appears to be a suitable maximum cut-off for the mobility threshold, for protection against substances that are permeable to quick bank filtration.

A more empirical justification beyond these theoretical and modelling arguments is the log K_{oc} values of the REACH registered substances that were detected in groundwater and drinking water, presented in the literature review in Chapter 2. This distribution of values is presented in Figure 6, with raw data presented in the Annex Table A1.

Figure 6: Distribution of log K_{OC} values of REACH registered substances detected in drinking water and groundwater from a review of monitoring studies



Source: Original figure

Figure 6 presents the distribution of the 88 out of 142 substances for which experimental K_{oc} data was available. There were 11 substances with a log K_{oc} between 3.0 and 4.0 (or 13% of considered substances), implying that they meet the M criterion but not the vM criterion. There are only 5 substances (or 6% of 88 substances) that do not meet the M criteria, having a log K_{oc} ranging from 4.0 to 5.4, implying these are false negatives (substances in drinking water not meeting the M criteria). Possible explanations for these false negatives are extremely high emissions, emissions close to the recipient, and direct contamination (e.g. leachate from pipes). Overall the selection of the M criteria appears empirically justifiable: lowering the vM and M criteria further would increase the number of false negatives,

which is considered insufficiently conservative. Also shown in this Figure is the "analytical gap", which roughly corresponds to substances with a log K_{oc} below 0, which are chemicals that are difficult to detect using standard non-target analysis via gas chromatography or reverse phase liquid chromatography, and require either dedicated or state-of-the-methods for detection (Reemtsma et al., 2016). This analytical gap is shown to underscore that there may be more substances detected if more non-target or dedicated analytical methods were available for highly polar substances.

Regarding substances for which log K_{oc} data are not available, the use of the lowest pH dependant D_{ow} for ionisable substances or K_{OW} less than 4.5 is recommended as an indication criterion for mobility (see Box 3). The D_{ow} in the pH range 4-9 can be derived from K_{ow} if the dissociation constant (pKa) is known, such as for monoprotic acids and bases through the following relationships:

$$D_{ow} = (1/(1+10^{pH - pKa}))K_{ow} \text{ (for monoprotic acids)} \quad (4)$$

$$D_{ow} = (1 - 1/(1+10^{pH - pKa}))K_{ow} \text{ (for monoprotic bases)} \quad (5)$$

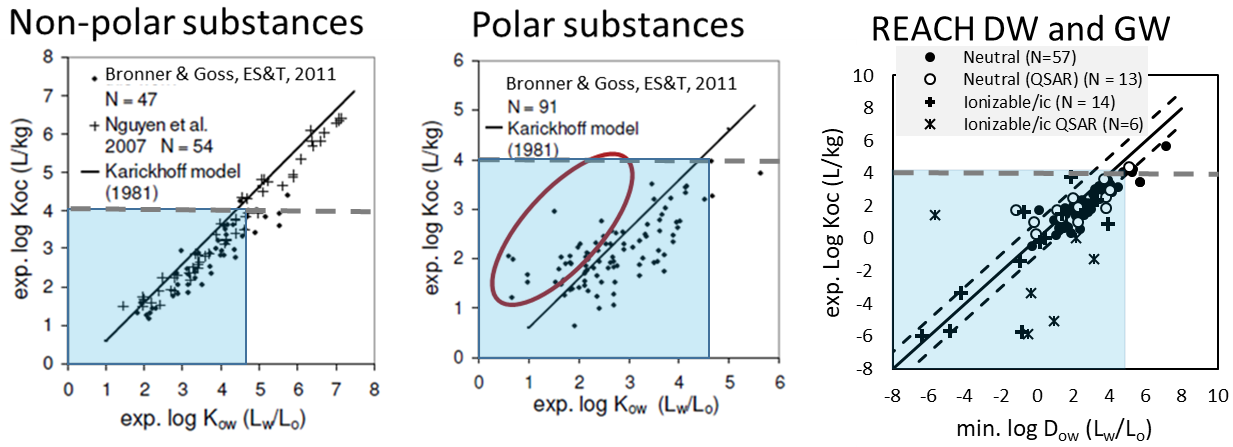
K_{ow} is already used as an indicator and screening criterion for the bioaccumulation (B) assessment. Specifically, substances with a log K_{ow} larger than 4.5 should be evaluated for B either through direct measurement of bioconcentration factors (BCF) or alternatively using a weight-of-evidence approach (ECHA, 2017a). If this data is not available, QSAR models for K_{ow} and pKa need to be used. Further guidance to approach the use of QSARs is presented in Annex 2, as well as in Arp et al. (2017).

The immense regulatory advantage of this screening cut-off is that persistent substances having a log D_{ow} or log K_{ow} above 4.5 should be assessed for B, and those below should be assessed for M. This provides a seamless integration with the indicator threshold for the bioaccumulation (B) assessment (ECHA, 2017a). However, this "sharp" cut-off between screening for B and screening for M is expected to be most representative for non-polar, neutral molecules. Correlations between K_{oc} and D_{ow} for polar, ionisable or ionic compounds are scattered; similar to correlations between BCF and D_{ow}. Consequently, some polar, ionisable or ionic substances can be both B and M simultaneously. A log D_{ow} value of 4.5 should therefore not be considered as a strict boundary between B and M substances, but rather an indicator for prioritizing whether to screen for B or M first.

The use of K_{ow} as a K_{oc} surrogate dates back to the late 1970's, when the two parameters were found to be closely correlated for neutral, non-polar molecules, particularly in the work of Karickhoff et al. (1979), who presented the general correlation: log K_{oc} = log K_{ow} - 0.21. As implied by this correlation, log K_{ow} values are generally slightly larger than log K_{oc} values for non-polar chemicals. This is supported by more recent data from Bronner and Goss (Bronner and Goss, 2010), as shown in the left panel of Figure 7. However, this correlation is not as good for polar substances, as is presented in the middle panel of the same Figure 7. For some polar substances log K_{ow} can be orders of magnitude smaller than log K_{oc}, as circled in the middle panel of Figure 7, implying a substance is less mobile than would be expected based on log K_{ow}. However, as is evident, there are several examples of a polar substance being more mobile than expected based on K_{ow}. In the right panel of Figure 7, the 88 REACH registered substances with experimental log K_{oc} available, that are also used in Figure 6, are plotted against the minimum log D_{ow} or log K_{ow}. It becomes clear to see that the correlation between log K_{oc} and the minimum log D_{ow}/log K_{ow} is much better for neutral substances than for ionisable and ionic substances, as expected.

The substances meeting the M criteria of log K_{oc} less than 4.0 and the screening criterion of the minimum log D_{ow} of 4.5 in the pH range of 4 to 9 is outlined using blue boxes in Figure 7. As is evident, most substances meeting the M criteria also have a log D_{ow} < 4.5; though there are some exceptions. The screening criterion captures most M substances but not all. Increasing to a higher threshold D_{ow} value is not recommended due to the practical reason of the aforementioned integration with the screening criteria for B.

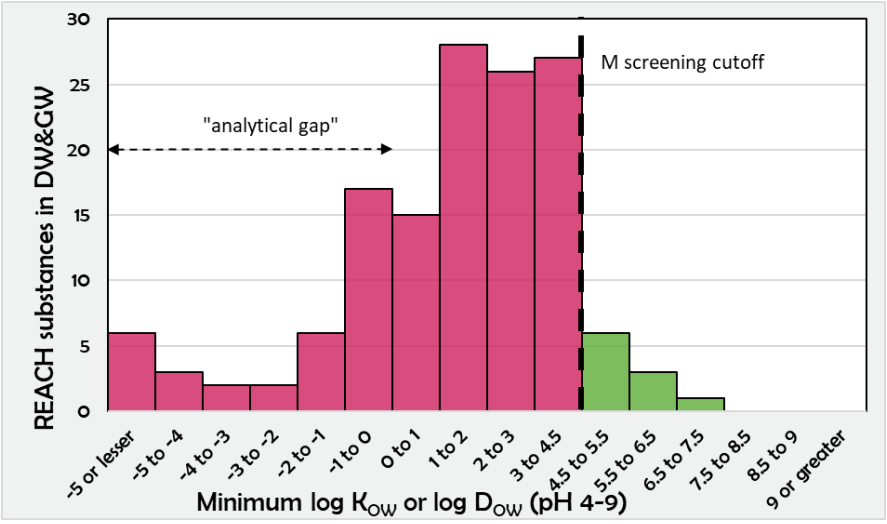
Figure 7: The log-log correlation between experimental K_{OC} and K_{OW}/D_{OW} for: left, non-polar substances (defined as having a mass fraction of oxygen + nitrogen atoms in the molecule ≤ 12%); middle, polar substances; right, REACH registered substances detected in drinking water (DW) and groundwater (GW).



Grey dashed horizontal lines show the M-criteria cut-off (log K_{OC} 4.0) and the blue boxes show the substances meeting both the M-criteria cut-off (y-axis) and the M screening value of a minimum log K_{OW} or log Dow (p 4-9) of 4.5 (x-axis). The red circle shows that for polar substances, log K_{OC} can sometimes be larger than K_{OW} by orders of magnitude which rarely occurs for non-polar substances. As shown in the right panel for the REACH registered substances detecting in drinking water and groundwater, substantial positive and negative deviations between D_{OW} and K_{OC} can occur for ionizable and ionic substances. Source: This left two panels were adapted with the permission from Bronner and Goss (2010) and the right panel is an original figure.

To validate the suitability of the M screening parameter, the 142 REACH registered substances detected in drinking water and groundwater are categorized by their K_{ow} or lowest D_{ow} (pH 4-9) in Figure 8. Unlike experimental K_{oc} values, for which data could only be found for 88 of the 142 substances, K_{ow} or lowest D_{ow} data could be found for all substances. Further, the screening cut-off of less than 4.5 captures 132 (93%), leaving only 10 false negatives (7%), indicating its suitability as a screening parameter.

Figure 8: Distribution of 142 REACH registered substances detected in drinking water and groundwater from the review of monitoring studies, organized by their minimum K_{OW} or D_{OW} (pH 4 to 9).



Source: Original figure

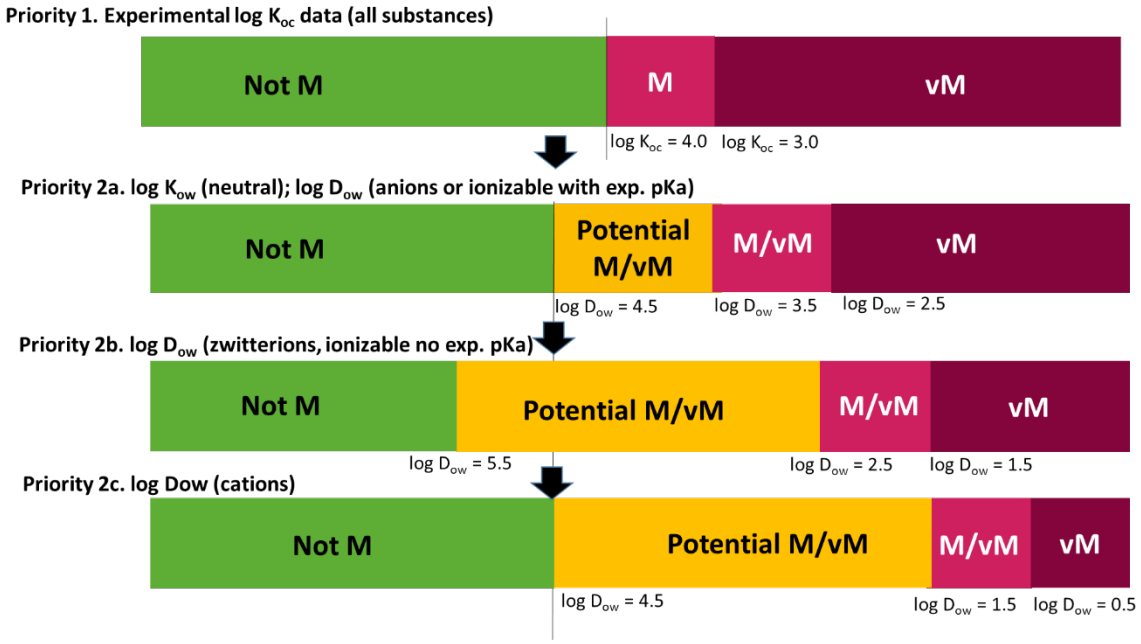
6.2 Guidelines for M and vM assessment

The M/vM criteria are based on K_{OC}. This parameter represents partitioning between soil-water, sediment-water or sludge-water, normalised to these media's organic carbon fractions (by weight). This means that high-quality data to these or related media containing organic carbon is suitable for the final K_{OC} assessment. The K_{OC} values should ideally be experimentally determined using partitioning studies in accordance with Section 9.3.1 of Annex VIII of REACH. The K_{OC} value can be inferred from field studies or monitoring studies (e.g. soil column leaching studies, batch studies, lysimeter studies, field observations, water treatment breakthrough studies and modelling studies) provided that their suitability and reliability can be reasonably demonstrated. ECHA has published guidelines for recommended approaches to measure K_{OC}, including: "Adsorption control within an inherent biodegradability test" (OECD TG 302B), "OECD TG 121; EU C.19: Estimation of the Adsorption Coefficient (Koc) on Soil and on Sewage Sludge using High Performance Liquid Chromatography (HPLC)", "Batch equilibrium method (OECD TG 106; EU C.18: Absorption – Desorption Using a Batch Equilibrium Method", "OECD TG 312: Leaching in Soil Columns", simulation tests and direct field measurements (ECHA, 2017b). Peer-reviewed experimental K_{OC} values determined using other methods can also be used for this assessment.

If log K_{OC} measured for different soils, sediments or sludges are available, the minimum log K_{OC} (between pH 4 and 9) should be selected, unless it can be reasonably demonstrated that soil, sediment or sludge type resulting in the minimum value is not representative. A minimum, high-quality log K_{OC} (between pH 4 and 9) value is considered as **Priority 1** for the mobility assessment, where the substances either meets the criteria as Not M (green), M (red) or vM (dark red) (Figure 9).

If high-quality experimental K_{OC} data is not available, screening assessments based on log D_{OW} or log K_{OW} values are to be conducted as **Priority 2**. The K_{ow} should be experimentally determined in accordance with Section 7.8 of Annex VII of REACH or estimated by (Q)SAR models in accordance with Section 1.3 of Annex XI of REACH. K_{ow} is required for organic substances in Section 9.1 of Annex II ("Requirements for the compilation of safety data sheets") and for volumes of more than 1 tonne per year, according to Section 7.7 - 7.8 of Annex VII of REACH. As with K_{OC}, if multiple high-quality K_{ow} data are available, the minimum experimental value should be used, and if not available the minimum of high-quality QSAR predictions. For ionizable substances, conversion to the minimum D_{OW} can be carried out using equations like equations 4 and 5 along with the pKa or estimated by (Q)SAR models in accordance with Section 1.3 of Annex XI of REACH. Determining the pKa is required under Section 7.16 of Annex IX of REACH when volumes are over 100 tonnes per year. At the Priority 2 level, a new category "Potential M/vM" is introduced, indicated as yellow in the traffic light system (Table 1).

Figure 9: Schematic representation of the approach used here to evaluate M and vM based on the best quality data available.



Source: Original figure

The basis for the "Potential M/vM" category is the degree to which log D_{OW} and log K_{OW} are correlated with log K_{OC}. In general, these correlations are poorer for ionic and ionisable substances (Figure 7). To elaborate briefly on the theoretical reason for this, equations 4 and 5, describing the relation between log D_{OW} and log K_{OW}, describe an octanol-water system where any molecule with an ionic charge will leave the octanol phase and enter the water phase. This is not necessarily the case for soil organic matter. Soil organic matter, unlike octanol, has acidic and basic functional groups that can be both positively and negatively charged. As a result, whether the substance in question is neutral, ionisable, cationic, anionic or zwitterionic has some influence as to how well D_{OW} can be used as a proxy for K_{OC}.

Priority 2a for neutral substances, ionisable and anionic substances with high-quality experimental pKa data.

For this assessment, neutral, ionisable and anionic substances are defined as follows:

> Neutral - no net ionic charge is present on >90% of a constituent in aqueous solution at any pH between 4 – 9; the K_{OW} can be used for such constituents.
>
> Ionisable - at some pH within the range of 4-9, at least 10% of molecules will transition from being neutral to having a cationic or anion charge present on the molecule. This category can be further subcategorized into ionisable acids (if log D_{OW} at pH 4 > log D_{OW} at pH 9) and ionisable bases (if log D_{OW} at pH 4 < log D_{OW} at pH 9). In such cases the log D_{OW} at pH 9 is used for acids and the log D_{OW} at pH 4 used for bases.
>
> Anions - over the entire pH range of 4-9, an anionic charge will be present on at least 90% of the constituent molecules, and no cationic charge is present above 10%.

With this data, as presented in Figure 9, if the minimum log D_{OW} (pH 4-9) is between 4.5 and 3.5 then the constituent is considered "Potential M/vM". Between log D_{OW} values of 3.5 and 2.5 the substance is considered "M/vM", which implies "M though potentially vM at the screening level". At values greater than log D_{ow} 2.5, the substance is considered as "vM at the screening level". The main justification for

this range for "Potential M/vM" is that the best performing QSARs for log K_{OW} are generally, at best, accurate within an order of magnitude (Arp et al., 2017).

Priority 2b for zwitterions and ionisable substances with no experimental pKa values.

For this assessment zwitterions are defined as follows:

> Zwitterions - at least one negative charge and one positive charge exist simultaneously on at least 10% of the constituent molecules over the entire pH range of 4-9.

There is comparatively little literature on the sorption zwitterions in soil, and the information that is there shows that their sorption behaviour can be very complex and hard to generalize across zwitterions. Further, for ionisable substances, if the pKa is not known, QSARs are needed, which can result in large uncertainties when estimating the D_{OW} value (Arp et al., 2017). Therefore, a broader range of minimum log D_{OW} values are selected for the "Potential M/vM" category, being between 5.5 and 2.5. Constituents with minimum log D_{OW} values between 2.5 and 1.5 are considered "M/vM", and less than 1.5 as "vM at the screening level".

Priority 2c for cations.

For this assessment cations are defined as follows:

> Cations - at least one positive charges exist on the molecule that is stable over a pH range of 4-9, and no anionic charge is present or occurs

Owing to the fact that cations generally sorb strongly to soils, due to the frequent presence of cation exchange sites in both soils and minerals in soils (Droge and Goss, 2013),the range of minimum log D_{OW} values used to define the "Potential M/vM" category is shifted from 4.5 to 1.5, with values between 1.5 and 0.5 defined as " M/vM", and values less than 0.5 as "vM at the screening level".

6.3 Conclusion of the M and vM assessment

The distribution of the primary organic constituents of the 9742 REACH registered substances in terms of neutral, ionisable, anionic, cationic and zwitterionic is presented in Table 3. Over 52% of substances (5107) had a neutral species as their primary organic constituent, followed by ionisable (33%), anions (11%), cations (3%) and zwitterions (1%).

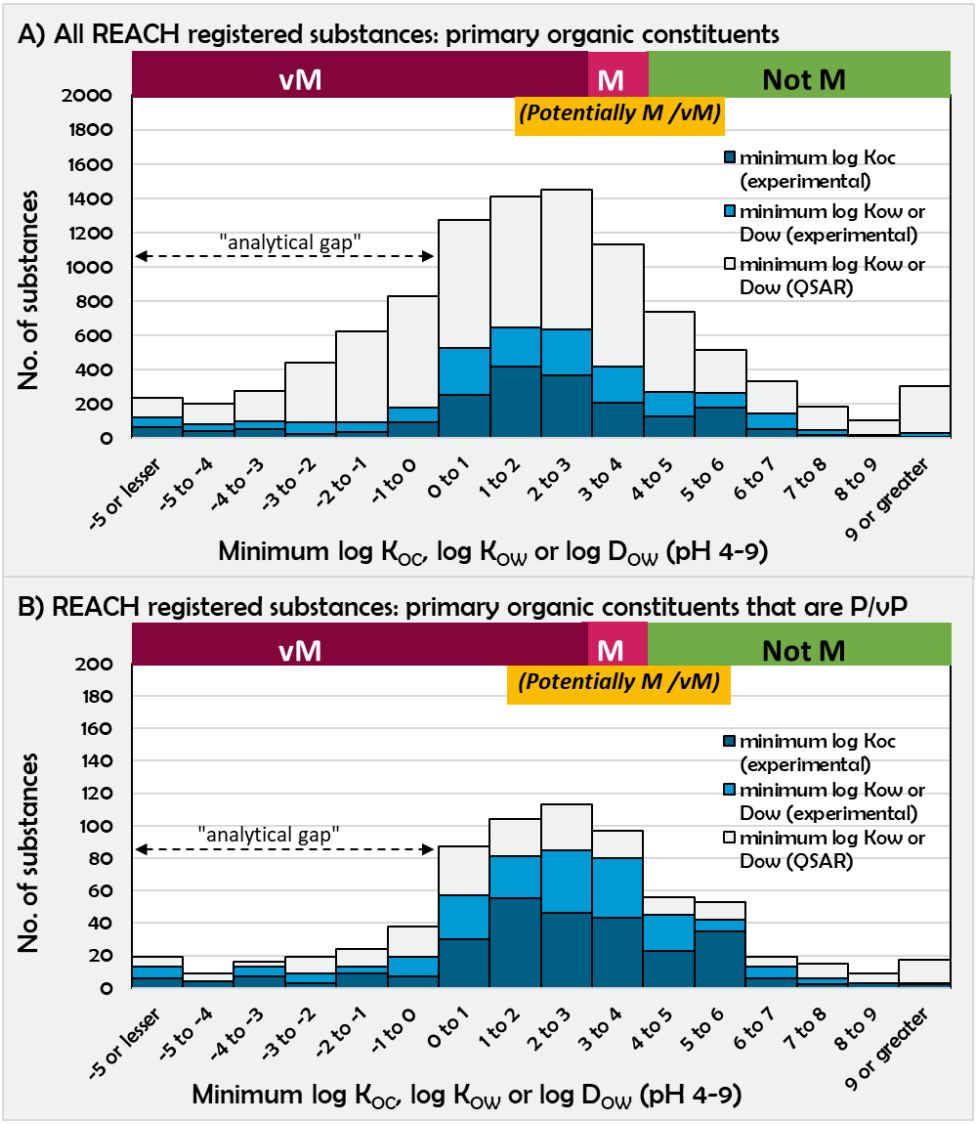
Table 3: Distribution of primary organic constituent types, based on ionizability and charge, across the 9742 REACH registered substances for which structural information was available.

Type of primary organic constituent	Number of REACH registered substances
Neutral	5107
Ionisable	3189
Anionic	1086
Cationic	300
Zwitterion	60

For each of these substances, K_{OC}, pKa, D_{OW}, and K_{OW} data was collected, with QSAR estimates only being used when no experimental data could be found. The sources of these data are presented in Annex 2. A histogram presenting the best available data for the mobility assessment for each of these substances, organized according to log K_{OC}, log D_{OW} or log K_{OW} value is presented in Figure 10a for all 9742 substances. In Figure 10b a similar histogram is presented, but only for the 716 substances that were

concluded to be vP, vP or Potential P/vP++ in Chapter 5, as the mobility assessment is only required for substances fulfilling the P/vP criteria.

Figure 10: Distribution of best available minimum log K_{OC} (experimental), log D_{OW} or log K_{OW} (experimental and QSAR) values over a pH range of 4 to 9 for a) the largest known organic fragment amongst all REACH registered substances and b) only substances where the Potential P/vP++, P or vP criterion is met (716 substances). Also shown is the "analytical gap", where analysis is difficult.



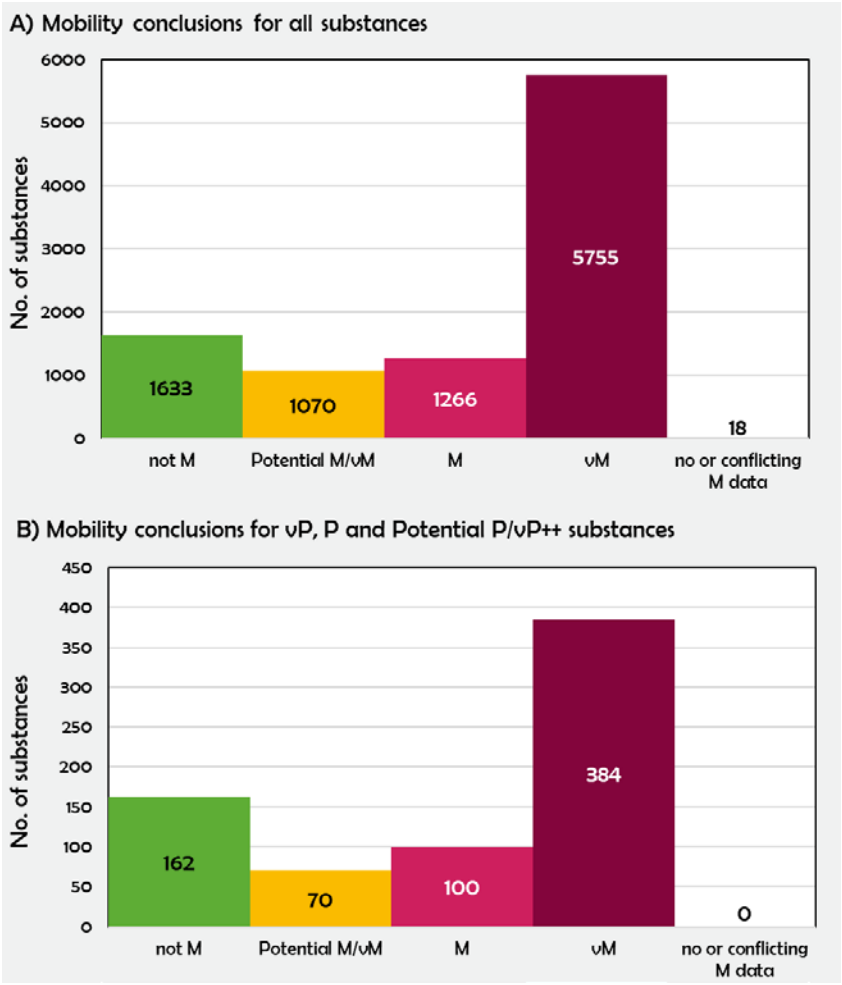
The "analytical gap" refers to substances were quantification requires either dedicated methods or state-of-the-art methods (Reemtsma et al., 2016).Source: Original figure

From Figure 10, it can be seen that the distribution of log K_{OC} and log D_{OW} is spread over 14 orders of magnitude from below log -5 to greater than log 9. There is a somewhat bell-like distribution, with the peak of the distribution between 2 and 3 log units. Several substances have a log K_{OC} or log D_{OW} value below 0, which has recently been referred to as the "analytical gap" (Reemtsma et al. 2016). This is because these substances are too mobile to be measured by traditional gas chromatography and reverse-phase liquid chromatography and require either dedicated or state-of-the-art methods for analysis. The distribution between all primary organic constituents in REACH registered substances (Figure 10a) and those meeting the persistency criteria (Figure 10b) is visually very similar. The most striking difference is that there is more experimental log K_{OC} (dark blue) and log D_{OW}/log K_{OW} (light blue) data for substances meeting the P, vP and Potential P/vP++ criteria. An explanation for this is that

substances with high quality P and vP data tend to have experimental log K_{OC} or log D_{OW}/log K_{OW} data available as well.

The data in Figure 10 is replotted in terms of M/vM conclusions in Figure 11 for all the REACH registered substances (Figure 11a) and just those where the P, vP or Potential P/vP++ criteria were met (Figure 11b). In both cases, more than half of the substances received a vM conclusion (59% and 54%, respectively) or M conclusion (13% and 14%, respectively). A conclusion of "Not M" was drawn for 17 and 22% of substances, respectively. Only a minority of substances were concluded to be "Potential M/vM" (13% and 11%, respectively) and only in rare cases could no conclusions for mobility be made. Unlike the P criteria, the data needed to draw a M conclusion are more readily available. Reasons for this are that log $K_{OC,}$ log K_{OW} and pKa tests are cheaper and less time consuming to conduct than half-life simulations, log K_{OW} is a mandatory reporting requirement at the 1 tonne per annum level, and QSARs for log K_{OW} and pKa are more accurate relatively speaking than QSARs for persistency half-lives (Arp et al., 2017).

Figure 11: Distribution of mobility conclusions for a) the 9742 REACH registered substances containing a known organic constituent greater than 0.1%, and b) only those that met the P, vP and Potential P/vP++ criteria (716 substances).



Source: Original figure

According to the PMT, vPvM assessment scheme (shown in Figure 3), only PM and vPvM substances are evaluated further for toxicity. Based on this analysis, of the 716 substances that met the P, vP or Potential P/vP++ criteria, 162 are considered "Not M", 70 are considered "Potential M/vM", 100 as M and 384 as vM. There are therefore 484 substances that meet the PM or vPvM criteria and need to be evaluate for toxicity.

7 Toxicity

The PMT/vPvM criteria for Toxicity (T) is based on those of Annex XIII for the PBT assessment (situations a, b and c in Box 4), though contains additional considerations specifically for drinking water exposure (Neumann and Schliebner, 2019) as presented in Box 4.

Box 4. T criterion

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 or 1B), germ cell mutagenic (category 1A or 1B), or toxic for reproduction (category 1A, 1B, or 2) according to Regulation EC No 1272/2008;

(c) there is other evidence of chronic toxicity, as identified by the substance meeting the criteria for classification: specific target organ toxicity after repeated exposure (STOT RE category 1 or 2) according to Regulation EC No 1272/2008;

The preceding situations are those described in Annex XIII, 1.1.3 of REACH. Beyond these situations, there might be cases, where it is necessary to identify persistent and mobile (PM) substances with other properties posing a risk to human health and the environment. In such cases an equivalent level of concern to the T-criteria set out in Annex XIII, 1.1.3 of REACH, should be demonstrated. Aspects to be considered are comparable to the SVHC-identification for respiratory sensitizers and include:

- Type and severity of possible health effects,
- Irreversibility of health effects,
- Delay of health effects,
- Is derivation of a 'safe concentration' possible?
- Effects on quality of life and societal concern,
- Others.

Evidence (so called indicators) for significant risk to human health and the environment for persistent and mobile (PM) substances in arises in any of the following situations:

(d) the substance meets the criteria for classification as carcinogenic (category 2), or germ cell mutagenic (category 2) according to the CLP Regulation EC No 1272/2008;

(e) the substance meets the criteria for classification as additional category for "effects on or via lactation", according to Regulation EC No 1272/2008;

(f) the Derived-No-Adverse-Effect-Level (DNEL) is ≤ 9 µg/kg/d (oral, long term, general population), as derived according to Annex I of REACH;

(g) the substance acts as an endocrine disruptor in humans and/or wildlife species according to the WHO/IPCS definition of an endocrine disruptor.

Source: Neumann and Schliebner (2019)

7.1 Justification of the T criteria

REACH considers exposure to the general human population, including pregnant women, children and the elderly. A central concern with persistent and mobile substances is that they could build up over time in the sources of our drinking water to levels that may eventually cause hazardous effects, either alone or as mixtures, to vulnerable populations, and remain in the environment for some time after emissions have ceased. Considering that human populations and remote environments will be exposed to such substances over long time scales, a chronic exposure hazard-based approach to their

identification is warranted. The T criterion within the PMT/vPvM assessment reflects this. Substances that lower the aesthetic quality of drinking water should be considered as well, as expressed in Annex 1, article 0.10 of REACH that states "*particular effects, such as […] strong odour and tainting*" to drinking water should be avoided.

Some of the additional T aspects considered in the PMT assessment, compared to those presented in REACH Annex XIII for the PBT assessment, are carcinogenic category 2, cell mutagenic category 2, and endocrine disrupting properties. These criteria were previously included in an earlier version of the PBT assessment, before Annex XIII was established (Matthies et al., 2016). Another T-consideration unique to the PMT assessment is including a Derived-No-Adverse-Effect-Level (DNEL) of ≤ 9 µg/kg/d (oral, long term, general population). This DNEL cut-off within the PMT/vPvM assessment was justified by Kalberlah et al., (2014) based on a study that derived "thresholds for toxicological concern" (TTC), and found that 9 µg/kg/d was the DNEL (oral, long term, general population) cut-off for 95% of substances exhibiting "moderate or low biological activity" (Barlow, 2005; Kalberlah et al., 2014).

7.2 Guidelines for the T assessment

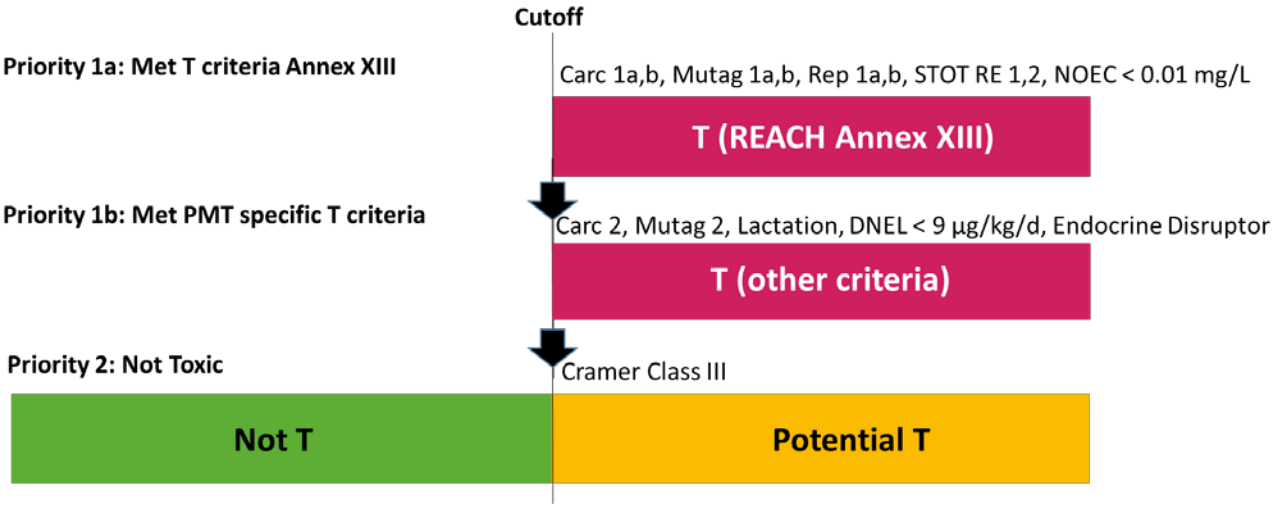
The T assessment is a combination of hazard categories and threshold concentrations. Ideally harmonized classifications for the hazard categories (CMR, STOT RE, lactation effects) should be utilized, and the NOEC/EC10 and DNEL threshold concentrations should be based on high-quality experimental values. If multiple NOEC/EC10 and DNEL values exist, the lowest value should be used, unless there is a reasonable explanation as to why this is not suitable.

Carcinogenic categories (1A, 1B, and 2), germ cell mutagenic categories (1A, 1B and 2), toxic for reproduction (1A, 1B and 2), specific target organ toxicity after repeated exposure (STOT RE category 1 or 2) and effects on lactation are mandatory for reporting according to the CLP registration (Regulation (EC) No 1272/2008); therefore, this data is already required during REACH registration. The threshold concentrations for the NOEC or EC10 for marine or freshwater organisms are less than 0.01 mg/l and the DNEL ≤ 9 µg/kg/d (oral, long term, general population). An assessment of NOEC or EC10 is mandatory as part of the PBT assessment in Annex XIII of REACH. The DNEL criteria, which is unique to the PMT/vPvM criteria (Kalberlah et al., 2014; Neumann and Schliebner, 2019), is required under REACH for substances registered with volumes of 10 t/y and that fulfil the criteria for classification in any of the hazard classes or categories listed in Article 14(4) of REACH as amended on 1st December 2010 by Article 58(1) of Regulation (EC) No 1272/2008 (CLP Regulation). Therein, the DNEL of the most predominant exposure pathway is to be reported, with key exceptions being intermediates and substances where it is not technically possible to derive DNELs (ECHA, 2012). The "oral, long term, general population" DNEL is not always the dominant exposure pathway, and therefore not as commonly reported as other toxicological properties in the T assessment. Nevertheless, a determination of this value for all substances considered to be PM, as part of the PMT/vPvM assessment, is recommended (Neumann and Schliebner, 2019). Similarly, an assessment of "endocrine disruption" is recommended for PM substances, even though this is not required as part of the REACH registration. An assessment of endocrine disruption has recently been required for plant protection products and biocides (Commission Regulation (EU) 2018/605 and Commission Delegated Regulation (EU) 2017/2100, respectively). Thereby assessments of endocrine disruption may exist for those REACH registered substances that are also plant protection products and biocides. The first step to assess if a substance is an endocrine disruptor is to see if it fulfils the hazard criteria of the WHO/IPCS definition of an endocrine disruptor. Guidance on how to interpret results from various assays providing endocrine relevant endpoint information is given in the OECD Guidance Document 150 and in the EFSA/ECHA guidance document (Andersson et al., 2018). It should be noted that substances that are identified as endocrine disruptors, though have not yet been identified as such under REACH, should additionally be proposed as an SVHC following the WHO/IPCS definition of an endocrine disruptor and the equivalent level of concern argument of Art. 57 (f).

Regarding multi-constituent and UVCB substances, different constituents within the substance will be responsible for the harmonized T criteria (which can apply to the whole substance mixture, see REACH Annex XIII section 1.1.3). The constituents that are T within the substance mixture may be different than those fulfilling the PM criteria within the mixture. In this special case, the multi-constituent or UVCB substance would be considered PMT until it is proven that the PM constituents are not T.

The overall guideline for the T assessment is presented in Figure 12. This figure shows that if a PM or vPvM substance fulfils the T criteria according to Annex XIII of REACH (**Priority 1a** in Figure 8) as part of the PBT assessment, it would be considered PMT, or possibly vPvMT. If a substance does not meet the T criteria based on Annex XIII, the substance is assessed for situations relevant to PM substances in drinking water (i.e. situations d – g in Box 4; **Priority 1b** in Figure 12). If the substance does not meet any of the Priority 1a or Priority 1b T criteria, the chemical structure of the substance should be screened using the Cramer classification scheme, which is used to make a "Threshold of Toxicological Concern" estimation (Kalberlah et al., 2014). Within this classification, Class I and Class II Cramer classes are considered "Not T", but a Class III definition implies *"…chemical structures that permit no strong initial impression of safety and may even suggest a significant toxicity*" (Cramer et al., 1976). As part of **Priority 2**, Class III structures are considered "Potential T", and Yellow according to the traffic light system for data quality (Table 1).

Figure 12: Schematic representation of the approach used to evaluate T

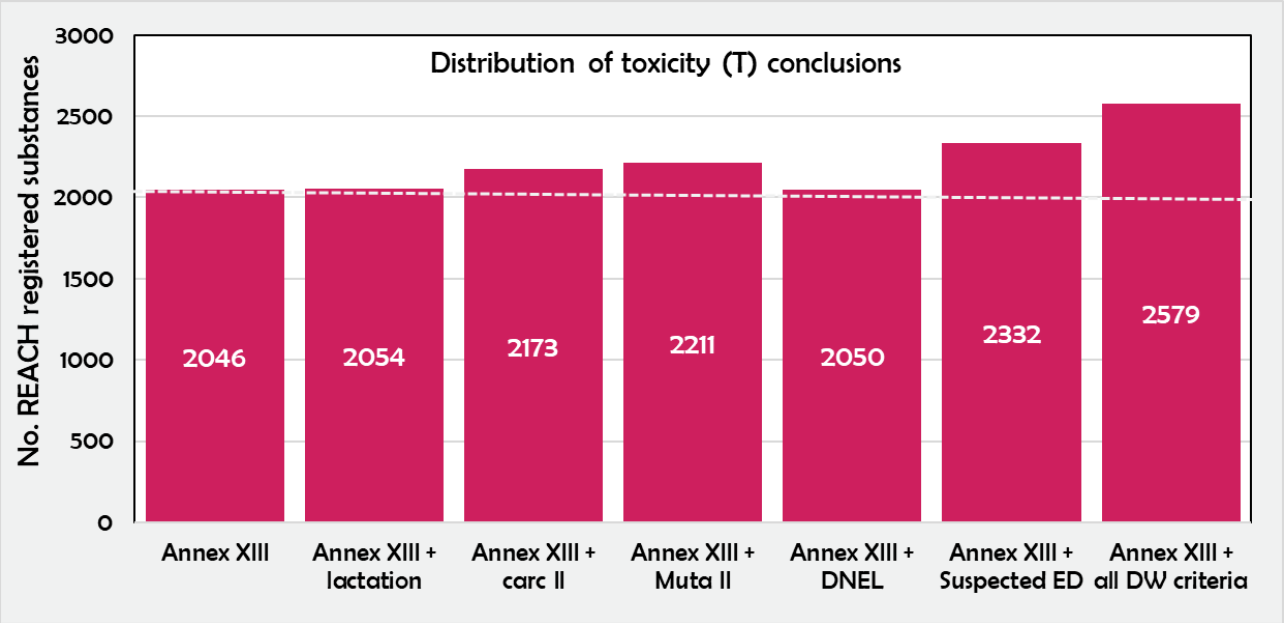


Source: Original figure

7.3 Conclusion of the T assessment

The T assessment was conducted according the guidelines above and data sources presented in Annex 2. The conclusions for the 9742 REACH registered substances registered as of May 2017 with identifiable organic constituents is presented in Figure 13.

Figure 13: Number of the 9742 REACH registered substances registered as of May 2017 containing organic constituents that fulfil the Annex XIII T criterion, along with additional T situations specific to the PMT assessment

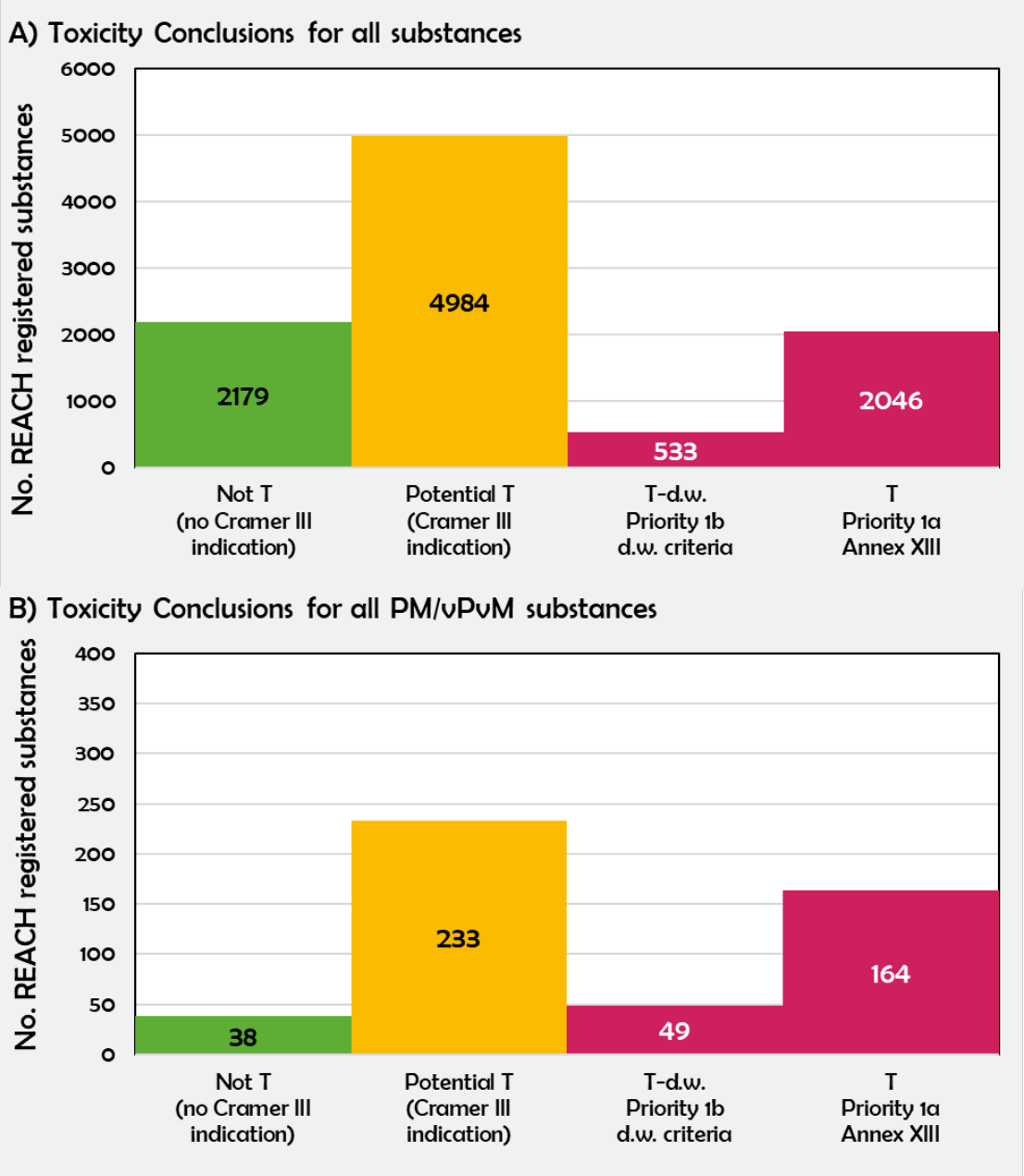


Source: Original figure

The additional toxicity situations in the PMT assessment (situations d – g in Box 4) only result in a moderate increase in the number of substances fulfilling the T criteria, from 21% (2046 of 9742) using the REACH Annex XIII criteria to 26% (2479 of 9742) using the PMT criteria. This is mostly due to including carcinogenic Category 2 (127 additional substances), mutagenic Category 2 (165 additional substances) and *suspected* endocrine disruptors (286 additional substances). It is emphasized that these are "suspected" endocrine disruptors (see Annex 2), as this assessment did not use the most recent commission regulations (i.e. Commission Regulation (EU) 2018/605 and Commission Delegated Regulation (EU) 2017/2100). Including the DNEL-criterion only had a minor effect (14 substances considered T that would not have been otherwise). This is due to DNEL (oral, general population) data being only available for a minority of substances.

The T conclusions for all 9742 REACH registered substances for which a dominant organic constituent above 0.1% could be identified is presented in Figure 14a. This figure shows that 2579 substances (26%) are considered T, 2179 substances (22%) considered "Not T" and 4984 substances (51%) are considered "Potential T". In Figure 14b, the T conclusions are presented for the 484 substances that are considered PM and vPvM (i.e. those meeting the M or vM criteria, along with P, vP or Potential P/vP++ criteria, see Chapter 6.3). Of these, only 213 substances (46% of the PM/vPvM) are considered T, whereas 38 substances (8%) are considered "Not T" and 233 substances (46%) as "Potential T" because of their Cramer Class III structure.

Figure 14: Distribution of toxicity conclusions for a) all 9742 REACH registered substances containing a known organic constituent greater than 0.1% and, b) just the 484 REACH registered substances meeting the PM and vPvM criteria with sufficient data quality



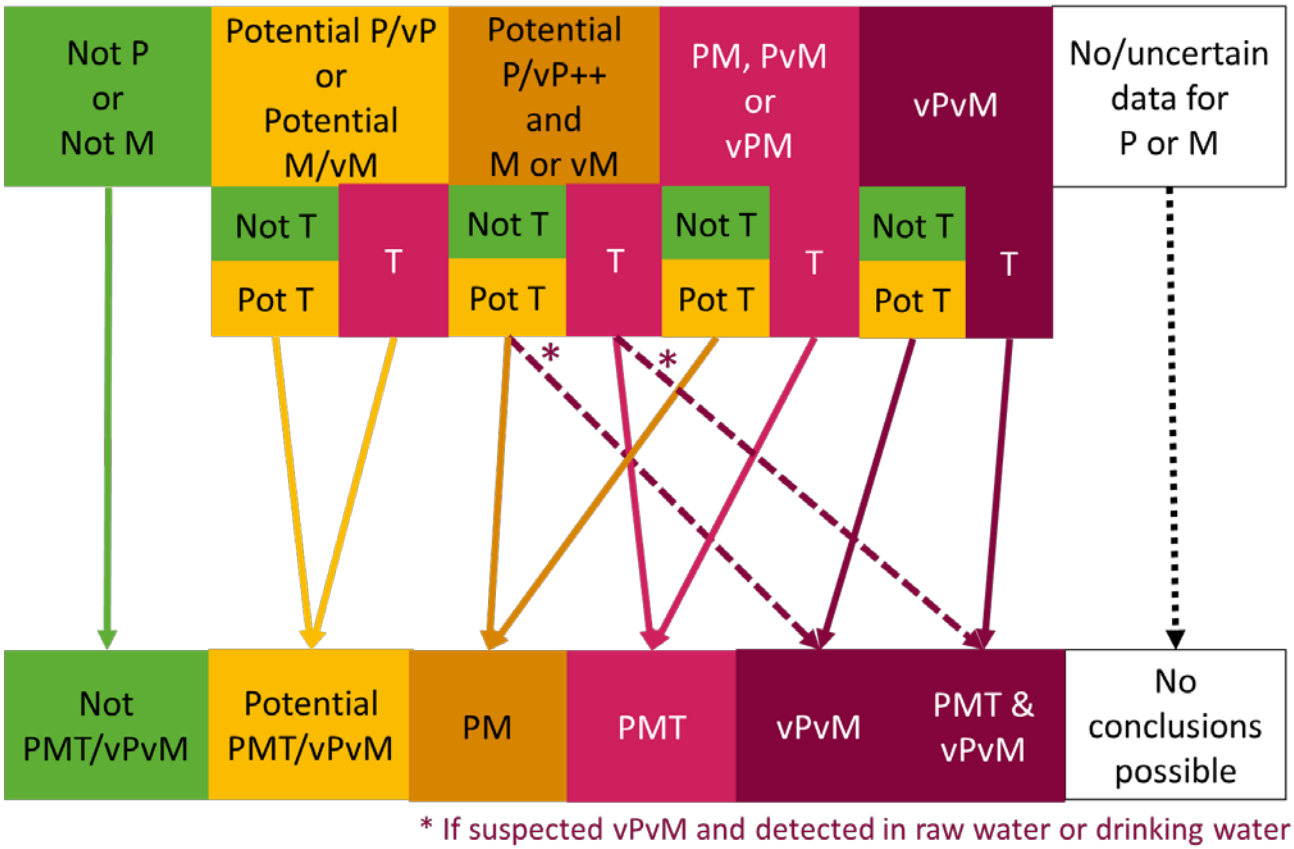
Source: Original figure

8 PMT/vPvM assessment

8.1 Guidelines for the PMT/vPvM assessment

Based on the "traffic light" system of the P, M and T assessment, as presented in Table 1, the final PMT/vPvM conclusion is only definitive in cases where each criterion is clearly met (red) or not met (green). The approach for integrating the conclusions of the P, M and T assessment following the "traffic light" system is illustrated in Figure 15.

Figure 15: Guidelines for making the final PMT/vPvM assessment based on individual P, M and T conclusions, using the "traffic light" system to address data quality.



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Seven different final conclusions from the PMT/vPvM assessment can result, depending on which criteria are met and their relative degree of certainty.

No conclusions possible –Either data for a P or M assessment at the screening level is lacking (white). Efforts should be made to obtain appropriate screening data.

PMT & vPvM - Indicates there is sufficient weight of evidence that the substance meets both the vP and vM criteria as well as the T criterion.

vPvM - Indicates there is sufficient weight of evidence that the substance meets both the vP and vM criteria but not the T criterion.

PMT - Indicates that there is sufficient weight of evidence that the substance meets the P, M and T criteria.

PM – Indicates there is sufficient weight of evidence that the substance meets both the P and M criteria but does not met the T criterion nor the vPvM criteria. These comprise of PM, vPM and PvM substances, but not PMT/vPvM substances. Though these substances are not prioritized

as a risk to the sources of our drinking water, investigating these substances further for potential hazards if they become widespread in the environment, such as in the case of high emissions or the formation of PMT/vPvM transformation products, is recommended.

Potential PMT/vPvM – Indicates that only screening or low-quality data is available for P, M or both, and that either a conclusion of "Potential P/vP" and/or "Potential M/vM" was obtained. Such screening or low-quality data cannot rule out the conclusion of P or M. Efforts should be made to obtain half-lives or K_{OC} data, or equivalent information.

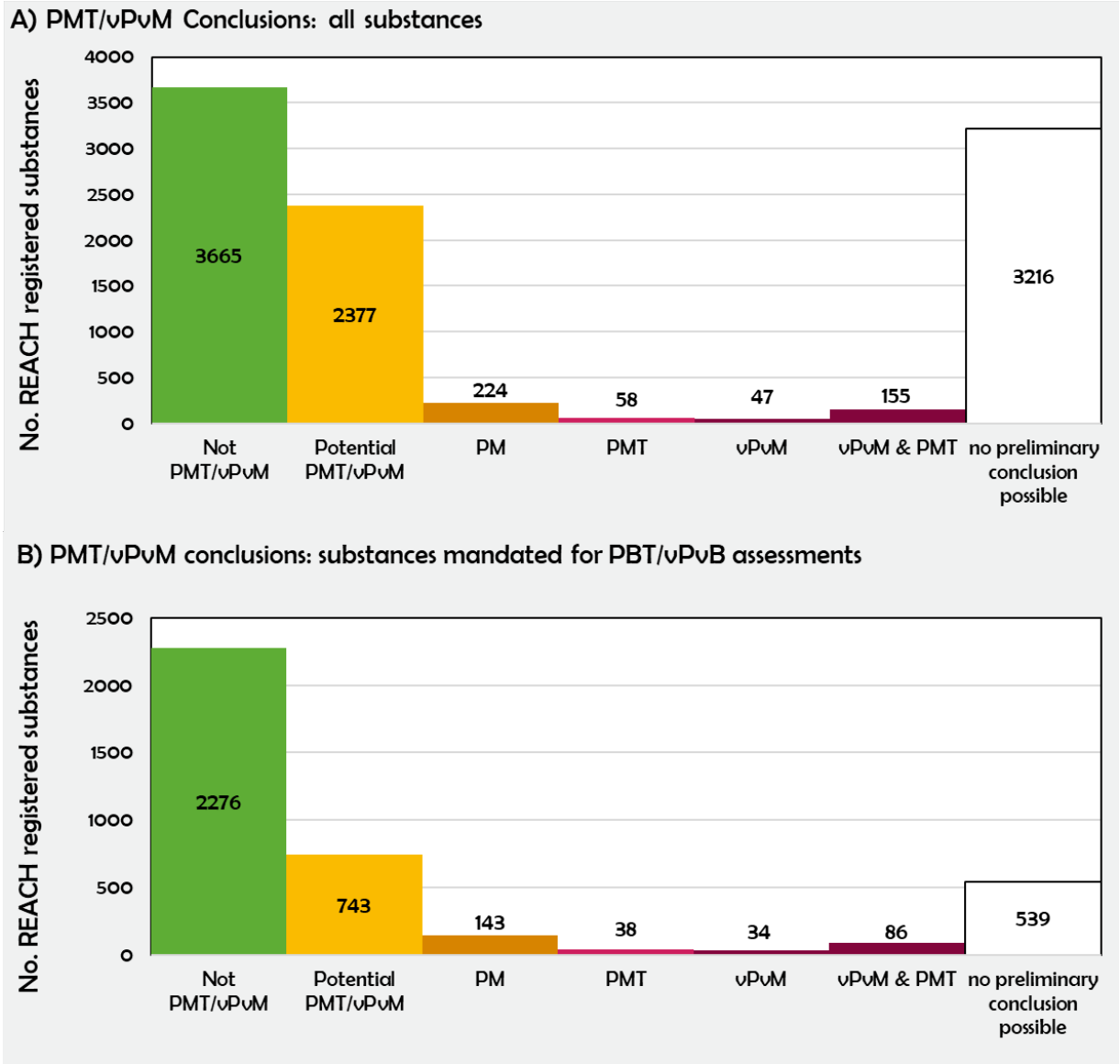
Not PMT/vPvM – Indicates that either the criteria for "Not P" or "Not M" was met with sufficient weight of evidence (green), the substance is therefore neither PMT nor vPvM.

A special case for drawing the conclusions PM, PMT and vPvM is when the persistency assessment results in "Potential P/vP++" (dark yellow). As described in Section 5.2, this assessment means that there is sufficient weight of evidence that the substance meets the P criterion, but it is unknown if it meets the vP criteria. To resolve this, the following method is recommended (as illustrated with dashed, red arrows in Figure 15). If a substance meeting the "Potential P/vP++" criteria meets the vM criteria and has been observed in a drinking water or a raw water monitoring study, or if the weight of evidence leans more toward vP than P, it is considered vPvM; otherwise it is considered PM. Such substances may then be considered "vPvM & PMT" or "PMT" depending on if they also meet the T criterion.

8.2 Conclusion of the PMT/vPvM assessment

The overall outcome of the PMT/vPvM assessment of all 9742 REACH registered substances as of May 2017 is presented in Figure 16a. Figure 16b presents the outcome for 3859 of those substances where a PBT/vPvB assessment is required (i.e. those are produced or imported in amounts more than 10 tonnes per year and not are used as intermediate (according to Article 14(1) of the REACH regulation, see Chapter 4.2.). This data is presented as a similar exemption could be foreseen for the PMT/vPvM assessment.

Figure 16: Distribution of PMT/vPvM conclusions for a) 9742 REACH registered substances containing an organic constituent greater than 0.1%, b) the 3859 substances which are mandated for PBT/vPvB assessments



Source: Original figure

The number (and percentage) of substances where no PMT/vPvM conclusion could be drawn were 3216 (33%) for all REACH registered substances and 539 (14%) for those substances for which a PBT/vPvB assessment is required. This decrease in percentage can be attributed to an increase in available P data for substances requiring a PBT/vPvB assessment. There were only 12 substances from all the REACH registered substances as of May 2017 where an M assessment could not be carried out. These few substances were outside the application domain of the implemented QSAR methods for estimating D_{ow}. It is apparent from this assessment that P remains the largest data gap for both the PMT/vPvM assessment, as it is for the PBT/vPvB assessment (Strempel et al., 2012).

Of the substances where it was possible to draw a conclusion, the most frequent conclusion was "Not PMT/vPvM" (green), which applied to 3665 (36%) of all REACH registered substances and 2276 (58%) substances for which a PBT/vPvB was required. In most cases this was due to the "Not P" conclusion (i.e. 2525 of all REACH registered substances), otherwise it was due to "Not M" (i.e. 980 of all

REACH registered substances). In cases where no P data was available, a conclusion of "Not PMT/vPvM" could be reached if the substances was considered "not M", which applied to 538 (6%) and 170 (4%) of the complete list of REACH registered substances and just those mandated for PBT/vPvB assessments, respectively.

The conclusion "Potential PMT/vPvM" was reached for 2377 (24%) of all REACH registered substances and 743 (19%) of those where the PBT/vPvB assessment was required. Recall from Table 1 that "Potential PMT/vPvM" refers to substances in which the available screening or low quality data cannot result in a conclusion of "Not PMT/vPvM", but at the same time there is not enough evidence to conclude "PMT/vPvM". In approximately 80% of these cases, the "Potential PMT/vPvM" classification was due exclusively to only screening or low-quality data for P being available (at the Priority 2 or Priority 3 level, according to Figure 4). For the remainder of cases this was due to only screening or low-quality data being available for both P and M. It was very rare that "Potential PMT/vPvM" was assigned to substances which met the P criteria due to high quality half-life data in combination with a "Potential M/vM" conclusion (due to a lack of K_{OC} and the D_{OW} or K_{OW} being near the screening cut-off (see Figure 9). This occurred only for 12 of all REACH registered substances.

There were 224 (2%) and 143 (4%) substances considered PM of all REACH registered substances and those where the PBT/vPvB assessment was required, respectively. Most of these (approximately 80%) had the conclusions of PvM or "Potential P/vP++" and M; therefore, it is possible that some of these could become PMT/vPvM in the future if new data becomes available that indicates toxicity or more environmental persistence than has currently been demonstrated.

Ultimately, only 260 (3%) of all REACH registered substances with an organic constituent were considered PMT, vPvM or vPvM & PMT (comprising of 58, 47 and 155 substances respectively). The corresponding result for the substances where PBT/vPvB assessment was required was 158 (4%) being considered PMT, vPvM or vPvM & PMT (comprising of 38, 34 and 86 substances, respectively).

There were four substances registered as PBT that also met the PMT criteria in this assessment. These are anthracene (CAS 120-12-7), 4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol (CAS 561-41-1), PFOS (CAS 56773-42-3) and dimethyl naphthalene-2,6-dicarboxylate (CAS 840-65-3).

The final list of REACH registered substances that were considered to meet the PMT, vPvM or both is presented in Annex 1.

9 Impact Assessment

Potential impacts the implementation of the PMT/vPvM criteria could have on the status quo of the chemical industry and drinking water sector in the EU is a topic of ongoing discussion. Key questions relating to this potential impact are:

- How many REACH registered substances fulfil the PMT/vPvM criteria?
- How many of these substances are emitted, or could be emitted, into the environment in a way that contaminates the sources of our drinking water?
- How many of the REACH registered PMT/vPvM substances are already subject to regulation?
- What are the potential costs / benefits of acting upon such a list?

9.1 Proportion of REACH registered substances considered PMT/vPvM

The previous chapter reported that the number of substances meeting the PMT/vPvM criteria ranged from 158 to 260, depending on whether only substances requiring the PBT/vPvB assessment are considered or whether all REACH registered substances are considered. This is only 1.0% to 1.7% of the complete list of 15469 REACH registered substances (as of May 2017), respectively. This is considered a minor portion of REACH registered substances. Over time this proportion could change as new and better-quality data becomes available that could add or remove PMT/vPvM substances from the list, including data related to transformation products and impurities that would add substances to the list.

Two other recent studies present a similar result that only a minor amount of REACH registered substances is considered PMT/vPvM. The first is a study from the Danish Environmental Protection Agency and the Technical University of Denmark (DTU) (Holmberg et al., 2019), which will be referred to here as the "Danish study"; the second is the "Hot-Target" approach, carried out by the German Water Centre of the German Gas and Waterworks Association (Nödler et al., 2019).

The Danish study (Holmberg et al., 2019) used an earlier version of the PMT/vPvM assessment criteria to develop an independent QSAR based approach to screen for PMT/vPvM substances utilizing the Danish QSAR database (http://qsar.food.dtu.dk). Similar to the present report, the Danish study was also based on primary organic constituents and not on transformation products and impurities. The Danish study considered: 1) different levels of strictness of the QSARs used to evaluate P (i.e. different simulated thresholds that correspond to the P-criteria, accounting for data uncertainty); 2) a sensitivity analysis of different D_{OW} values for the M criterion; and 3) only mono-constituent substances with volumes produced at 10 tonnes per year per manufacturer or importer, for which CAS or structural information could be found (by June 2017). These three conditions corresponded to 2073 REACH registered substances. The Danish study reported that between 16 and 96 substances were considered to meet the vPvM criteria and between 37 and 166 substances were considered to meet the PMT criteria. The number of substances depended on the QSAR approach used and how output uncertainty was considered. Considering all the QSAR approaches tested, 53 to 268 substances were determined to be either PMT/vPvM in at least one of the approaches. Therefore, here again, a relatively minor portfolio of REACH registered substances (0.3 to 1.7%) were considered to meet the PMT/ vPvM criteria from this assessment.

The Hot-Target approach (Nödler et al., 2019) has both differences and similarities with the current PMT/vPvM assessment approach. The Hot-Target approach uses not only REACH registered substances as a starting point, but also includes substances from other databases of chemicals (such as pharmaceuticals and pesticides). Like the Danish study, the Hot-Target approach is mainly based on QSAR screening first, rather than on experimental data prioritized in this PMT/vPvM assessment. The

Hot-Target criteria for persistency was primarily based on the Biowin QSAR. The Hot-Target criteria for mobility were a) log D_{OW} ≤ 4.5 at pH 8, b) cation exchange ≤ 60% at pH 8 and c) a molecular mass less than 200 Daltons. Another unique consideration in the Hot-Target approach is that after an initial list of "Hot Targets" were identified, it applied additional screening criteria to further consider risk, such as tonnages, screening studies, and ability to penetrate state-of-the-art drinking water treatments via resistance to ozonolysis and sorption to activated charcoal (using a criterion of D_{OW} ≤ 2.5). Finally, substances that met these subsequent criteria were considered individually for a final risk assessment on a case-by-case bases, to differentiate true Hot-Targets from Hot-Target candidates that are not perceived to be of concern to drinking water. Based on these differences, the Hot-Target approach can be considered as a more risk-based approach than the purely hazard-based PMT/vPvM criteria. The results of the Hot-Target study can be summarized as follows. Starting from approximately 10400 substances, a total of 2671 was considered as potentially drinking water relevant PM(T) substances. This number was reduced to 763 substances that could not be removed efficiently from drinking water, and ultimately manually refined to 89 substances that were considered as Hot-Targets based on additional considerations. Here again, considering a broad database of substances, only a minor fraction (0.9%) was considered relevant to pose a threat to the sources of our drinking water.

Though all three studies conclude PMT/vPvM substances are rare within REACH, the substances that were flagged as PMT/vPvM or Hot-Target was not identical across studies. This is related to the complexity of using different starting sets of substances, differences between the use of experimental and QSAR data, differences in criteria, etc. As an example, in the guidelines presented in Chapter 5 in this report, QSAR data is not used for the P assessment unless it forms part of a weight of evidence evaluation; however, in the Danish study and Hot-Target study P assessments primarily relied on QSARs. Though QSARs for P are quite useful due to the extreme lack of experimental data, they are associated with substantial uncertainty (Strempel et al., 2012; Arp et al., 2017). Nevertheless, despite the uncertainty with QSAR based approaches, substances flagged as PMT/vPvM based on this study, the Danish study and the Hot-Target study deserve special attention; as these were independently identified as relevant for drinking water using different methodology. In Annex 1, Table A1, which presents the PMT/vPvM substances identified in this study, it is indicated which of these substances were also identified as PMT/vPvM substances using the Danish study or the Hot Target approach.

9.2 Impact of PMT/vPvM vs PBT/vPvB substances

PMT/vPvM substances may be considered of an equivalent level of concern to PBT/vPvB substances (Neumann and Schliebner, 2019), based on the following rationales given in ECHA's PBT/vPvB guidance *"PBT or vPvB substances may have the potential to contaminate remote areas that should be protected from further contamination by hazardous substances resulting from human activity because the intrinsic value of pristine environments should be protected"* […] *"the effects of such accumulation are unpredictable in the long-term"* […] *"such accumulation is in practice difficult to reverse as cessation of emission will not necessarily result in a reduction in substance concentration"* (ECHA, 2017a) as these concerns apply equivalently to PMT/vPvM substances. PBT/vPvB substances can potentially bioaccumulate in biota to levels that cause harmful effects; PMT/vPvM substances can potentially accumulate in the sources of our drinking water to levels that cause adverse effects through chronic exposure. For both, "*the level of uncertainty in identifying long-term risk cannot be estimated with sufficient accuracy*" (ECHA, 2014). The long-term risks are often only identified retrospectively. Once these risks occur, "*consequences of an underestimation of adverse effects are not easily reversible by regulatory action*" (ECHA, 2014). Actions to reduce emissions would be slow to take effect, because of the persistency of the substance, with the potential for the risk to persist over multiple generations and even intergenerational time scales. Even after regulatory measures, mobile substances are still problematic, e.g. MTBE (Goldenman et al., 2017) and certain chlorinated solvents (Di Lorenzo et al., 2015). A strategy to precautionarily minimize emissions is needed. Post hoc reactions to observed harm are too late.

Collectively, vPvM and vPvB substances would comprise many vP substances, which are in general problematic: "*From the standpoint of public health, environmental protection and economic growth, it appears desirable to take a more precautionary and proactive approach and to prevent and/or minimise releases of vP chemicals in the future*" (EC, 2017).

The main inherent difference between persistent and bioaccumulative and persistent and mobile substances is their pathways of exposure and transport. For PBT/vPvB substances, human and animal exposure is primarily via the food chain through bioaccumulation. For PMT/vPvM substances, human and ecosystem exposure is primarily through freshwater systems and accumulation in the sources of our drinking water, though other pathways are also possible, such as enrichment in edible crops (Blaine et al., 2013; Felizeter et al., 2014). ECHA's PBT/vPvB guidance concludes that "*a "safe" concentration in the environment cannot be established using the methods currently available with sufficient reliability for an acceptable risk to be determined in a quantitative way*". This conclusion applies also to PMT/vPvM substances.

9.3 Monitoring and Emissions of PMT/vPvM substances

As outlined in Annex I (4.0.2) of REACH, for substances that meet the PBT/vPvB criterion, the registrant must carry out, "Step 2: Emission Characterisation". The emission characterisation for PMT/vPvM substances could follow a similar procedure as is already in place for PBT/vPvB substances, particularly based on the argument in the previous section that PMT/vPvM substances are of an equivalent level of concern as PBT/vPvB substances. Details of how this characterization can be carried out are given in sections R.11.3.4 and R.11.4.1.4 of the REACH PBT guidance document (ECHA, 2017a). The purposes of this emission characterization are:

- *to identify and estimate the amount of releases of a "PBT or vPvB-substance" to the environment;*
- *to identify exposure routes by which humans and the environment are exposed to a "PBT or vPvB-substance".* (ECHA, 2017a)

With this information, it is possible to develop risk management measures (RMM) to prevent or minimize such exposure from occurring. In some cases, the emission characterization would indicate that a given PBT/vPvB substances is not being emitted substantially and does not require a RMM. In other cases, this data can provide a starting point for the development of RMM to reduce exposure.

In addition to the "Emission Characterization" following that of PBT/vPvB substances, for PMT/vPvM assessments, water cycle enrichment and potential accumulation in local sources of drinking water should be focussed on and included. Here two components to be considered in this regard are presented. The first is monitoring data to investigate if the substance is detected in sources of our drinking water and the second is the consideration of the likelihood of emissions based on what the substance is used for.

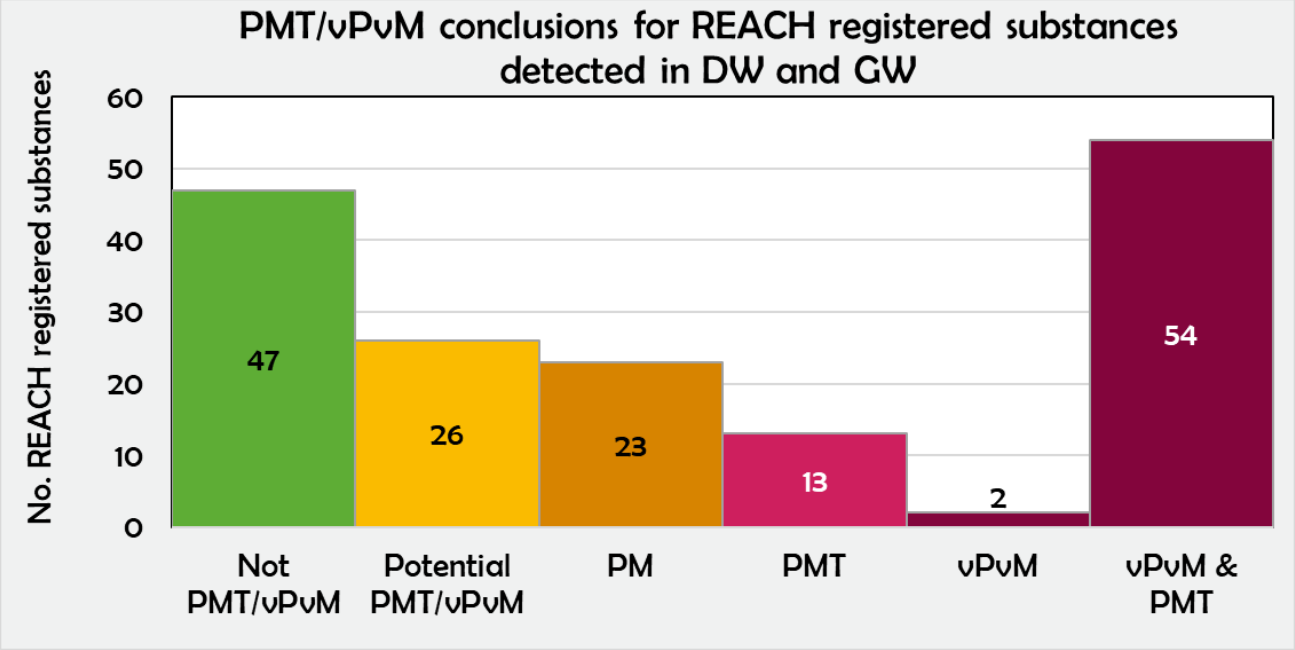
9.3.1 Monitoring of PMT/vPvM substances

Chapter 2 presented a review of REACH registered substances that have been detected in drinking water and groundwater. In addition to that chapter, a new investigation of REACH registered substances in drinking water and also raw water in different European watersheds has recently been published (Schulze et al., 2019). The Schulze et al. (2019) paper is of special importance as it selected 57 REACH registered substances prior to monitoring, purely based on whether they were persistent and mobile (PM substances) as well as if their REACH registered uses indicated a potential to be emitted. The procedure used by Schulze et al. (2019) for the PM assessment was presented in an earlier publication (Schulze et al., 2018). Schulze et al. (2019) were able to detect 43 of the 57 chosen PM analytes after hypothesizing they would be present; 23 of which were never detected in the environment before. It is

highly likely that the 14 they did not detect was in large part due to uncertainties with the emission likelihood, more so than the persistency and mobility evaluation. This provides direct support that the PMT/vPvM assessment can be used – with some success – to predict that the substance will be found in the sources of our drinking water after emissions are established. The discovery of so many PM substances for the first time gives further support to the argument that there are more PM/PMT/vPvM substances in the environment than we are aware of, due in large part to the lack of methods and standards currently available to identify many mobile substances in environmental samples (Reemtsma et al., 2016). The PMT/vPvM criteria in combination with emission information is therefore useful to identify substances for monitoring programs, such as the Norman List for emerging substances, to help both develop analytical methods and to help identify emerging substances in the sources of our drinking water.

Figure 17 presents the outcome of the PMT/vPvM assessment for the 166 REACH registered substances detected in drinking water, groundwater and raw water, where 142 of these were presented in Chapter 2 along with an additional 24 unique substances that were identified by Schulze et al. (2019) not included in Chapter 2. The PMT/vPvM assessment for these 166 substances presented in Figure 17 can be found in Annex 1, Table A1.

Figure 17: PMT/vPvM assessment of 166 REACH registered substances that have been detected in drinking water (DW), groundwater (GW) and raw water



Source: Original figure.

Figure 17 shows that not all substances that are present in drinking water, groundwater or raw water meet the PMT/vPvM criteria. A total of 47 of the 166 substances (28%) in Figure 17 are considered "Not PMT/vPvM". Such substances could appear in the sources of drinking water for several reasons, including large environmental emissions, the source of contamination being very local (e.g. additives in water pipes that leach) or only minimalistic water treatment being used. "Not PMT/vPvM" substances that are present in the sources of our drinking water are not considered as problematic PMT/vPvM substances. When the emission sources of "Not PMT/vPvM" substances are removed it is expected that their concentrations in the environment and in drinking water are reversible and will decrease and disappear within a reasonable time frame, and in addition that the contamination is local

and will not spread rapidly to pristine areas. PM and PMT/vPvM substances, on the other hand, are more problematic, and have more potential to be widespread and recalcitrant long after their emissions have ceased. The majority of substances in Figure 13 are either PM, PMT, vPvM or Potential PMT/vPvM (72%), with 54 of the 166 substances (33%) being considered both PMT and vPvM.

9.3.2 Emission Likelihood

It was not possible to carry out an emission characterization for individual substances on a case-by-case basis according the PBT guidelines (ECHA, 2017a) in this research project. This would require extensive amounts of production and use data. Instead, a more simplistic screening approach was used. This approach is referred to as the "Emission Likelihood", and is based on the Emission-Score (E-Score) system (Schulze et al., 2018), which only requires REACH registered data as input, as presented in Equation 6:

$$\text{E-score} = \log(\text{tonnage} + 1.1) \times \Sigma\text{UC-scores} \quad (6)$$

where "tonnage" is the tonnage registered in REACH and "ΣUC-scores" is the sum of scores from seven individual "Use Characteristics" (UC). The different UCs and their UC-scores are presented in Table 4 as well as the REACH categories they refer to. This includes "Environmental Release Categories", "Process Categories" and "Life Cycle Categories". More information about what the different type of categories are and how they are assigned can be found in the relevant guidance document on "Use Descriptions" (ECHA, 2015). If any of the REACH categories in Table 4 belonging to a given UC were registered then the "UC-score if True" was assigned to that specific UC, otherwise the "UC-score if False" was assigned. As an example, if for a given substance the "Environmental Release Category 2: Formulation into mixture" is registered in REACH then the substance would get a score of 7 for UC 1: High Release to the Environment. However, if for the same substance it was not registered with the "Life cycle category: "Consumer Uses", the score of 0.5 would be given for UC 6: Consumer use. The maximum and minimum values for "ΣUC-scores" are 21 and 6, respectively (Schulze et al., 2018).

Table 4: Use Characteristics (UCs) included in the calculation of the E-Score.

Use Characteristic (UC)	UC-score if True	UC-score if False	REACH categories
1: High release to environment	7	3	Environmental Release Categories: 2, 5, 8a, 8c, 8d, 8f, 10b, 11b, or 12b
2: Wide dispersive use	4	1	Environmental Release Categories: 8, 9, 10 or 11; Process Categories: 10, 11, 13, 15, 17, 18 or 19
3: Intermediate use	0	3	Registered as an Intermediate according to Article 3(15)
4: Closed system use	1	3	Process Categories: 1, 2 or 3
5: Professional use	1.5	0.5	Life cycle category: "Widespread uses by professional workers"
6: Consumer use	2	0.5	Life cycle category: "Consumer Uses"
7: Substance in article	0.5	0	Live cycle category "Article service life"

The maximum ΣUC-scores of 21 results from True for UC1, UC2, UC5, UC6 and UC7, and False for UC3 andUC4; similarly, the minimum score of 6 would be from the opposite. Source: Adapted from (Schulze et al., 2018)

Herein the tonnage information for the E-score was obtained from confidential dossiers from the REACH registration process, to which the authors had access. The UCs were obtained directly from publicly available REACH registration dossiers. To simplify the output of the E-score system, a final

"REACH emission likelihood" system was developed based on E-score and monitoring data, as presented in Table 5.

Table 5: REACH emission likelihood categories.

REACH emission likelihood	Detected in raw water, drinking water or groundwater	Registration type in REACH	E-score
Very High	Yes	Full	Top 50'th percentile
High	No	Full	Top 50'th percentile
Medium	Yes	Full	Lower 50'th percentile
	Yes	Intermediate	n/a
Low	No	Full	Lower 50'th percentile
	No	Intermediate	n/a

n/a= not applicable, all E-score percentiles considered

The "REACH emission likelihood" for PMT/vPvM substances and substances detected in drinking water and groundwater is presented in Annex 1, Table A1. Of the 260 PMT/vPvM substances registered under REACH there are 48 substances with a "Very High" REACH emission likelihood ranking (i.e. detected in sources of drinking water and associated with a high E-score), 99 with a "High" ranking (i.e. not detected in sources of drinking water but associated with a high E-score), 34 with a "Medium" ranking (i.e. detected in sources of drinking water, but not associated with a high E-score; contamination could come from non-REACH uses if primary use is pharmaceuticals, biocides or plant protection products) and 79 with a "Low" REACH emission likelihood ranking (i.e. not detected in sources of drinking water, and associated with a low E-score).

In addition to this generic REACH emission likelihood criteria, there are several individual case-by-case reasons why a substance may be considered to have a low REACH emission likelihood, or to only be problematic under specific situations, which the REACH emission likelihood criteria does not capture. As examples, four ionic yellow dyes with large molecular weights (> 350 Daltons) were considered vPvM with a high REACH emission likelihood score, yet these have never been detected in the environment (these are Pigment Yellow 17 CAS 5468-75-7, Pigment Yellow 13 CAS 5567-15-7, Pigment Yellow 139 CAS 36888-99-0 and Pigment Yellow 127 CAS 68610-86-6). Similarly, some substances are considered volatile (i.e. have a high Henry's Law coefficient) and are therefore easy to remove during water treatment. These are only relevant to sources of drinking water under specific contexts, like direct consumption of untreated groundwater. Of the PMT/vPvM substances suspected to have high emissions in Annex 1, there are three volatile substances identified (i.e. Chloromethane CAS 74-87-3, Chloroethane CAS 75-00-3, and Dimethyl ether CAS 115-11-6).

Another general issue with REACH registered substances is that sometimes different substances contain the same chemical constituent; as a result, the same chemical constituent that has received a PMT/vPvM assessment may occur in more than one REACH registered substance. Accordingly, the number of chemical constituents that are PMT/vPvM is herein smaller than the number of PMT/vPvM substances. Examples are two REACH registered substances that are considered PMT/vPvM because the contain cyanamide (calcium cyanamide CAS 156-62-7 and neutral cyanamide CAS 420-04-2), and another two substances which contain melamine (melamine CAS 108-78-1 and melamine cyanurate CAS 37640-57-6).

When risk considerations such as REACH emission likelihood are taken in to account, the number of chemical constituents that would be prioritized for further scrutiny decreases. Here, starting from the

260 substances registered under REACH, only 144 of these have a REACH emission likelihood of medium to very high and are required to undergo PBT/vPvB assessment. Removing the four dyes, three volatiles and two duplicates leaves 135 chemical constituents (or 0.9% of REACH registered substances as of May 2017).

9.4 PMT/vPvM substances known by European authorities

Twenty-one of the identified PMT/vPvM substances registered under REACH (Annex 1, Table A1) are already acknowledged by European Authorities as existing or potential pollutants. Some are on the candidate list of substances of very high concern (SVHC) for authorisation under REACH, others are listed as priority substances under the Water Frame Work Directive (2013/39 EU), others are included in water quality recommendations via the Drinking Water Directive (98/83/EC), or have other European guidelines/directives regarding their use. These are summarized in Table 6. The fact that there are relatively few substances that fall in to this category demonstrates a regulatory gap for substances that pose a hazard to the sources of our drinking water.

The REACH registered substance ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate (i.e. Gen X CAS 62037-80-3) in Table 6 was the most recent to be added to the candidate list of SVHC (in July 2019). A large part of the justification was its presence in the environment and arguments that it has PMT/vPvM properties, which result in an equivalent level of concern (ELoC) to PBT/vPvB substances (Article 57 (f)).

The substances listed in Table 6 do not need to be assessed for their PMT/vPvM properties as they are under regulatory scrutiny. This reduces the number of PMT/vPvM substances identified in this assessment and recommended for further follow-up by 13, as five are already exempted from follow-up due to low REACH emission likelihood or because they are exempted for PBT/vPvB assessments under REACH article 14. This brings the total number of PMT/vPvM substances recommended herein for follow-up from 135 to 122 (or 0.8% of the REACH registered list of May 2017).

Table 6: PMT/vPvM substances currently regulated in the EU.

CAS	Name	PMT/vPvM	REACH Emission Likelihood	Regulation
79-01-6	Trichloroethylene	PMT	very high	SVHC
107-06-2	1,2-dichloroethane	PMT	very high	SVHC
96-18-4	1,2,3-trichloropropane	vPvM&PMT	very high	SVHC
111-96-6	Bis(2-methoxyethyl) ether	vPvM&PMT	very high	SVHC
88-85-7	Dinoseb	vPvM&PMT	high	SVHC
85-42-7	Cyclohexane-1,2-dicarboxylic anhydride	vPvM&PMT	high	SVHC
25550-51-0	Hexahydromethylphthalic anhydride	vPvM&PMT	high	SVHC
840-65-3	Dimethyl naphthalene-2,6-dicarboxylate	PMT	high	SVHC
62037-80-3	ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate	vPvM&PMT	medium	SVHC
561-41-1	4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol	vPvM&PMT	low	SVHC
101-80-4	4,4'-oxydianiline	vPvM&PMT	low	SVHC
127-18-4	Tetrachloroethylene	vPvM&PMT	very high	DWD
330-54-1	Diuron	vPvM&PMT	very high	WFD
1634-04-4	tert-butyl methyl ether	vPvM&PMT	very high	EU Directive 98/70/EC
3380-34-5	Triclosan	vPvM&PMT	very high	Decision (EU) 2016/110
PMT/vPvM substances that are currently low tonnage or as intermediates				
120-12-7	Anthracene	PMT	medium	SVHC
98-95-3	Nitrobenzene	vPvM&PMT	medium	SVHC
115-96-8	Tris(2-chloroethyl) phosphate	vPvM&PMT	medium	SVHC
120-71-8	6-methoxy-m-toluidine	vPvM&PMT	Low	SVHC
56773-42-3	Tetraethylammonium heptadecafluorooctanesulphonate (PFOS)	vPvM & PMT	medium	Stockholm Convention
1912-24-9	Atrazine	vPvM&PMT	medium	WFD

SVHC: the substance is regulated under the REACH Candidate List as a Substance of very high concern (SVHC); DWD: The Drinking Water Directive (Council Directive 98/83/EC of 3 November 1998 on the quality of water intended for human consumption); WFD: Daughter Directive 2013/39 EU of the Water Framework Directive ("Directive 2000/60/EC of the European Parliament and of the Council establishing a framework for the Community action in the field of water policy"); Stockholm Convention: listed in the Stockholm Convention for Persistent Organic Pollutants.

9.5 Costs/Benefits

A previous cost-benefit analysis focusing on substances that have already been restricted under REACH concluded that restriction of these substances was in societies favour, according to the ECHA report: " Cost and benefit assessments in the REACH restriction dossiers" (ECHA, 2016a). This report estimated costs as of April 2016 of the 18 substances that have gone through the REACH restriction procedure of €290 million per year; however, the report concluded this cost is more than

compensated by health benefits of €700 million per year (via a reduction of 190 tonnes of SVHC, removing risks for approximately 81000 consumers and workers) (ECHA, 2016a).

It is beyond the scope of this study to address the costs verses the benefits of implementing risk mitigation measures for the 122 prioritized PMT/vPvM substances individually; rather, herein we discuss the costs verses benefits of introducing risk mitigation measures for PMT/vPvM substances in general. Some benchmarks to consider when implementing RMMs are:

For registrants and down-stream users:

1) Cost of substituting to a non PMT/vPvM
2) Cost of reducing emissions
3) Cost of monitoring and legislation compliance

For registrants, down-stream users and society

4) Cost of contaminated site remediation and monitoring
5) Cost of upgrading water treatment infrastructure to reduce exposure
6) Cost of ecosystem services potentially compromised
7) Health costs or benefits of using a PMT/vPvM substance for an essential purpose compared to available non-PMT/vPvM alternatives

An assessment of costs related to PBT substance reductions found that substitution costs are generally lower than emission reduction costs or contaminated site remediation costs, though this is not necessary generally applicable in all cases (Oosterhuis and Brouwer, 2015). Costs of contaminated site remediation can be quite substantial in the case of PMT/vPvM substances. As an example, clean-up costs in the United States of America for protecting drinking water from military bases contaminated with perfluorinated substances (a portion of which meet the PMT/vPvM criteria) are estimated at 2 billion USD (Knickmeyer, 2019). Drinking water purification to remove PMT/vPvM substances is also quite costly, as the same properties of persistence and mobility in the environment can also lead to contaminant breakthroughs using conventional and even state-of-the art drinking water purification technologies (Reemtsma et al., 2016; Neumann and Schliebner, 2017). It is anticipated that the greater the persistency and mobility of the substance, the more likely expensive remediation methods are needed for removal. The more mobile the substance implies that activated carbon filtration or other filtration would be less effective, as filtration ultimately relies on sorption. Even expensive, state-of-the-art methods, like reverse osmosis, are not completely effective for very mobile substances for drinking water production (Albergamo et al., 2019). It was estimated in the tandem UBA report presenting the PMT/vPvM criteria that costs of up to 0.8 – 1.5 billion €/year are required for only partial removal of vPvM substances in Germany alone (Neumann and Schliebner, 2019). Thus, it is not unreasonable when extrapolating from Germany to all of Europe and all existing PMT/vPvM substances that the clean-up and drinking water purification could costs in the range of several hundreds of billions of Euros, and this is not even factoring in potential health-care costs or costs from the reduction of ecosystem services.

It is not always clear who should bear the costs of contamination, and with PMT/vPvM substances this can be especially difficult. Because they are mobile substances they transport far from the point of emissions, potentially obscuring who the polluters are. It can become legally and scientifically complicated to identify who covers the remediation, removal, health-effects and ecosystem service loss costs; placing not only a potential health burden on the consumers of drinking water, but a potential financial one as well. The utilization of the PMT/vPvM criteria under REACH could help avoid or minimize such costs and conflicts in the future.

10 Recommendations

The criteria guidelines

Using the guidelines presented here, registrants could voluntarily apply the PMT/vPvM criteria to substances in their existing and future portfolios, and even consider the criteria as part of their product development procedure. Another application is the integration of the PMT/vPvM criteria within a substance alternatives assessment, to help choose the most benign of two or more chemical alternatives for a specific use. This would be advantageous to both registrants and down-stream users. Recently, a method for integrating the PMT/vPvM criteria into alternatives assessment has been proposed (Zheng et al., 2019). In cases where uses of a PMT/vPvM substance are essential, registrants are encouraged to perform an emission characterization to see if RMM should be put in place, using the same protocols that exist for PBT/vPvB substances (ECHA, 2017a), though with a focus on the sources of our drinking water and freshwater ecosystem services. Finally, the guidelines for implementing the PMT/vPvM criteria presented could be used in the development of future legislation or regulations, such as future REACH or CLP amendments (Neumann and Schliebner, 2019).

The list of substances fulfilling the PMT/vPvM criteria

Though care was taken to ensure accuracy regarding the PMT/vPvM list presented in Annex 1, there are likely some substances on the PMT/vPvM list that would no longer be considered as such if more data was available, or if inaccurate data was used here in their assessment. Similarly, there are also REACH registered substances that were not on the PMT/vPvM list, but would be if better quality data was available, or if the weight of evidence was interpreted differently; particularly regarding transformation products.

The substances in Table A1 could be included in monitoring programs, particularly those mentioned in Categories 1 to 3 of the list (see Annex 1), and even more so if local industrial sources of these substances are known. Not all of these substances may have analytical methods available due to the "analytical gap" for very mobile substances (Reemtsma et al., 2016) and in this case method development would be needed.

Researchers working with water treatment technology and contaminated land remediation could also consider if their technologies can remove/remediate the substances on this list. It could be that some of the state-of-the-art methods that address one PMT/vPvM substance can address others as well. As stated in the previous section, it is anticipated that the greater the persistency and mobility of a substance, the more expensive the technology required to remove it. Following the ideals of the polluter pays principle, such research or technology implementation should be supported by producers of PMT/vPvM substances.

Registrants and downstream users of substances presented in Table A1 should conduct their own PMT/vPvM assessment to see if they agree with the conclusions, and when necessary, develop RMMs to avoid future costs.

Regulators are encouraged to consider if substances mentioned in Table A1 require further attention, particularly those where the PMT/vPvM conclusions were supported with high quality data and there is a large chance of emissions. In some cases, substances may be worth considering under Article 57f of REACH, to demonstrate "scientific evidence of probable serious effects to human health or the environment which give rise to an equivalent level of concern" as a PBT/vPvB substance. The only inherent difference between PBT/vPvB and PMT/vPvM substances is their main pathways of exposure and transport (see section 9.2).

Though the relative percentage of REACH registered substances meeting the PMT/vPvM criteria is not substantial, the potential health and economic costs of not acting on them are.

11 List of Annexes

- Annex 1. Substances registered under REACH fulfilling the PMT/vPvM criteria and/or detected in drinking water or groundwater
- Annex 2. Data sources used in the PMT/vPvM assessment

12 References

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Annex 1. Substances registered under REACH fulfilling the PMT/vPvM criteria and/or detected in drinking water or groundwater

This Annex contains a list of REACH registered substances (as of May 2017) that are either considered a hazard to the sources of our drinking water because they fulfil the PMT/vPvM criteria, or otherwise have been detected in drinking water or groundwater without fulfilling the PMT/vPvM criteria. This list, presented in Table A1, is subdivided into the following seven categories:

Cat. 1. Priority PMT/vPvM substances for follow up

These substances are considered of the highest priority for follow up, either to confirm their PMT/vPvM status or to further investigate their presence in the sources of our drinking water.

122 substances with unique structures, 39 detected in monitoring studies

Cat. 2. Established PMT/vPvM substances

PMT/vPvM substances that are already receiving attention by European authorities (as presented in Table 6).

21 substances with unique structures, 14 detected in monitoring studies

Cat. 3. Down-prioritized PMT/vPvM substances

PMT/vPvM substances that are considered easy to remove during drinking water treatment or are associated with a low REACH emission likelihood. Though down-prioritized, it is still worthwhile to consider this list for follow-up.

19 substances with unique structures, 2 detected in groundwater

Cat.4. Exempted PMT/vPvM substances

These substances met the PMT/vPvM criteria, but as of May 2017 they were exempt from PBT/vPvB assessment under REACH Article 14 and they are, by proxy, considered exempt from the PMT/vPvM assessment. Changes in use, such as an increase in volume, would make them non-exempt.

96 substances with unique structures, 27 detected in monitoring studies

Cat. 5. Detected PM substances

Substances detected in drinking water and groundwater that met the PM criteria (but not the PMT/vPvM criteria). *11 substances*

Cat. 6. Detected Potential PMT/vPvM substances

Substances detected in drinking water and groundwater that met the Potential PMT/vPvM criteria. *26 substances*

Cat. 7. Detected Non PMT/vPvM substances

Substances detected in drinking water and groundwater did not meet the PMT/vPvM criteria. *47 substances*

Additionally, Table A2 presents the references to literature sources for the compilation of drinking water and groundwater monitoring data in Chapter 2. Table A3 compiles substances detected in drinking water and groundwater not registered under REACH but were reported in the references for Chapter 2.

Table A1: List of REACH registered substances (as of May 2017) evaluated as either PMT, vPvM or both, as well as the outcome of PMT/vPvM assessments for all substances reported in drinking water and groundwater (Chapter 2). See footnotes to the table for an explanation of terms.

CAS Number	Name	REACH Emission Likelihood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
Category 1. Prioritized PMT/vPvM substances *124 substances, 122 unique chemical constituents, 39 detected in monitoring studies*													
108-78-1	Melamine	very high	Y	**vPvM & PMT**	HQ	**vP**	All biodegradation results in 301C and 302B tests imply no significant biodegradation. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	**vM**	exp min. log Dow/Kow = -2.3 (ionizable cmpd.)	**T**	Carc_2 STOTRE_2	E; F; Z (DW: det.)	HOT-L
80-08-0	Dapsone	very high	Y	**vPvM & PMT**	HQ	**vP**	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. (Berger et al. 2018)	**vM**	exp min. log Doc/Koc = 1.8 (neutral cmpd.)	**T**	STOTRE_1 STOTRE_2_Suspected ED	F (DW: det.)	pharmaceutical
37640-57-6	1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6-triamine (1:1)	high	Y	**vPvM & PMT**	HQ	**vP**	measured half-life = 913 d (soil)	**vM**	read-across min. log Dow/Kow = 2.0 (neutral cmpd.)	**T**	STOTRE_2		melamine duplicate
3622-84-2	N-butylbenzenesulphonamide	very high	Y	**vPvM & PMT**	HQ	**vP**	measured half-life = 1 011 d (fresh water)	**vM**	exp min. log Dow/Kow = 2.0 (neutral cmpd.)	**T**	STOTRE_2	S (DW: 0.05)	
95-50-1	1,2-dichlorobenzene	very high	Y	**vPvM**	HQ	**vP**	measured half-life = 191 d (soil)	**vM**	exp min. log Doc/Koc = 2.7 (neutral cmpd.)	**Pot. T**	Cramer Class III	H;O (DW&GW: >10)	DK-study
123-91-1	1,4-dioxane	very high	Y	**PMT**	HQ	**P**	No significant biodegradation in 301F testimated The PBT assessment evaluates the substance to be persistent. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	**vM**	exp min. log Doc/Koc = -0.5 (neutral cmpd.)	**T**	Carc_2 STOTRE_1 STOTRE_2	E;S; T (DW: 0.6)	HOT-H
126-86-3	2,4,7,9-tetramethyldec-5-yne-4,7-diol	very high	Y	**PMT**	HQ	**P**	All biodegradation results in 301B and 302B tests imply no significant biodegradation. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	**vM**	exp min. log Doc/Koc = 1.6 (neutral cmpd.)	**T**	STOTRE_2	N (DW: 0.24)	DK-study

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
288-88-0	1,2,4-triazole	very high	Y	PMT	HQ	P	All biodegradation results in 301A and 302B tests imply no significant biodegradation. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	vM	exp min. log Doc/Koc = 1.6 (ionizable cmpd.)	T	Rep_2	E; Z (DW: det.)	HOT-H
834-12-8	Ametryn	very high	Y	PMT	HQ	P	measured half-life = 143 d (soil)	vM	exp min. log Doc/Koc = 1.8 (ionizable cmpd.)	T	ecotox	H; Z (DW&GW: det.)	DK-study
2855-13-2	3-aminomethyl-3,5,5-trimethylcyclohexylamine	very high	Y	PMT	HQ	P	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. (Berger et al. 2018)	vM	exp min. log Dow/Kow = -1.3 (ionizable cmpd.)	T	Suspected ED	Z (det.)	
51-28-5	2,4-dinitrophenol	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	this is not persistent in soil, but some data in the dossier suggests the vP criteria in fresh water is met. Further, it is found in monitoring studies, there were consistent indications of P across tested QSARs, and this substances was also considered as prioritized by Nödler et al.	vM	exp min. log Doc/Koc = -3.4 (ionizable cmpd.)	T	muta_2 Rep_2 STOTRE_1 STOTRE_2 DNEL_Suspected ED	A;H (DW&GW: 333)	HOT-H, DK-study
56-23-5	Carbon tetrachloride	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 97d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 1.9 (neutral cmpd.)	T	Carc_1b Carc_2 Rep_2 STOTRE_1 STOTRE_2	H;O (DW&GW: 2.24)	
56-93-9	Benzyltrimethylammonium chloride	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 21d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	QSAR min. log Dow/Kow = -1.0 (single_cation cmpd.)	T	muta_2	F; Z (DW: det.)	
67-66-3	Chloroform	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 45d, weight-of-evidence by discovery in monitoring studies, available QSARs and no biodeg. observed in majority of biodegradation screen tests e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Doc/Koc = 2.0 (neutral cmpd.)	T	Carc_2 muta_2 Rep_2 STOTRE_1 STOTRE_2	H;O;P (DW&GW: 34.6)	HOT-H
75-35-4	1,1-dichloroethylene	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 28d, weight-of-evidence by discovery in monitoring studies, available QSARs and no biodeg. observed in majority of	vM	exp min. log Doc/Koc = 1.4 (neutral cmpd.)	T	Carc_1b Carc_2 STOTRE_1 STOTRE_2	O (GW: >10)	HOT-H

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
							biodegradation screen tests e.g. 301 D (Ready Biodegradability: Closed Bottle Test)						
75-71-8	Dichlorodifluoro-methane	very high	Y	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 44d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 1.0 (neu-tral cmpd.)	Pot. T	Cramer Class III	O (GW: 5-10)	
76-05-1	Trifluoroacetic acid	very high	Y	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 20d, weight-of-evidence by discovery in monitoring studies, available QSARs and no biodeg. observed in majority of biodegradation screen tests e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	QSAR min. log Dow/Kow = -0.6 (ionizable cmpd.)	Pot. T	Cramer Class III	E;U;V (DW&GW: 0.15)	HOT-L
78-51-3	Tris(2-butoxyethyl) phosphate	very high	Y	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 10d, weight-of-evidence by discovery in monitoring studies, available QSARs and no biodeg. observed in majority of biodegradation screen tests e.g. 302 C (Inher-ent Biodegradability: Modified MITI Test (II))	vM	exp min. log Doc/Koc = 2.5 (neu-tral cmpd.)	Pot. T	Cramer Class III	H (DW: 0.35)	
78-87-5	1,2-dichloropropane	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	P data for this substance is variable and difficult to conclude; however, its identification in moni-toring studies in DW and GW indicates it is per-sistent enough.	vM	exp min. log Doc/Koc = 1.3 (neu-tral cmpd.)	T	Carc_1b	H;O (DW&GW: 1.71)	HOT-H, DK-study
95-14-7	Benzotriazole	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 18d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 1.5 (ioniz-able cmpd.)	T	muta_2	A; B; E;S (DW&GW: 1.5)	HOT-L
97-39-2	1,3-di-o-tolylguani-dine	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 107d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Dow/Kow = -3.0 (ionizable cmpd.)	T	Carc_1b Rep_2	F; Z (DW: det.)	
102-06-7	1,3-diphenylguanidine	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 68d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Dow/Kow = 1.4 (ion-izable cmpd.)	T	Rep_2	F; Z (DW: det.)	DK-study

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
106-93-4	1,2-dibromoethane	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 20d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 0.3 (neu-tral cmpd.)	T	Carc_1a Carc_1b Carc_2_Su spected ED	O (GW: 0.2-0.5)	HOT-H
108-20-3	Diisopropyl ether	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 25d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 0.6 (neu-tral cmpd.)	T	Rep_2	O (GW: >10)	fuel oxygenate
108-80-5	Cyanuric acid	very high	Y	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 20d, detected in several water samples in Schulze et al. (2019) and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 1.7 (neu-tral cmpd.)	Not T	-	F; Z (DW: det.)	
108-90-7	Chlorobenzene	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 23d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 2.4 (neu-tral cmpd.)	T	Carc_1a muta_1b Rep_2 STOTRE_1	O (GW: 5-10)	
119-61-9	Benzophenone	very high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 18d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	M	exp min. log Doc/Koc = 3.1 (neu-tral cmpd.)	T	Carc_2 STO-TRE_2_ED	N (DW: 0.26)	
121-47-1	3-aminobenzenesul-phonic acid	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 44d, detected in several water samples in Schulze et al. (2019) and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -2.0 (ionizable cmpd.)	T	Suspected ED	Z (det.)	
121-82-4	Perhydro-1,3,5-tri-nitro-1,3,5-triazine	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 33d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Dow/Kow = 0.9 (ne-utral cmpd.)	T	STOTRE_1 STOTRE_2	H (DW: 1.1)	HOT-H
156-60-5	trans-dichloroeth-ylene	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 28d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = 2.0 (ne-utral cmpd.)	T	STOTRE_2	O (GW: >10)	
280-57-9	1,4-diazabicyclooc-tane	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 42d, detected in several water samples in Schulze et al. (2019) and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 1.0 (ioniz-able cmpd.)	T	STOTRE_2	Z (det.)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
541-73-1	1,3-dichlorobenzene	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 48d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 2.6 (neu-tral cmpd.)	T	STO-TRE_2_Sus pected ED	H (DW: 0.1)	
1493-13-6	Trifluoromethanesul-phonic acid	very high	Y	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 39d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Dow/Kow = 0.3 (ne-utral cmpd.)	Pot. T	Cramer Class III	F;W; Z (DW: 1)	
5165-97-9	Sodium 2-methyl-2-[(1-oxoal-lyl)amino]propanesul-phonate	very high	Y	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 19d, detected in several water samples in Schulze et al. (2019) and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -2.4 (single_anion cmpd.)	Pot. T	Cramer Class III	Z (det.)	DK-study
13674-87-8	Tris[2-chloro-1-(chloromethyl)ethyl] phosphate	very high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 231d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	M	exp min. log Doc/Koc = 3.7 (neu-tral cmpd.)	T	Carc_2 STOTRE_2	H:J (DW: 0.51)	DK-study
52556-42-0	Sodium 3-(allyloxy)-2-hydroxypropanesul-phonate	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 15d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	QSAR min. log Dow/Kow = -2.9 (single_anion cmpd.)	T	Rep_2	Z (det.)	
6331-96-0	2-amino-4,5-dichloro-benzenesulfonic acid	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 152d, detected in several wa-ter samples in Schulze et al. (2019) and con-sistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -0.7 (ionizable cmpd.)	T	Suspected ED	Z (det.)	
29420-49-3	PFBS - Potassium 1,1,2,2,3,3,4,4,4-no-nafluorobutane-1-sul-phonate	very high	Y	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 327d, weight-of-evidence by discovery in monitoring studies, available QSARs and no biodeg. observed in at least one biodegradation screen test e.g. OECD Guideline 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	exp min. Dow/Kow = -1.7 (ionizable cmpd.)	Pot. T	Cramer Class III	A;H;I;L;M (DW&GW: 0.025)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
75-01-4	Chloroethylene	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 17d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 0.8 (neu-tral cmpd.)	T	Carc_1a muta_2	H;O (DW&GW: 5-10)	volatile
81-07-2	1,2-benzisothiazol-3(2H)-one 1,1-dioxide	medium	Y	vPvM & PMT	MQ	Pot. P/vP ++	the reported t1/2 in soil is 30d; however, it is detected in several water samples in Schulze et al. (2019) and consistent indications of P across tested QSARs. Thus it is considered sufficiently P in the environment	vM	exp min. log Dow/Kow = -0.7 (ionizable cmpd.)	T	Carc_2 muta_2 Rep_2	Z (det.)	
78-67-1	2,2'-dimethyl-2,2'-azodipropiononitrile	high	Y	vPvM	HQ	vP	measured half-life = 1 093 d (fresh water)	vM	exp min. log Doc/Koc = 2.0 (neu-tral cmpd.)	Pot. T	Cramer Class III		HOT-L
91-76-9	6-phenyl-1,3,5-tria-zine-2,4-diyldiamine	high	Y	vPvM	HQ	vP	No significant biodegradation in 301C and E tests. The PBT assessment evaluates the sub-stance to be persistent. Therefore, this sub-stance is assessed to be persistent in water. (Berger et al. 2018)	vM	exp min. log Doc/Koc = 1.4 (ioniz-able cmpd.)	Pot. T	Cramer Class III		
121-03-9	4-nitrotoluene-2-sul-phonic acid	high	Y	vPvM	HQ	vP	No significant biodegradation in 301E and C tests. The PBT assessment evaluates the sub-stance to be persistent. Therefore, this sub-stance is assessed to be persistent in water. (Berger et al. 2018)	vM	QSAR min. log Dow/Kow = -0.9 (ionizable cmpd.)	Pot. T	Cramer Class III		
156-62-7	Calcium cyanamide	high	Y	vPvM	HQ	vP	measured half-life = 242 d (soil)	vM	exp min. log Dow/Kow = -2.0 (ionizable cmpd.)	T	Carc_2 Rep_2 STOTRE_2		cyanamide du-plicate
382-28-5	2,2,3,3,5,5,6,6-oc-tafluoro-4-(trifluoro-methyl)morpholine	high	Y	vPvM	HQ	vP	estimated t1/2 = 918d, weight-of-evidence (this study) based on all known QSARs and no bio-deg. observed in majority of biodegradation screen tests, e.g. 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)	vM	exp min. log Doc/Koc = 0.2 (ioniz-able cmpd.)	Pot. T	Cramer Class III		DK-study
420-04-2	Cyanamide	high	Y	vPvM & PMT	HQ	vP	measured half-life = 242 d (soil)	vM	exp min. log Dow/Kow = -2.0 (ionizable cmpd.)	T	Carc_2 Rep_2 STOTRE_2		cyanamide
115-27-5	1,4,5,6,7,7-hexa-chloro-8,9,10-trinor-born-5-ene-2,3-dicar-boxylic anhydride	high	Y	vPvM & PMT	HQ	vP	estimated t1/2 = 1 113d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 302 C (Inherent	vM	exp min. log Doc/Koc = 0.9 (neu-tral cmpd.)	T	Carc_1a Carc_2 STOTRE_2		DK-study

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
							Biodegradability: Modified MITI Test (II)),301 F (Ready Biodegradability: Manometric Respi-rometry Test)						
556-88-7	1-nitroguanidine	high	Y	vPvM	HQ	vP	measured half-life = 102 d (fresh water)	vM	QSAR min. log Dow/Kow = -1.1 (ionizable cmpd.)	Pot. T	Cramer Class III		
593-85-1	Diguanidinium car-bonate	high	Y	vPvM	HQ	vP	measured half-life = 174 d (fresh water)	vM	QSAR min. log Dow/Kow = -4.2 (multiple_anion cmpd.)	Not T	-		
3033-62-3	N,N,N',N'-tetrame-thyl-2,2'-oxybis(ethyl-amine)	high	Y	vPvM	HQ	vP	All biodegradation results in 301F and 302B im-ply no significant biodegradation. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	vM	exp min. log Dow/Kow = 0.5 (ion-izable cmpd.)	Pot. T	Cramer Class III		
41583-09-9	1,3,5-triazine-2,4,6-triamine phosphate	high	Y	vPvM	HQ	vP	measured half-life = 913 d (soil)	vM	exp min. log Dow/Kow = -2.3 (ionizable cmpd.)	Pot. T	Cramer Class III		
68987-63-3	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, chlorinated	high	Y	vPvM	HQ	vP	estimated t1/2 = 1 537d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	read-across min. log Dow/Kow = 1.2 (ion-izable cmpd.)	Not T	-		
73037-34-0	Disodium ox-ybis[methylbenzene-sulphonate]	high	Y	vPvM	HQ	vP	No significant biodegradation in 301F and C tests. The PBT assessment evaluates the sub-stance to be persistent. Therefore, this sub-stance is assessed to be persistent in water. (Berger et al. 2018)	vM	QSAR min. log Dow/Kow = -1.7 (multiple_anion cmpd.)	Pot. T	Cramer Class III		
90268-24-9	Butanamide, 2,2'-[(3,3'-dichloro[1,1'-bi-phenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(4-chloro-2,5-dimethoxy-phenyl and 2,4-xylyl) derivs.	high	Y	vPvM	HQ	vP	estimated t1/2 = 1 379d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Dow/Kow = 1.3 (ion-izable cmpd.)	Pot. T	Cramer Class III		

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
83016-70-0	2-[(2-[2-(dimethyla-mino)eth-oxy]ethyl)methyla-mino]ethanol	high	Y	vPvM	HQ	vP	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. (Berger et al. 2018)	vM	QSAR min. log Dow/Kow = -2.9 (ionizable cmpd.)	Pot. T	Cramer Class III		
1671-49-4	4-mesyl-2-nitrotolu-ene	high	Y	vPvM & PMT	HQ	vP	All biodegradation results in 301F and 302B tests imply no significant biodegradation. Therefore, this substance is assessed to be per-sistent in water. (Berger et al. 2018)	vM	exp min. log Doc/Koc = 2.3 (neu-tral cmpd.)	T	Rep_2		
3030-47-5	Bis(2-dimethylami-noethyl)(me-thyl)amine	high	Y	vPvM	HQ	vP	All biodegradation results in 301C and E and 302B imply no significant biodegradation. Therefore, this substance is assessed to be per-sistent in water. (Berger et al. 2018)	vM	exp min. log Dow/Kow = 0.1 (ion-izable cmpd.)	Pot. T	Cramer Class III		
107-46-0	Hexamethyldisiloxane	high	Y	vPvM & PMT	HQ	vP	measured half-life = 231 d (soil)	vM	exp min. log Doc/Koc = 2.7 (neu-tral cmpd.)	T	ecotox Carc_2		
22042-96-2	[[(phosphonome-thyl)imino]bis[(eth-ylenenitrilo)bis(meth-ylene)]]tetrakisphos-phonic acid, sodium salt	high	Y	vPvM	HQ	vP	estimated t1/2 = 1 303d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	QSAR min. log Dow/Kow = -14.3 (single_anion cmpd.)	Pot. T	Cramer Class III		Chelating agent, DK-study
34690-00-1	[[(phosphonome-thyl)imino]bis[hexa-methylenenitrilo-bis(meth-ylene)]]tetrakisphos-phonic acid	high	Y	vPvM & PMT	HQ	vP	estimated t1/2 = 1 619d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	QSAR min. log Dow/Kow = -11.0 (ionizable cmpd.)	T	STOTRE_2		Chelating agent, DK-study
61792-09-4	Pentasodium pen-tahydrogen [[(phos-phonatome-thyl)imino]bis[ethane-2,1-diylnitrilo-bis(meth-ylene)]]tetrakisphos-phonate	high	Y	vPvM	HQ	vP	estimated t1/2 = 1 303d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	QSAR min. log Dow/Kow = -14.3 (multiple_anion cmpd.)	Pot. T	Cramer Class III		Chelating agent, DK-study

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
129909-90-6	4-amino-N-(1,1-di-methylethyl)-4,5-di-hydro-3-(1-meth-ylethyl)-5-oxo-1H-1,2,4-triazole-1-car-boxamide	high	Y	vPvM	HQ	vP	Due to lack of other information the substance was assessed by PBT assessment in water. Therefore, this substance is assessed to be per-sistent in water. (Berger et al. 2018)	vM	exp min. log Doc/Koc = 1.4 (ioniz-able cmpd.)	Not T	-		HOT-L
2312-35-8	Propargite	high	Y	PMT	HQ	vP	measured half-life = 169 d (soil)	M	exp min. log Doc/Koc = 3.6 (neu-tral cmpd.)	T	ecotox Carc_2		DK-study
12108-13-3	Tricarbonyl(methylcy-clopentadienyl)man-ganese	high	Y	PMT	HQ	vP	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. (Berger et al. 2018)	M	exp min. log Doc/Koc = 3.4 (single_anion cmpd.)	T	Carc_2 STOTRE_1		
87-62-7	2,6-xylidine	high	Y	PMT	HQ	P	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. (Berger et al. 2018)	vM	exp min. log Doc/Koc = 1.3 (ioniz-able cmpd.)	T	Carc_2		
123-30-8	4-aminophenol	high	Y	PMT	HQ	P	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. (Berger et al. 2018)	vM	exp min. log Doc/Koc = 0.6 (ioniz-able cmpd.)	T	muta_2 STOTRE_2		
622-40-2	2-morpholinoethanol	high	Y	PMT	HQ	P	No significant biodegradation in 302B testi-mated Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	vM	exp min. log Doc/Koc = -1.9 (ion-izable cmpd.)	T	Carc_1b		
2226-96-2	4-hydroxy-2,2,6,6-tet-ramethylpiperidinoxyl	high	Y	PMT	HQ	P	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. (Berger et al. 2018)	vM	QSAR min. log Dow/Kow = 0.1 (ion-izable cmpd.)	T	STOTRE_2		
4065-45-6	Sulisobenzone	high	Y	PMT	HQ	P	All biodegradation results in 301F and 302B tests imply no significant biodegradation. Therefore, this substance is assessed to be per-sistent in water. (Berger et al. 2018)	vM	exp min. log Doc/Koc = 2.0 (ioniz-able cmpd.)	T	Rep_2_Sus pected ED		
5281-09-4	Calcium 3-hydroxy-4-[(4-methyl-2-sulpho-natophenyl)azo]-2-naphthoate	high	Y	PMT	HQ	P	Biodegradation results in 301 C test <20% and persistence due to PBT assessment. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	vM	exp min. log Dow/Kow = 0.7 (multiple_anion cmpd.)	T	STOTRE_2		red pigment

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13472-08-7	2,2'-azobis[2-methyl-butyronitrile]	high	Y	PMT	HQ	P	No significant biodegradation in 301D testi-mated The PBT assessment evaluates the sub-stance to be persistent. Therefore, this sub-stance is assessed to be persistent in water. (Berger et al. 2018)	vM	exp min. log Dow/Kow = 2.1 (ne-utral cmpd.)	T	STOTRE_2		HOT-L
37971-36-1	2-phosphonobutane-1,2,4-tricarboxylic acid	high	Y	PMT	HQ	P	measured half-life = 139 d (soil)	vM	QSAR min. log Dow/Kow = -7.7 (ionizable cmpd.)	T	STOTRE_2		
98362-33-5	2,3-Epoxypropyl ne-odecanoate, oligo-meric reaction prod-ucts with toluene-4-sulfonic acid	high	Y	PMT	HQ	vP	estimated t1/2 = 1 218d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. log Dow/Kow = 3.5 (ne-utral cmpd.)	T	muta_2		DK-study
67-68-5	Dimethyl sulfoxide	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 15d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 0.6 (neu-tral cmpd.)	T	Carc_2 muta_2 STOTRE_2		
75-77-4	Chlorotrimethylsilane	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 18d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)	vM	read-across min. log Dow/Kow = 1.2 (neutral cmpd.)	T	Carc_2		
75-91-2	tert-butyl hydroper-oxide	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 22d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. log Dow/Kow = 0.8 (ne-utral cmpd.)	T	muta_2		HOT-L
76-03-9	Trichloroacetic acid	high	Y	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 35d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	exp min. log Doc/Koc = 1.0 (ioniz-able cmpd.)	Pot. T	Cramer Class III		HOT-H

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77-73-6	3a,4,7,7a-tetrahydro-4,7-methanoindene	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 18d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	M	exp min. log Dow/Kow = 2.8 (ne-utral cmpd.)	T	Rep_1a Rep_2 STOTRE_1 STOTRE_2		
78-40-0	Triethyl phosphate	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 10d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. log Doc/Koc = -0.3 (neu-tral cmpd.)	T	Carc_1b muta_2		
80-15-9	α,α-dimethylbenzyl hydroperoxide	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 24d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test) (1981)	M	exp min. log Doc/Koc = 3.1 (neu-tral cmpd.)	T	muta_2 STOTRE_1 STOTRE_2		DK-study
80-43-3	Bis(α,α-dimethylben-zyl) peroxide	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 51d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	M	exp min. log Doc/Koc = 4.0 (neu-tral cmpd.)	T	Rep_2		
80-51-3	4,4'-oxydi(benzene-sulphonohydrazide)	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 80d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	QSAR min. log Dow/Kow = 0.2 (ion-izable cmpd.)	T	muta_2 STOTRE_2		
88-72-2	2-nitrotoluene	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 39d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 1.9 (neu-tral cmpd.)	T	Carc_1b Carc_2 muta_1b Rep_2		HOT-L

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88-73-3	1-chloro-2-nitroben-zene	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 64d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 2.5 (neu-tral cmpd.)	T	Carc_1b Carc_2 muta_2 Rep_2 STOTRE_1 STOTRE_2		
97-74-5	Tetramethylthiuram monosulphide	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 24d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	exp min. log Dow/Kow = 1.2 (ne-utral cmpd.)	T	STOTRE_2		HOT-L
99-99-0	4-nitrotoluene	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 39d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 2.0 (neu-tral cmpd.)	T	STO-TRE_2_Sus pected ED		HOT-L
100-43-6	4-vinylpyridine	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 22d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Dow/Kow = 0.2 (ion-izable cmpd.)	T	muta_2		
100-61-8	N-methylaniline	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 25d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. log Doc/Koc = 0.3 (ioniz-able cmpd.)	T	STOTRE_1 STOTRE_2		
100-97-0	Methenamine	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 249d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Dow/Kow = -7.5 (ionizable cmpd.)	T	Rep_2 STOTRE_1		DK-study

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102-08-9	1,3-diphenyl-2-thiou-rea	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 17d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	M	exp min. log Dow/Kow = 2.0 (ion-izable cmpd.)	T	Rep_2 STOTRE_2		
107-66-4	Dibutyl hydrogen phosphate	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 9d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. log Doc/Koc = -8.3 (single_anion cmpd.)	T	Carc_2		
108-42-9	3-chloroaniline	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	From data in the dossier, the water half-life is near the criteria for P, and the sediment vP cri-teria is met in a water-sediment system,	vM	exp min. log Doc/Koc = 1.5 (ioniz-able cmpd.)	T	ecotox Carc_1b STOTRE_1 STOTRE_2		DK-study
109-01-3	1-methylpiperazine	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 24d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. log Doc/Koc = 2.9 (ioniz-able cmpd.)	T	Rep_2		
119-64-2	1,2,3,4-tetrahy-dronaphthalene	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 24d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 2.7 (neu-tral cmpd.)	T	Carc_2_Su spected ED		
345-92-6	Bis(4-fluorophenyl) ketone	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 155d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	M	exp min. log Dow/Kow = 3.4 (ne-utral cmpd.)	T	Suspected ED		DK-study
482-89-3	2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 98d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen	vM	exp min. log Doc/Koc = 2.9 (ioniz-able cmpd.)	T	STOTRE_2		

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
	1,2-dihydro-3H-indol-3-one						tests for substance/main transformation products, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)						
584-84-9	4-methyl-m-phenylene diisocyanate	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 26d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	M	read-across min. log Dow/Kow = 3.4 (neutral cmpd.)	T	Carc_2 STOTRE_1		
599-61-1	3,3'-sulphonyldianiline	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 109d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 1.8 (ionizable cmpd.)	T	STOTRE_2_Suspected ED		
1758-73-2	Aminoimino-methanesulphinic acid	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 18d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 301 A (new version) (Ready Biodegradability: DOC Die Away Test)	vM	QSAR min. log Dow/Kow = -4.3 (zwitterion cmpd.)	T	STOTRE_2		
1761-71-3	4,4'-methylenebis(cyclohexylamine)	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 17d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Doc/Koc = -3.6 (ionizable cmpd.)	T	STOTRE_2_Suspected ED		
2440-22-4	2-(2H-benzotriazol-2-yl)-p-cresol	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 27d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. log Doc/Koc = 3.0 (ionizable cmpd.)	T	STOTRE_2_Suspected ED		DK-study
2554-06-5	2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane	high	Y	PMT	MQ	Pot. P/vP ++	The P conclusion remains controversial; currently D4 is being considered as SVHC based on vPvB and PMT properties	M	exp min. log Doc/Koc = 3.8 (neutral cmpd.)	T	ecotox		

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
							(https://echa.europa.eu/docu-ments/10162/50488161-546d-2048-828a-b6d9ef29f310)						
284-95-7, 2680-03-7	N,N-dimethylacryla-mide	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 11d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 1.3 (neu-tral cmpd.)	T	muta_2		
3006-86-8	Cyclohexyli-denebis[tert-butyl] peroxide	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 107d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test) 17th July 1992	vM	exp min. log Doc/Koc = 2.7 (neu-tral cmpd.)	T	Carc_2 muta_2		
3468-63-1	1-[(2,4-dinitro-phenyl)azo]-2-naph-thol	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 295d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	M	exp min. log Dow/Kow = 2.5 (ion-izable cmpd.)	T	ecotox Carc_2 muta_2_S uspected ED		
3710-84-7	N,N-diethylhydroxyla-mine	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 14d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	exp min. log Dow/Kow = -0.2 (ionizable cmpd.)	T	muta_2		
5026-74-4	p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypro-pyl)aniline	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 114d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test) July 17, 1992	vM	exp min. log Doc/Koc = 1.9 (ioniz-able cmpd.)	T	Carc_2 muta_2 Rep_2 STOTRE_2		DK-study
6674-22-2	1,8-diazabicy-clo[5.4.0]undec-7-ene	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 19d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation	vM	exp min. log Doc/Koc = -6.0 (ion-izable cmpd.)	T	Carc_1b muta_2		

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
							products, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)						
6864-37-5	2,2'-dimethyl-4,4'-methylenebis(cyclo-hexylamine)	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 20d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. log Doc/Koc = -2.2 (ion-izable cmpd.)	T	STO-TRE_2_Sus pected ED		
7226-23-5	Tetrahydro-1,3-dime-thyl-1H-pyrimidin-2-one	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 19d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 E (Ready biodegradability: Modi-fied OECD Screening Test)	vM	exp min. log Doc/Koc = 0.9 (neu-tral cmpd.)	T	Rep_2		HOT-L
25321-09-9	Diisopropylbenzene	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 27d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	M	exp min. log Doc/Koc = 3.8 (neu-tral cmpd.)	T	STOTRE_2		
26471-62-5	m-tolylidene diisocya-nate	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 26d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	M	exp min. log Dow/Kow = 3.4 (ne-utral cmpd.)	T	Carc_2 STOTRE_1		
38083-17-9	Climbazole	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 72d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	M	exp min. log Doc/Koc = 3.5 (ioniz-able cmpd.)	T	ecotox		
53988-10-6	1,3-dihydro-4(or 5)-methyl-2H-benzimid-azole-2-thione	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 25d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation	vM	exp min. log Doc/Koc = 1.9 (ioniz-able cmpd.)	T	Rep_2 STOTRE_2		DK-study

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
							products, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))						
68937-41-7	Phenol, isopropy-lated, phosphate (3:1)	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 66d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	M	exp min. log Doc/Koc = 3.7 (neu-tral cmpd.)	T	Rep_2 STOTRE_2		
71604-74-5	m-(2,3-epoxypro-poxy)-N,N-bis(2,3-epoxypropyl)aniline	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 114d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. log Doc/Koc = 1.9 (ioniz-able cmpd.)	T	muta_2 STOTRE_2		DK-study
71868-10-5	2-methyl-1-(4-methyl-thiophenyl)-2-mor-pholinopropan-1-one	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 140d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. log Doc/Koc = 1.9 (ioniz-able cmpd.)	T	Rep_1b		
110553-27-0	4,6-bis(octylthiome-thyl)-o-cresol	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 20d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. log Doc/Koc = 2.0 (neu-tral cmpd.)	T	ecotox		
27955-94-8	4,4',4''-(ethan-1,1,1-triyl)triphenol	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 38d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. log Doc/Koc = 1.7 (ioniz-able cmpd.)	T	Suspected ED		
74091-64-8	2,5-bis-isocyanatome-thyl-bicy-clo[2.2.1]heptane	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 26d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation	vM	exp min. log Doc/Koc = 0.2 (ioniz-able cmpd.)	T	STOTRE_1		HOT-L

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
							products, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))						
162881-26-7	Phenyl bis(2,4,6-tri-methylbenzoyl)-phos-phine oxide	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 107d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. log Doc/Koc = 3.9 (neu-tral cmpd.)	T	ecotox		
94239-04-0	2-fluoro-6-trifluoro-methylpyridine	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 183d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	vM	exp min. log Doc/Koc = 1.7 (neu-tral cmpd.)	T	STOTRE_2		
25068-38-6	4,4'-Isopropylidenedi-phenol, oligomeric re-action products with 1-chloro-2,3-epoxy-propane	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 30d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	exp min. log Doc/Koc = 2.1 (neu-tral cmpd.)	T	Suspected ED		
1112-39-6	Dimethoxydime-thylsilane	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 19d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)	vM	exp min. log Doc/Koc = 0.7 (neu-tral cmpd.)	T	Rep_1b Rep_2 STOTRE_1		
Category 2. Established PMT/vPvM substances *21 substances with unique structures, 14 detected in monitoring studies*													
62037-80-3	ammonium 2,3,3,3-tetrafluoro-2-(hep-tafluoropropoxy)pro-panoate	medium	Y	vPvM & PMT	HQ	vP	All biodegradation results in 301B and 302C im-ply no significant biodegradation. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	vM	exp min. log Doc/Koc = -5.1 (single_anion cmpd.)	T	STOTRE_2	M (DW: 0.011)	SVHC

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
88-85-7	Dinoseb	high	Y	vPvM & PMT	HQ	vP	measured half-life = 314 d (soil)	vM	exp min. log Doc/Koc = -2.3 (ion-izable cmpd.)	T	SVHC		SVHC, HOT-L
561-41-1	4,4'-bis(dimethyla-mino)-4''-(methyla-mino)trityl alcohol	low	Y	vPvM & PMT	HQ	vP	Due to lack of other information the substance was assessed by PBT assessment in water. Therefore, this substance is assessed to be per-sistent in water. (Berger et al. 2018)	vM	exp min. log Dow/Kow = -0.6 (ionizable cmpd.)	T	SVHC		SVHC, DK-study
330-54-1	Diuron	very high	Y	vPvM & PMT	HQ	vP	measured half-life = 2 241 d (soil)	vM	exp min. log Doc/Koc = 2.1 (neu-tral cmpd.)	T	ecotox Carc_2 STO-TRE_2_Sus pected ED	A;E;H;Q;S (DW&GW: 2.1)	WFD substance
127-18-4	Tetrachloroethylene	very high	Y	vPvM & PMT	HQ	vP	No significant biodegradation in 301 C tests. The PBT assessment evaluates the substance to be persistent. Therefore, this substance is as-sessed to be persistent in water. (Berger et al. 2018)	vM	exp min. log Doc/Koc = 2.2 (neu-tral cmpd.)	T	Carc_1b Carc_2 Rep_2 STO-TRE_2_ED	G;H;J (DW: 180)	DWD substance
56773-42-3	Tetraethylammonium heptadecafluorooc-tanesulphonate	medium	N	vPvM & PMT	HQ	vP	on SVHC list - vPvB substance	vM	exp min. log Doc/Koc = 0.0 (single_anion cmpd.)	T	SVHC	A;E;H;I;L;S (DW&GW: 0.14)	SVHC
79-01-6	Trichloroethylene	very high	Y	PMT	HQ	P	No significant biodegradation in 301C and D tests. The PBT assessment evaluates the sub-stance to be persistent. Therefore, this sub-stance is assessed to be persistent in water. (Berger et al. 2018)	vM	exp min. log Doc/Koc = 2.2 (neu-tral cmpd.)	T	SVHC	G;H;O;S (DW&GW: 21.6)	SVHC, HOT-H, DK-study
107-06-2	1,2-dichloroethane	very high	Y	PMT	HQ	P	Due to lack of other information the substance was assessed by PBT assessment in water. Therefore, this substance is assessed to be per-sistent in water. (Berger et al. 2018)	vM	exp min. log Doc/Koc = 1.1 (neu-tral cmpd.)	T	SVHC	H;O (DW&GW: 81.9)	SVHC, HOT-H, DK-study
120-12-7	Anthracene	medium	N	PMT	HQ	P	On SVHC list - PBT substance	M	exp min. log Doc/Koc = 3.6 (neu-tral cmpd.)	T	SVHC	H (GW: det.)	SVHC
96-18-4	1,2,3-trichloropro-pane	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	P data for this substance is variable and difficult to conclude; however, its identification in moni-toring studies in DW and GW indicates it is per-sistent enough.	vM	exp min. log Doc/Koc = 1.9 (neu-tral cmpd.)	T	SVHC	O (GW: 1-5)	SVHC, HOT-H, DK-study

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
111-96-6	Bis(2-methoxyethyl) ether	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 38d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. log Dow/Kow = -0.4 (ne-utral cmpd.)	T	SVHC	S (DW: 0.150)	SVHC, HOT-L
85-42-7	Cyclohexane-1,2-di-carboxylic anhydride	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 21d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. log Doc/Koc = 2.3 (neu-tral cmpd.)	T	SVHC		SVHC
101-80-4	4,4'-oxydianiline	low	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 58d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 1.2 (ioniz-able cmpd.)	T	SVHC		SVHC, DK-study
25550-51-0	Hexahydro-methylphthalic anhy-dride	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 32d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	read-across min. log Dow/Kow = 2.1 (neutral cmpd.)	T	SVHC		SVHC
3380-34-5	Triclosan	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	The P conclusion of triclosan remains contro-versial, with P assessment still under develop-ment. It is observed in monitoring studies, indi-cating it may be P enought to reach drinking water.	vM	exp min. log Doc/Koc = 0.9 (ioniz-able cmpd.)	T	ecotox_ED	A; D; K; N; R (DW&GW: 2.110)	restricted bio-cide (Decision (EU) 2016/110), DK-study
1634-04-4	tert-butyl methyl ether	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	Though definitive P conclusions can not be found an evaluation of dossier information could not rule out definitely that the P criteria was not met.	vM	exp min. log Doc/Koc = 0.2 (neu-tral cmpd.)	T	ED	E;H;O;S (DW&GW: 57.8)	regulated fuel oxygenate (EU Directive 98/70/EC)
98-95-3	Nitrobenzene	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	biodegradation screening tests give conflicting results, but this is detected in monitoring stud-ies	vM	exp min. log Doc/Koc = 1.7 (neu-tral cmpd.)	T	SVHC	H (DW: 100)	SVHC, HOT-L

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
115-96-8	Tris(2-chloroethyl) phosphate	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 35d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 0.7 (neu-tral cmpd.)	T	SVHC	D; E; J; K (DW&GW: 0.74)	SVHC, HOT-H
120-71-8	6-methoxy-m-tolui-dine	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 25d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Dow/Kow = 1.1 (ion-izable cmpd.)	T	SVHC		SVHC
1912-24-9	Atrazine	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 153d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 1.5 (neu-tral cmpd.)	T	STO-TRE_2_Sus pected ED	A; E;H;K;Q (DW&GW: 3.45)	WFD substance
840-65-3	Dimethyl naphtha-lene-2,6-dicarbox-ylate	high	Y	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 8d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	M	exp min. log Dow/Kow = 3.5 (ne-utral cmpd.)	T	SVHC		SVHC
Category 3. Down-prioritized PMT/vPvM substances *19 substances with unique structures, 2 detected in groundwater*													
74-87-3	Chloromethane	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 16d, weight-of-evidence by discovery in monitoring studies, available QSARs and no biodeg. observed in majority of biodegradation screen tests e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 1.1 (neu-tral cmpd.)	T	Carc_2 Rep_2 STOTRE_2	O (GW: >10)	volatile
75-00-3	Chloroethane	very high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 17d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 0.8 (neu-tral cmpd.)	T	Carc_2	O (GW: 1-5)	volatile
90268-23-8	Butanamide, 2,2'-[(3,3'-dichloro[1,1'-bi-phenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(p-anisyl and Ph) derivs.	low	Y	vPvM	HQ	vP	estimated t1/2 = 613d, weight-of-evidence (this study) based on all known QSARs and no bio-deg. observed in majority of biodegradation screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Dow/Kow = 1.4 (ion-izable cmpd.)	Pot. T	Cramer Class III		

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
5468-75-7	2,2'-[(3,3'-di-chloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methylphenyl)-3-oxo-butyramide]	high	Y	vPvM	HQ	vP	estimated t1/2 = 773d, weight-of-evidence (this study) based on all known QSARs and no bio-deg. observed in majority of biodegradation screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Dow/Kow = 0.5 (ion-izable cmpd.)	Pot. T	Cramer Class III		Dye (large MW)
5567-15-7	2,2'-[(3,3'-di-chloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-chloro-2,5-dimethoxy-phenyl)-3-oxobutyra-mide]	high	Y	vPvM	HQ	vP	estimated t1/2 = 716d, weight-of-evidence (this study) based on all known QSARs and no bio-deg. observed in majority of biodegradation screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Dow/Kow = 0.0 (ion-izable cmpd.)	Pot. T	Cramer Class III		Dye (large MW)
36888-99-0	5,5'-(1H-isoindole-1,3(2H)-diylidene)dibarbituric acid	high	Y	vPvM	HQ	vP	Due to lack of other information the substance was assessed by PBT assessment in water. Therefore, this substance is assessed to be per-sistent in water. (Berger et al. 2018)	vM	exp min. log Dow/Kow = 0.3 (ion-izable cmpd.)	Not T	-		Dye (large MW), DK-study
68610-86-6	Butanamide, 2,2'-[(3,3'-dichloro[1,1'-bi-phenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(o-anisyl and 2,4-xylyl) derivs.	high	Y	vPvM	HQ	vP	estimated t1/2 = 861d, weight-of-evidence (this study) based on all known QSARs and no bio-deg. observed in majority of biodegradation screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Dow/Kow = 0.8 (ion-izable cmpd.)	Pot. T	Cramer Class III		Dye (large MW)
1217271-49-2	1,6-Bis[2,2-dimethyl-3-(N-morpholino)-propylideneamino]-hexane	low	Y	vPvM	HQ	vP	estimated t1/2 = 900d, weight-of-evidence (this study) based on all known QSARs and no bio-deg. observed in majority of biodegradation screen tests, e.g. 301 D (Ready Biodegradabil-ity: Closed Bottle Test) July 17, 1992	vM	QSAR min. log Dow/Kow = 0.1 (ion-izable cmpd.)	Pot. T	Cramer Class III		
22094-93-5	2,2'-[(2,2',5,5'-tetra-chloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]	low	Y	vPvM	HQ	vP	estimated t1/2 = 1 619d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Dow/Kow = 0.5 (ion-izable cmpd.)	Pot. T	Cramer Class III		Dye (large MW)
199119-58-9	sodium (4,6-di-methoxypyrimidin-2-yl)carbamoyl-[[3-	low	Y	vPvM & PMT	HQ	vP	measured half-life = 170 d (soil)	vM	exp min. log Doc/Koc = 1.5 (single_anion cmpd.)	T	ecotox		DK-study

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
	(2,2,2-trifluoroeth-oxy)-2-pyridyl]sul-fonyl]azanide												
849608-59-9	Tetra potassium 5,5'-[ethane-1,2-diylbis[thio-1,3,4-thia-diazole-5,2-diyldi-azene-2,1-diyl(5-amino-3-tert-buyl-1H-pyrazole-4,1-diyl)]}diisophthalate	low	Y	vPvM	HQ	vP	estimated t1/2 = 2 706d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	QSAR min. log Dow/Kow = -3.4 (multiple_anion cmpd.)	Pot. T	Cramer Class III		Large MW
88-19-7	Toluene-2-sulphona-mide	low	Y	PMT	HQ	P	No significant biodegradation in 301C testi-mated The PBT assessment evaluates the sub-stance to be persistent. Therefore, this sub-stance is assessed to be persistent in water. (Berger et al. 2018)	vM	QSAR min. log Dow/Kow = 0.9 (ne-utral cmpd.)	T	Carc_1a Carc_2		
13676-54-5	1,1'-(methylenedi-p-phenylene)bismalei-mide	low	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 83d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	exp min. log Doc/Koc = 3.0 (neu-tral cmpd.)	T	muta_2		
115-10-6	Dimethyl ether	high	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 16d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test) Slightly Modified.	vM	exp min. log Doc/Koc = -0.4 (neu-tral cmpd.)	T	Carc_1a muta_1b		volatile
80-73-9	1,3-dimethylimidazol-idin-2-one	low	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 17d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	QSAR min. log Dow/Kow = -0.4 (ne-utral cmpd.)	T	Rep_2 STOTRE_2		
154279-60-4	4,4'-methylenebis(N-sec-butylcyclohexa-mine)	low	Y	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 33d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen	vM	exp min. log Doc/Koc = -1.0 (ion-izable cmpd.)	T	ecotox		

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
							tests for substance/main transformation products, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))						
85-27-8	4-(1-Phenylethyl)-benzene-1,3-diol	low	Y	**vPvM & PMT**	MQ	**Pot. P/vP ++**	estimated t1/2 = 19d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	**vM**	exp min. log Doc/Koc = 1.5 (ionizable cmpd.)	**T**	Suspected ED		
2781-10-4	Dibutyltin bis(2-ethylhexanoate)	low	Y	**PMT**	MQ	**Pot. P/vP ++**	estimated t1/2 = 14d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	**M**	exp min. log Dow/Kow = 2.6 (neutral cmpd.)	**T**	muta_2 Rep_1b Rep_2 STOTRE_1 STOTRE_2 DNEL		
26898-17-9	Dibenzyltoluene	low	Y	**PMT**	MQ	**Pot. P/vP ++**	estimated t1/2 = 44d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	**M**	exp min. log Doc/Koc = 3.6 (neutral cmpd.)	**T**	ecotox		
Category 4. Exempted PMT/vPvM substances *96 substances with unique structures, 27 detected in monitoring studies*													
542-02-9	6-methyl-1,3,5-triazine-2,4-diyldiamine	medium	N	**vPvM**	HQ	**vP**	No significant biodegradation in an enhanced 301E testimated PBT assessment evaluates this substance to be persistent. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	**vM**	exp min. log Dow/Kow = -0.7 (ionizable cmpd.)	**Pot. T**	Cramer Class III	Z (det.)	
768-94-5	Amantadine	medium	N	**PMT**	HQ	**P**	No significant biodegradation in 302B tests. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	**vM**	QSAR min. log Dow/Kow = 0.5 (ionizable cmpd.)	**T**	Rep_2	Z (det.)	
87-61-6	1,2,3-trichloroben-zene	medium	N	**vPvM**	MQ	**Pot. P/vP ++**	estimated t1/2 = 88d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen	**vM**	exp min. log Doc/Koc = 2.9 (neutral cmpd.)	**Pot. T**	Cramer Class III	H (DW: 0.16)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
							tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))						
15307-86-5	Diclofenac	medium	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 99d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	M	exp min. log Doc/Koc = 3.8 (ioniz-able cmpd.)	T	Lact Rep_2 STOTRE_1	A; B;D;H;R (DW&GW: 0.59)	pharmaceutical
7704-67-8	Erythromycin thiocya-nate	medium	N	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 13d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = 0.0 (ion-izable cmpd.)	Pot. T	Cramer Class III	B (GW: >1)	antibiotic
60-80-0	Phenazone	medium	N	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 24d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = 0.9 (ne-utral cmpd.)	Not T	-	B;D;H;R;S (DW&GW: 3.95)	HOT-L
50-48-6	Amitriptyline	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 100d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = -1.3 (ion-izable cmpd.)	T	Rep_2	R (DW: 0.0014)	
57-41-0	Phenytoin	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 43d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = 1.1 (ion-izable cmpd.)	T	Carc_1a Carc_1b Carc_2 muta_1b Rep_1a Rep_1b STOTRE_1	H;K;R (DW: 0.019)	
57-68-1	Sulfadimidine	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 83d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -0.7 (ionizable cmpd.)	T	Lact Rep_2	C; D; H;Q (GW: 0.616)	biocide
68-35-9	Sulfadiazine	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 66d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -1.7 (ionizable cmpd.)	T	Lact Rep_2	B; H;Q (GW: >0.1)	antibiotic
71-55-6	1,1,1-trichloroethane	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 65d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 1.7 (neu-tral cmpd.)	T	Carc_1b Carc_2 STOTRE_2	O (DW&GW: >10)	HOT-L
79-00-5	1,1,2-trichloroethane	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 47d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 1.7 (neu-tral cmpd.)	T	Carc_1b Carc_2	H (DW: 0.1)	HOT-H

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
100-02-7	4-nitrophenol	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 31d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = -1.4 (ion-izable cmpd.)	T	STO-TRE_2_ED	A (GW: 0.122)	HOT-L
114-07-8	Erythromycin	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 768d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = 0.1 (ion-izable cmpd.)	T	Rep_2	B (GW: >1)	antibiotic
144-83-2	Sulfapyridine	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 88d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = 0.5 (ion-izable cmpd.)	T	Rep_2_Sus pected ED	Q (GW: 0.104)	
117-96-4	3,5-diacetamido-2,4,6-triiodobenzoic acid	medium	N	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 797d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = 1.1 (ion-izable cmpd.)	Pot. T	Cramer Class III	B;S;R (DW&GW: >1)	
120-82-1	1,2,4-trichloroben-zene	medium	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 88d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	M	exp min. log Doc/Koc = 3.4 (neu-tral cmpd.)	T	Suspected ED	H (DW: 0.92)	
139-40-2	Propazine	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 186d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 1.8 (neu-tral cmpd.)	T	Carc_2_Su spected ED	A;H;Q (DW&GW: 0.025)	
15687-27-1	Ibuprofen	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 18d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 2.5 (neu-tral cmpd.)	T	Rep_1b Rep_2 STOTRE_2	A;B;C;D;N; R (DW&GW: 12)	HOT-L, pharma-ceutical
18559-94-9	Salbutamol	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 13d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. log Dow/Kow = -0.6 (ionizable cmpd.)	T	Suspected ED	Q (GW: 0.009)	pharmaceutical
66108-95-0	Iohexol	medium	N	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 224d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -2.5 (ne-utral cmpd.)	Pot. T	Cramer Class III	H;S (DW: 11)	Contrasting agent
137862-53-4	(2S)-3-methyl-2-(N-{[2'-(1H-1,2,3,4-te-trazol-5-yl)-[1,1-bi-phenyl]-4-	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 22d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation	vM	exp min. log Dow/Kow = 1.2 (ion-izable cmpd.)	T	Rep_1a Rep_2	E (DW: det.)	HOT-L

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
	yl]methyl}pentan-amido)butanoic acid						products, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)						
139481-59-7	2-ethoxy-1-[[2'-(1H-tetrazol-5-yl)biphenyl-4-yl]methyl]-1H-benzimidazole-7-carboxylic acid	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 48d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -0.6 (ionizable cmpd.)	T	Rep_2	X (DW: det.)	HOT-L
152459-95-5	Benzamide, 4-[(4-methyl-1-piperazinyl)methyl]-N-[4-methyl-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 881d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -0.7 (ionizable cmpd.)	T	Carc_2 muta_2 Rep_1b Rep_2 STOTRE_2	B (GW: >0.1)	
83905-01-5	2R,3R,4R,5R,8R,10R,11R,13S,14R)-11-[(2S,3R,4S,6R)-4-dimethylamino-3-hydroxy-6-methyl-oxan-2-yl]oxy-2-ethyl-3,4,10-trihydroxy-13-[(2S,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyl-oxan-2-yl]oxy-3,5,6,8,10,12,14-heptamethyl-1-oxa-6-azacyclopentadecan-15-one	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 1 469d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -0.5 (ionizable cmpd.)	T	STOTRE_2	X (DW: det.)	antibiotic
93413-69-5	1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol	medium	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 83d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = 1.4 (ionizable cmpd.)	T	Lact Rep_1a	L (DW: 0.0011)	
144689-24-7	4-(Hydroxy-1-methyethyl)-2-propyl-1-[[2'-[1H-tetrazol-5-yl]-1,1'-biphenyl-4-	medium	N	vPvM	MQ	Pot. P/vP ++	estimated t1/2 = 112d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = 1.5 (ionizable cmpd.)	Pot. T	Cramer Class III	X (DW: det.)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
	yl]methyl]-1H-imidaz-ole-5-carboxylic acid												
25321-14-6	Dinitrotoluene	low	N	vPvM & PMT	MQ	Pot. P/vP ++	P data for this substance is variable and difficult to conclude; it is not readily biodegradable, QSARs collectively anticipate persistence, yet soil half-life studies indicates it is nor persistent. In lieu of the high volumes and toxicity of this substance, it is considered potentially P	vM	exp min. log Doc/Koc = 1.0 (neu-tral cmpd.)	T	Carc_1b muta_2 Rep_2 STOTRE_2		
79-46-9	2-nitropropane	high	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 16d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = -1.7 (ion-izable cmpd.)	T	Carc_1b muta_2		
96-12-8	1,2-dibromo-3-chloro-propane	low	N	PMT	HQ	vP	measured half-life = 529 d (soil)	M	QSAR min. log Dow/Kow = 2.5 (ne-utral cmpd.)	T	Carc_1b muta_1b muta_2 Rep_1a STO-TRE_2_Sus pected ED		
118-79-6	2,4,6-tribromophenol	low	N	vPvM & PMT	HQ	vP	measured half-life = 370 d (soil)	vM	exp min. log Doc/Koc = -0.4 (ion-izable cmpd.)	T	Rep_2 STO-TRE_2_ED		
55-56-1	Chlorhexidine	low	N	PMT	HQ	vP	estimated t1/2 = 837d, weight-of-evidence (this study) based on all known QSARs and no bio-deg. observed in majority of biodegradation screen tests, e.g. 301 D (Ready Biodegradabil-ity: Closed Bottle Test)	M	QSAR min. log Dow/Kow = 2.4 (ion-izable cmpd.)	T	ecotox		disinfectant
4404-43-7	4,4'-bis[4-[bis(2-hy-droxyethyl)amino]-6-anilino-1,3,5-triazin-2-yl]amino]stilbene-2,2'-disulphonic acid	low	N	vPvM	HQ	vP	estimated t1/2 = 2 317d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 A (old version) (Ready Bio-degradabiltiy: Modified AFNOR Test)	vM	exp min. log Doc/Koc = 2.5 (zwit-terion cmpd.)	Pot. T	Cramer Class III		Dye (large MW)
6022-22-6	Disodium 4,4'-dia-mino-9,9',10,10'-tet-rahydro-9,9',10,10'-	low	N	vPvM	HQ	vP	estimated t1/2 = 693d, weight-of-evidence (this study) based on all known QSARs and no bio-deg. observed in majority of biodegradation	vM	QSAR min. log Dow/Kow = -1.1	Pot. T	Cramer Class III		

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	tetraoxo[1,1'-bian-thracene]-3,3'-disul-phonate						screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)		(multiple_anion cmpd.)				
6358-37-8	2,2'-[(3,3'-di-chloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-methylphenyl)-3-oxo-butyramide]	low	N	vPvM	HQ	vP	estimated t1/2 = 773d, weight-of-evidence (this study) based on all known QSARs and no bio-deg. observed in majority of biodegradation screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Dow/Kow = 1.1 (ion-izable cmpd.)	Pot. T	Cramer Class III		
52299-25-9	bis(nonafluorobu-tyl)phosphinic acid	low	N	vPvM	HQ	vP	estimated t1/2 = 1 556d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. log Dow/Kow = -1.1 (ionizable cmpd.)	Pot. T	Cramer Class III		
25956-17-6	Disodium 6-hydroxy-5-[(2-methoxy-4-sul-phonato-m-tolyl)azo]naphtha-lene-2-sulphonate	low	N	vPvM & PMT	HQ	vP	Due to lack of other information the substance was assessed by PBT assessment in water. Therefore, this substance is assessed to be per-sistent in water. (Berger et al. 2018)	vM	exp min. log Dow/Kow = 0.1 (multiple_anion cmpd.)	T	Suspected ED		Dye (large MW). DK-study
35453-19-1	5-amino-2,4,6-triio-doisophthalic acid	low	N	vPvM	HQ	vP	estimated t1/2 = 1 024d, weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	QSAR min. log Dow/Kow = 0.6 (ion-izable cmpd.)	Pot. T	Cramer Class III		
68391-08-2	Alcohols, C8-14, γ-ω-perfluoro	low	N	PMT	HQ	vP	measured half-life = 202 521 d (soil)	M	QSAR min. log Dow/Kow = 2.9 (ne-utral cmpd.)	T	Rep_2 STOTRE_2		
111453-32-8	rac-5-Amino-N-(2,3-dihydroxypropyl)-2,4,6-triiodoisophtha-lamic acid	low	N	vPvM	HQ	vP	estimated t1/2 = 755d, weight-of-evidence (this study) based on all known QSARs and no bio-deg. observed in majority of biodegradation screen tests, e.g. 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	QSAR min. log Dow/Kow = 0.1 (ion-izable cmpd.)	Pot. T	Cramer Class III		
1072957-71-1	N-[9-(dichloromethyli-dene)-1,2,3,4-tetrahy-dro-1,4-meth-anonaphthalen-5-yl]-3-(difluoromethyl)-1-	low	N	PMT	HQ	vP	measured half-life = 881 d (soil)	M	exp min. log Doc/Koc = 3.7 (ioniz-able cmpd.)	T	ecotox		

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	methyl-1H-pyrazole-4-carboxamide												
155661-07-7	rac-[(2R,4R)-2-(2,4-DI-CHLOROPHENYL)-2-(1H-1,2,4-TRIAZOL-1-YLMETHYL)-1,3-DIOX-OLAN-4-YL]METHYL METHANESULFONATE MONOHYDROCHLO-RIDE	low	N	PMT	HQ	P	estimated t1/2 = 489d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respi-rometry Test)	vM	exp min. log Doc/Koc = 2.5 (neu-tral cmpd.)	T	STOTRE_2		pharmaceutical
120-83-2	2,4-dichlorophenol	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 42d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 0.0 (ioniz-able cmpd.)	T	Suspected ED		
4433-79-8	4'-chloro-2',5'-di-methoxyacetoacetan-ilide	high	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 20d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	M	exp min. log Dow/Kow = 1.7 (ion-izable cmpd.)	T	STOTRE_2		
6610-29-3	4-methylthiosemi-carbazide	high	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 17d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. log Dow/Kow = -1.0 (ionizable cmpd.)	T	DNEL		HOT-L
68512-65-2	Resin acids and Rosin acids, esters with eth-ylene glycol	high	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 187d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	read-across min. log Dow/Kow = 2.4 (neutral cmpd.)	T	Rep_2		
-	Tin, dioctylbis(2,4-pentanedionato-κO2,κO4)-	high	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 32d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen	vM	exp min. log Doc/Koc = 0.9 (neu-tral cmpd.)	T	Rep_2 STOTRE_2		

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							tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)						
100-40-3	4-vinylcyclohexene	low	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 16d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	M	QSAR min. log Dow/Kow = 3.2 (ne-utral cmpd.)	T	Carc_2 Rep_2		
68-22-4	Norethisterone	low	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 78d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. log Dow/Kow = 2.7 (ne-utral cmpd.)	T	Carc_1b Carc_2 Lact Rep_1a Rep_1b Rep_2 STO-TRE_2_Sus pected ED		pharmaceutical
88-17-5	α,α,α-trifluoro-o-tolu-idine	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 96d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. log Dow/Kow = 2.3 (ne-utral cmpd.)	T	STOTRE_2		
81-11-8	4,4'-diaminostilbene-2,2'-disulphonic acid	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 251d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	QSAR min. log Dow/Kow = -2.7 (ionizable cmpd.)	T	Suspected ED		
88-75-5	2-nitrophenol	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 31d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = -1.3 (ion-izable cmpd.)	T	STOTRE_2		HOT-L

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88-44-8	4-aminotoluene-3-sul-phonic acid	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 50d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	QSAR min. log Dow/Kow = -1.7 (ionizable cmpd.)	T	Suspected ED		
97-00-7	1-chloro-2,4-dinitro-benzene	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 159d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. log Dow/Kow = 2.2 (ne-utral cmpd.)	T	muta_2 STOTRE_1 STOTRE_2		HOT-L
95-54-5	o-phenylenediamine	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 48d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Dow/Kow = -0.6 (ionizable cmpd.)	T	Carc_2 muta_2		
99-88-7	4-isopropylaniline	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 36d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 1.2 (ioniz-able cmpd.)	T	ecotox		
97-52-9	4-nitro-o-anisidine	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 46d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	exp min. log Dow/Kow = 1.2 (ion-izable cmpd.)	T	Carc_2 muta_2		
103-69-5	N-ethylaniline	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 26d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Dow/Kow = 1.1 (ion-izable cmpd.)	T	STOTRE_2		

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106-48-9	4-chlorophenol	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 23d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 0.9 (ioniz-able cmpd.)	T	Suspected ED		HOT-L
108-67-8	Mesitylene	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 19d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 2.9 (neu-tral cmpd.)	T	STOTRE_1		
109-09-1	2-chloropyridine	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 35d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 0.8 (neu-tral cmpd.)	T	STOTRE_2		
109-70-6	1-bromo-3-chloropro-pane	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 24d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. log Dow/Kow = 2.0 (ne-utral cmpd.)	T	Carc_1b Carc_2 muta_2 Rep_2 STOTRE_2		HOT-L
119-65-3	Isoquinoline	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 19d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 1.8 (ioniz-able cmpd.)	T	Carc_1b		
121-86-8	2-chloro-4-nitrotolu-ene	low	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 72d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	M	QSAR min. log Dow/Kow = 2.9 (ne-utral cmpd.)	T	STOTRE_2		

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434-03-7	Ethisterone	low	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 119d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	M	exp min. log Dow/Kow = 2.7 (ne-utral cmpd.)	T	ecotox Carc_2 Lact Rep_1a Rep_2_Sus pected ED		pharmaceutical
479-27-6	1,8-naphthylenedia-mine	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 64d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	QSAR min. log Dow/Kow = 1.3 (ion-izable cmpd.)	T	Carc_2 muta_2		
599-64-4	4-(α,α-dimethylben-zyl)phenol	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 27d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 3.0 (ioniz-able cmpd.)	T	STO-TRE_2_Sus pected ED		
611-06-3	1,3-dichloro-4-nitro-benzene	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 119d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	exp min. log Doc/Koc = 2.5 (neu-tral cmpd.)	T	Carc_1b Carc_2 muta_2 Rep_2		
615-60-1	4-chloro-o-xylene	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 32d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 1.2 (neu-tral cmpd.)	T	STOTRE_2		
920-66-1	1,1,1,3,3,3-hex-afluoropropan-2-ol	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 95d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = -0.5 (ion-izable cmpd.)	T	Rep_2		

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1185-81-5	Dibutylbis(do-decylthio)stannane	low	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 12d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	M	exp min. log Dow/Kow = 3.1 (ne-utral cmpd.)	T	muta_2 Rep_1b STOTRE_1		
1321-12-6	Nitrotoluene	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 39d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Doc/Koc = 1.9 (neu-tral cmpd.)	T	Carc_1b muta_1b Rep_2 STOTRE_2		
1570-64-5	4-chloro-o-cresol	low	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 26d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. log Dow/Kow = 2.2 (ion-izable cmpd.)	T	Suspected ED		
2243-62-1	1,5-naphthylenedia-mine	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 64d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	QSAR min. log Dow/Kow = 1.1 (ion-izable cmpd.)	T	Carc_2		
100-00-5	1-chloro-4-nitroben-zene	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 64d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 2.1 (neu-tral cmpd.)	T	Carc_2 muta_2 STOTRE_2		
2524-03-0	O,O-dimethyl phos-phorochloridothioate	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 24d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	QSAR min. log Dow/Kow = 1.4 (ne-utral cmpd.)	T	muta_2		

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3590-84-9	Tetraoctyltin	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 8d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	exp min. log Dow/Kow = -4.0 (ne-utral cmpd.)	T	STOTRE_2		antibiotic
5460-09-3	Sodium hydrogen 4-amino-5-hy-droxynaphthalene-2,7-disulphonate	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 90d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	QSAR min. log Dow/Kow = -4.2 (single_anion cmpd.)	T	Suspected ED		
6358-64-1	4-chloro-2,5-di-methoxyaniline	low	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 36d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	M	exp min. log Dow/Kow = 1.8 (ion-izable cmpd.)	T	STO-TRE_2_Sus pected ED		
6640-24-0	1-(m-chlorophenyl)pi-perazine	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 62d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	QSAR min. log Dow/Kow = 0.3 (ion-izable cmpd.)	T	Rep_2		
7336-20-1	Disodium 4,4'-diami-nostilbene-2,2'-disulphonate	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 251d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	QSAR min. log Dow/Kow = -3.1 (multiple_anion cmpd.)	T	Suspected ED		
7474-78-4	3,4-diaminobenzene-sulphonic acid	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 82d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	QSAR min. log Dow/Kow = -2.7 (ionizable cmpd.)	T	Suspected ED		

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
25376-45-8	Diaminotoluene	low	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 54d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	M	exp min. log Doc/Koc = 3.4 (ioniz-able cmpd.)	T	Carc_1b muta_2 Rep_2 STOTRE_2		
27310-25-4	7-aminonaphthalene-1,3,5-trisulphonic acid	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 174d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	QSAR min. log Dow/Kow = -5.0 (ionizable cmpd.)	T	Suspected ED		
49701-24-8	4-amino-2,5-di-methoxy-N-methylbenzenesul-phonamide	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 34d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 F (Ready Biodegradability: Mano-metric Respirometry Test)	vM	exp min. log Dow/Kow = 0.3 (ion-izable cmpd.)	T	Suspected ED		
67801-01-8	Barium bis[5-chloro-4-ethyl-2-[(2-hydroxy-1-naphthyl)azo]ben-zenesulphonate]	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 205d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	exp min. log Dow/Kow = 0.1 (sin-gle_anion cmpd.)	T	Suspected ED		
71786-67-9	Benzyl(3-hydroxy-phenacyl)me-thylammonium chlo-ride	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 26d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. log Dow/Kow = 0.5 (sin-gle_cation cmpd.)	T	Suspected ED		
73612-34-7	Barium bis[6-chloro-4-[(2-hydroxy-1-naph-thyl)azo]toluene-3-sulphonate]	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 122d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. log Dow/Kow = 2.0 (sin-gle_anion cmpd.)	T	Suspected ED		

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
84650-02-2	Distillates (coal tar), benzole fraction	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 21d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	vM	exp min. log Doc/Koc = 1.4 (neu-tral cmpd.)	T	Carc_1a Carc_1b muta_1b Rep_2 STOTRE_1		
93839-71-5	4-[[(2-aminophe-nyl)methyl]amino]cy-clohexyl acetate	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 26d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. log Dow/Kow = 0.3 (ion-izable cmpd.)	T	Suspected ED		
7305-71-7	2-amino-5-methylthi-azole	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 31d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	QSAR min. log Dow/Kow = 0.3 (ion-izable cmpd.)	T	STOTRE_2		
114772-54-2	4'-Bromomethylbi-phenyl-2-carbonitrile	low	N	PMT	MQ	Pot. P/vP ++	estimated t1/2 = 34d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. log Doc/Koc = 3.4 (neu-tral cmpd.)	T	muta_2		
54914-95-3	sodium 2-amino-5-methylbenzenesul-fonate	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 50d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	vM	QSAR min. log Dow/Kow = -1.7 (single_anion cmpd.)	T	Suspected ED		
3717-40-6	N,N-dimethyl-1-ada-mantanamine	low	N	vPvM & PMT	MQ	Pot. P/vP ++	estimated t1/2 = 61d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	QSAR min. log Dow/Kow = 0.9 (ion-izable cmpd.)	T	Rep_2		

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
91161-71-6	(2E)-N,6,6-trimethyl-N-(1-naphthylmethyl)hept-2-en-4-yn-1-amine	low	N	**vPvM & PMT**	MQ	**Pot. P/vP ++**	estimated t1/2 = 133d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	**vM**	exp min. log Dow/Kow = 0.3 (ionizable cmpd.)	**T**	ecotox		
641571-11-1	3-(4-Methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)aniline	low	N	**PMT**	MQ	**Pot. P/vP ++**	estimated t1/2 = 158d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	**M**	QSAR min. log Dow/Kow = 1.9 (ionizable cmpd.)	**T**	Suspected ED		
Category 5. Detected PM substances *11 substances*													
13674-84-5	Tris(2-chloro-1-methylethyl) phosphate	very high	Y	**PM**	HQ	**vP**	Biodegradation results in 301C and E tests <20% and persistence due to PBT assessment. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	**M**	QSAR min. log Dow/Kow = 2.9 (neutral cmpd.)	**Pot. T**	Cramer Class III	E; F; K; Z (DW: 0.5)	
1506-02-1	1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one	very high	Y	**PM**	MQ	**Pot. P/vP ++**	estimated t1/2 = 74d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	**M**	exp min. log Doc/Koc = 3.4 (neutral cmpd.)	**Not T**	-	H (DW: <0.1)	DK-study
15214-89-8	2-acrylamido-2-methylpropanesulphonic acid	very high	Y	**PM**	HQ	**P**	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. (Berger et al. 2018)	**vM**	exp min. log Dow/Kow = -3.7 (ionizable cmpd.)	**Pot. T**	Cramer Class III	F (DW: det.)	DK-study
21145-77-7	1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one	medium	N	**PM**	MQ	**Pot. P/vP ++**	estimated t1/2 = 74d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	**M**	exp min. log Doc/Koc = 3.4 (neutral cmpd.)	**Not T**	-	J (DW: 0.1)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
461-58-5	Cyanoguanidine	very high	Y	**PM**	HQ	**P**	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. (Berger et al. 2018)	**vM**	exp min. log Dow/Kow = 0.1 (neutral cmpd.)	**Pot. T**	Cramer Class III	F; Z (DW: det.)	
1561-92-8	Sodium 2-methylprop-2-ene-1-sulphonate	very high	Y	**PM**	HQ	**P**	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. (Berger et al. 2018)	**vM**	exp min. log Doc/Koc = -6.6 (single_anion cmpd.)	**Pot. T**	Cramer Class III	Z	
23386-52-9	Sodium 1,4-dicyclo-hexyl sulphonatosuc-cinate	very high	Y	**PM**	HQ	**P**	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. (Berger et al. 2018)	**vM**	exp min. log Dow/Kow = 0.0 (single_anion cmpd.)	**Pot. T**	Cramer Class III	Z	
3965-55-7	Sodium dimethyl 5-sulphona-toisophthalate	very high	Y	**PM**	HQ	**P**	All biodegradation results in 301C and 302B tests imply no significant biodegradation. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	**vM**	QSAR min. log Dow/Kow = -1.0 (single_anion cmpd.)	**Pot. T**	Cramer Class III	Z	
52722-86-8	4-hydroxy-2,2,6,6-tet-ramethylpiperidine-1-ethanol	very high	Y	**PM**	HQ	**P**	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. (Berger et al. 2018)	**vM**	exp min. log Doc/Koc = -3.7 (ionizable cmpd.)	**Pot. T**	Cramer Class III	Z	
55589-62-3	6-methyl-1,2,3-oxa-thiazin-4(3H)-one 2,2-dioxide, potassium salt	very high	Y	**PM**	HQ	**P**	All biodegradation results in 301A and 302B tests imply no significant biodegradation. Therefore, this substance is assessed to be persistent in water. (Berger et al. 2018)	**vM**	QSAR min. log Dow/Kow = -2.3 (single_anion cmpd.)	**Pot. T**	Cramer Class III	Z	
7365-45-9	4-(2-hydroxyethyl)pi-perazin-1-ylethanesulphonic acid	medium	Y	**PM**	HQ	**P**	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. (Berger et al. 2018)	**vM**	exp min. log Doc/Koc = 1.3 (zwitterion cmpd.)	**Pot. T**	Cramer Class III	Z	
Category 6. Detected Potential PMT/vPvM substances *26 substances*													

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
101-77-9	4,4'-methylenedianiline	very high	Y	Pot. PMT/vPvM	LQ	Pot. P/vP	P data for this substance is variable and difficult to conclude (see e.g. Berger et al. (2018)); however, its identification in monitoring studies in monitoring studies (Schulze et al. 2019) indicates it is persistent enough to be considered potentially P/vP	vM	exp min. log Doc/Koc = 0.8 (ionizable cmpd.)	T	SVHC	Z	SVHC, DK-study
104-23-4	4'-aminoazobenzene-4-sulphonic acid	very high	Y	Pot. PMT/vPvM	LQ	Pot. P/vP	P data for this substance is variable and difficult to conclude (see e.g. Berger et al. (2018)); however, its identification in monitoring studies in monitoring studies (Schulze et al. 2019) indicates it is persistent enough to be considered potentially P/vP	vM	exp min. log Dow/Kow = 0.4 (ionizable cmpd.)	T	Suspected ED	Z	DK-study
103-90-2	Paracetamol	medium	Y	Pot. PMT/vPvM	LQ	Pot. P/vP	estimated t1/2 = 11d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 0.0 (ionizable cmpd.)	T	Carc_2 muta_2 STOTRE_1 STOTRE_2	B; C; D; H; J;Q;R (DW&GW: 120)	
121-57-3	Sulphanilic acid	very high	Y	Pot. PMT/vPvM	LQ	Pot. P/vP	estimated t1/2 = 44d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -1.9 (ionizable cmpd.)	T	Suspected ED	F (DW: det.)	
131-57-7	Oxybenzone	very high	Y	Pot. PMT/vPvM	LQ	Pot. P/vP	estimated t1/2 = 16d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	Pot. M	exp min. log Dow/Kow = 3.6 (neutral cmpd.)	T	STOTRE_2_ED	H (DW: det.)	
140-01-2	Pentasodium (carboxylatomethyl)imino-bis(ethyleneni-trilo)tetraacetate	very high	Y	Pot. PMT/vPvM	LQ	Pot. P/vP	estimated t1/2 = 8d, weight-of-evidence by discovery in monitoring studies, available QSARs and no biodeg. observed in majority of biodegradation screen tests e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test),301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. log Dow/Kow = -15.6 (multiple_anion cmpd.)	T	Rep_1a Rep_2 STOTRE_2	E (DW: det.)	
143-24-8	Bis(2-(2-methoxyethoxy)ethyl) ether	very high	Y	Pot. PMT/vPvM	LQ	Pot. P/vP	estimated t1/2 = 83d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Dow/Kow = -0.8 (neutral cmpd.)	T	Rep_1b	E (DW: det.)	HOT-L
22204-53-1	Naproxen	medium	N	Pot. PMT/vPvM	LQ	Pot. P/vP	estimated t1/2 = 12d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = -0.2 (ionizable cmpd.)	T	Carc_2 Lact Rep_1b Rep_2 STOTRE_2	H (DW&GW: det.)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
288-13-1	Pyrazole	medium	N	**Pot. PMT/v PvM**	LQ	**Pot. P/vP**	estimated t1/2 = 13d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	**vM**	exp min. log Dow/Kow = 0.3 (ion-izable cmpd.)	**T**	Rep_2 STOTRE_1	E (DW: det.)	
532-02-5	Sodium naphthalene-2-sulphonate	very high	N	**Pot. PMT/v PvM**	LQ	**Pot. P/vP**	estimated t1/2 = 32d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	**vM**	QSAR min. log Dow/Kow = -1.5 (single_anion cmpd.)	**Pot. T**	Cramer Class III	E (DW: det.)	
57-83-0	Progesterone	medium	N	**Pot. PMT/v PvM**	LQ	**Pot. P/vP**	estimated t1/2 = 78d, and consistency across all tested QSARs	**Pot. M**	exp min. log Dow/Kow = 3.7 (ne-utral cmpd.)	**T**	Carc_1b Carc_2 Lact muta_1b muta_2 Rep_1a Rep_1b Rep_2_Sus pected ED	B;H;K (DW&GW: 0.1)	
60-00-4	Edetic acid	very high	Y	**Pot. PMT/v PvM**	LQ	**Pot. P/vP**	estimated t1/2 = 6d, weight-of-evidence by dis-covery in monitoring studies, available QSARs and no biodeg. observed in majority of biodeg-radation screen tests e.g. 301 A (new version) (Ready Biodegradability: DOC Die Away Test)	**vM**	QSAR min. log Dow/Kow = -7.2 (ionizable cmpd.)	**T**	Rep_2 STOTRE_1 STOTRE_2	B; E;S (DW&GW: 13.6)	
637-92-3	2-ethoxy-2-methylpropane	very high	Y	**Pot. PMT/v PvM**	LQ	**Pot. P/vP**	estimated t1/2 = 29d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	**vM**	exp min. log Doc/Koc = 0.6 (neu-tral cmpd.)	**Pot. T**	Cramer Class III	H (GW: det.)	
67-43-6	N-carboxyme-thyliminobis(eth-ylenenitrilo)tetra(ace-tic acid)	very high	Y	**Pot. PMT/v PvM**	LQ	**Pot. P/vP**	estimated t1/2 = 8d, weight-of-evidence by dis-covery in monitoring studies, available QSARs and no biodeg. observed in majority of biodeg-radation screen tests e.g. 301 D (Ready Biodeg-radability: Closed Bottle Test)	**vM**	QSAR min. log Dow/Kow = -8.8 (ionizable cmpd.)	**T**	Rep_2 STOTRE_2	B;S;E (DW&GW: 9)	
74-83-9	Bromomethane	medium	N	**Pot. PMT/v PvM**	LQ	**Pot. P/vP**	estimated t1/2 = 14d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	**vM**	exp min. log Doc/Koc = 0.7 (neu-tral cmpd.)	**T**	muta_2 STO-TRE_2_Sus pected ED	O (GW: 0.4)	HOT-L
74-95-3	Dibromomethane	medium	N	**Pot. PMT/v PvM**	LQ	**Pot. P/vP**	estimated t1/2 = 20d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	**vM**	exp min. log Doc/Koc = 1.3 (neu-tral cmpd.)	**Pot. T**	Cramer Class III	H (DW: 0.7)	HOT-L

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
76-74-4	Pentobarbital	medium	N	Pot. PMT/v PvM	LQ	Pot. P/vP	estimated t1/2 = 45d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	QSAR min. log Dow/Kow = 1.1 (ion-izable cmpd.)	T	Rep_2	B (GW: 1)	
791-28-6	Triphenylphosphine oxide	medium	N	Pot. PMT/v PvM	LQ	Pot. P/vP	estimated t1/2 = 31d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 3.0 (neu-tral cmpd.)	Pot. T	Cramer Class III	S (DW: 0.1)	
80-09-1	4,4'-sulphonyldiphe-nol	very high	Y	Pot. PMT/v PvM	LQ	Pot. P/vP	The 301C test indicates non readily biodegrada-ble; however, QSAR data and other indicators indicate is more persistent than BPA	vM	exp min. log Doc/Koc = -0.3 (ion-izable cmpd.)	T	_ED	F; Z (DW: det.)	
826-36-8	2,2,6,6-tetramethyl-4-piperidone	medium	N	Pot. PMT/v PvM	LQ	Pot. P/vP	estimated t1/2 = 32d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = -3.3 (ion-izable cmpd.)	Pot. T	Cramer Class III	E (DW: det.)	
83-32-9	Acenaphthene	medium	N	Pot. PMT/v PvM	LQ	Pot. P/vP	estimated t1/2 = 28d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	M	exp min. log Doc/Koc = 3.3 (neu-tral cmpd.)	Pot. T	Cramer Class III	H (GW: det.)	
85-98-3	1,3-diethyldiphenylu-rea	very high	Y	Pot. PMT/v PvM	LQ	Pot. P/vP	estimated t1/2 = 31d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 2.5 (neu-tral cmpd.)	Pot. T	Cramer Class III	X (DW: det.)	DK-study
91-20-3	Naphthalene	very high	Y	Pot. PMT/v PvM	LQ	Pot. P/vP	Data indicates certain conditions where Naph-thalene is persistent, but no definitive conclu-sion is given based on Nielsen et al. Environ. Sci. Technol., 1995, 30 (1), pp 31–37; further, many natural causes of naphthalene occur	vM	exp min. log Doc/Koc = 2.5 (neu-tral cmpd.)	T	Carc_2 STO-TRE_1_ED	H;O;P (DW&GW: 3)	DK-study
95-16-9	Benzothiazole	very high	Y	Pot. PMT/v PvM	LQ	Pot. P/vP	biodegradation screening tests give conflicting results	vM	exp min. log Dow/Kow = 2.0 (ne-utral cmpd.)	T	STOTRE_2	S (DW: 0.01)	
98-82-8	Cumene	very high	Y	Pot. PMT/v PvM	LQ	Pot. P/vP	Initial evidnce suggests this si not P under aero-bic conditions. This substance is observed in monitoring studies, but this could be mainly due to extensive emissions.	vM	exp min. log Doc/Koc = 2.9 (neu-tral cmpd.)	T	STOTRE_1	H;O (DW&GW: 3)	
994-05-8	2-methoxy-2-methyl-butane	very high	Y	Pot. PMT/v PvM	LQ	Pot. P/vP	estimated t1/2 = 29d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	vM	exp min. log Doc/Koc = 0.7 (neu-tral cmpd.)	T	Carc_1b	O (GW: 0.4)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
Category 7. Detected Non PMT/vPvM substances *47 substances*													
1222-05-5	1,3,4,6,7,8-hexahy-dro-4,6,6,7,8,8-hexa-methylindeno[5,6-c]pyran	very high	Y	**Not PMT**	HQ	**vP**	measured half-life = 203 d (soil)	**not M**	exp min. log Doc/Koc = 4.3 (neu-tral cmpd.)	**T**	Rep_2_ED	D;H;Q (DW&GW: 23)	
140-66-9	4-(1,1,3,3-tetra-methylbutyl)phenol	very high	Y	**Not PMT**	HQ	**P**	measured half-life = 49 d (fresh water)	**not M**	exp min. log Doc/Koc = 4.0 (neu-tral cmpd.)	**T**	SVHC	A; Q (GW: 1.8)	SVHC, DK-study
117-81-7	Bis(2-ethylhexyl) phthalate	very high	Y	**Not PMT**	HQ	**P**	measured half-life = 176 d (soil)	**not M**	exp min. log Doc/Koc = 5.7 (neu-tral cmpd.)	**T**	SVHC	N; Q (DW&GW: 5.7)	SVHC
140-31-8	2-piperazin-1-ylethyl-amine	very high	Y	**Not PMT**	HQ	**P**	All biodegradation results in 301D and F and 302B tests imply no significant biodegradation. Therefore, this substance is assessed to be per-sistent in water. (Berger et al. 2018)	**not M**	exp min. log Doc/Koc = 4.6 (ioniz-able cmpd.)	**T**	Rep_2 STOTRE_1	Z (det.)	
96-76-4	2,4-di-tert-butylphe-nol	very high	Y	**Not PMT**	HQ	**Pot. P/vP ++**	estimated t1/2 = 48d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	**not M**	exp min. log Dow/Kow = 4.8 (ne-utral cmpd.)	**T**	STO-TRE_2_Sus pected ED	X (DW: det.)	
128-37-0	2,6-di-tert-butyl-p-cresol	very high	Y	**Not PMT**	HQ	**Pot. P/vP ++**	estimated t1/2 = 53d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation prod-ucts, e.g. 301 C (Ready Biodegradability: Modi-fied MITI Test (I))	**not M**	exp min. log Doc/Koc = 4.4 (neu-tral cmpd.)	**T**	Carc_1b Carc_2 muta_1b muta_2 Rep_2 STO-TRE_2_ED	K; H (DW: 0.026)	DK-study
129-00-0, 1718-52-1	Pyrene	medium	N	**Not PMT**	HQ	**Pot. P/vP**	estimated t1/2 = 139d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	**not M**	exp min. log Doc/Koc = 4.1 (neu-tral cmpd.)	**T**	ecotox	H (GW: det.)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
104-40-5	p-nonylphenol	medium	N	Not PMT	HQ	Pot. P/vP	estimated t1/2 = 13d, weight-of-evidence by discovery in monitoring studies, and consistent indications of P across tested QSARs	not M	QSAR min. log Dow/Kow = 6.1 (neutral cmpd.)	T	SVHC	A; D;H;J; K; Q (DW&GW: 84)	SVHC
100-41-4	Ethylbenzene	very high	Y	Not PMT	HQ	not P	inherently biodeg: 302 C (Inherent Biodegradability: Modified MITI Test (II))	vM	exp min. log Doc/Koc = 2.7 (neutral cmpd.)	T	Carc_2 STOTRE_2	H;O (DW&GW: 10)	
100-42-5	Styrene	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 2.1 (neutral cmpd.)	T	SVHC	H (DW: 46.4)	SVHC
102-76-1	Triacetin	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. log Dow/Kow = 0.1 (neutral cmpd.)	Not T	-	E (DW: det.)	
106-46-7	1,4-dichlorobenzene	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 2.4 (neutral cmpd.)	T	Carc_2	O (GW: 10)	DK-study
107-07-3	2-chloroethanol	very high	Y	Not PMT	HQ	not P	readily biodeg: 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test),301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. log Doc/Koc = 0.3 (neutral cmpd.)	T	Carc_1a muta_1b STOTRE_1	X (DW: det.)	
108-88-3	Toluene	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Doc/Koc = 1.9 (neutral cmpd.)	T	Rep_1a Rep_2 STOTRE_1 STOTRE_2	H;O;P (DW&GW: 63.1)	
105-60-2	ε-caprolactam	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Doc/Koc = 1.8 (neutral cmpd.)	T	STOTRE_1	F; Z (DW: det.)	
120-18-3	Naphthalene-2-sulphonic acid	very high	Y	Not PMT	HQ	not P	OECD tests (301B and E) for surrogate imply no persistence. Therefore, the substance is assessed not to be persistent. (Berger et al. 2018)	vM	exp min. log Doc/Koc = -5.9 (ionizable cmpd.)	T	Carc_2	F (DW: det.)	
139-13-9	Nitrilotriacetic acid	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	exp min. log Doc/Koc = 1.4 (ionizable cmpd.)	T	Carc_2 muta_1b STOTRE_2	H (GW: det.)	
126-73-8	Tributyl phosphate	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Doc/Koc = 1.9 (neutral cmpd.)	T	Carc_2 STOTRE_2	J (DW: 0.2)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
25321-41-9	Xylenesulphonic acid	very high	Y	Not PMT	HQ	not P	Several read-across studies including 301B and D tests imply no persistence. Therefore, the substance is assessed not to be persistent. (Berger et al. 2018)	vM	exp min. log Dow/Kow = -6.0 (ionizable cmpd.)	Not T	-	F; Z (DW: det.)	
128-44-9	1,2-benzisothiazol-3(2H)-one 1,1-dioxide, sodium salt	very high	Y	Not PMT	HQ	not P	readily biodeg: 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)	vM	exp min. log Doc/Koc = -6.0 (single_anion cmpd.)	T	Carc_1a Carc_1b Carc_2	F (DW: det.)	
50-78-2	O-acetylsalicylic acid	very high	Y	Not PMT	HQ	not P	estimated t1/2 = 7d, and consistency across all tested QSARs	vM	exp min. log Doc/Koc = -5.7 (ionizable cmpd.)	T	Rep_1a Rep_1b Rep_2 STOTRE_2	B;S (GW: 0.1)	
131-11-3	Dimethyl phthalate	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	exp min. log Doc/Koc = 1.9 (neutral cmpd.)	T	Rep_2_Suspected ED	N (DW: 0.5)	
58-08-2	Caffeine	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 A (new version) (Ready Biodegradability: DOC Die Away Test)	vM	exp min. log Doc/Koc = 1.0 (neutral cmpd.)	Not T	-	A; B; C; D;H;J; L; Q;R (DW&GW: 110)	
70-55-3	Toluene-4-sulphonamide	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test)	vM	QSAR min. log Dow/Kow = 0.6 (neutral cmpd.)	T	Rep_2	X; Z (DW: det.)	
7085-19-0	Mecoprop	medium	N	Not PMT	HQ	not P	longest measured half-life all media = 50 d (sediment)	vM	exp min. log Dow/Kow = -4.2 (ionizable cmpd.)	Pot. T	Cramer Class III	A; E (DW&GW: 0.8)	
71-43-2, 1076-43-3	Benzene	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. log Doc/Koc = 1.4 (neutral cmpd.)	T	ecotox Carc_1a Carc_1b muta_1a muta_1b STOTRE_1	H;O;S (DW&GW: 25.8)	
75-09-2	Dichloromethane	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. log Doc/Koc = 0.9 (neutral cmpd.)	T	Carc_2 Lact muta_1a muta_2 Rep_1a	H (DW: 0.5)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
											STOTRE_1 STOTRE_2		
76-22-2	Bornan-2-one	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. log Doc/Koc = 2.1 (neutral cmpd.)	T	muta_2 Rep_1a STOTRE_2	H;J (DW: 0.017)	
77-93-0	Triethyl citrate	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. log Dow/Kow = 0.7 (neutral cmpd.)	T	Carc_1b muta_1b	H;J (DW: 0.082)	
80-05-7	4,4'-isopropylidenedi-phenol	very high	Y	Not PMT	HQ	not P	inherently biodeg: 302 A (Inherent Biodegradability: Modified SCAS Test)	vM	exp min. log Doc/Koc = 2.3 (ionizable cmpd.)	T	SVHC	A; B;D;H;J; K; Q (DW&GW: 9.3)	SVHC, DK-study
69-72-7	Salicylic acid	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Doc/Koc = -5.7 (ionizable cmpd.)	T	Rep_2 STOTRE_1	D; H (GW: 1.2)	
84-66-2	Diethyl phthalate	very high	Y	Not PMT	HQ	not P	estimated t1/2 = 6d, and consistency across all tested QSARs	vM	exp min. log Doc/Koc = 2.4 (neutral cmpd.)	T	Rep_2 STO-TRE_2_ED	N; Q;S (DW: 2.5)	
95-47-6	o-xylene	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. log Doc/Koc = 2.7 (neutral cmpd.)	T	Rep_2	H;O (DW&GW: 16.5)	
98-86-2	Acetophenone	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Doc/Koc = 1.5 (neutral cmpd.)	Not T	-	H (DW: 0.5)	
103-83-3	Benzyldimethylamine	very high	Y	Not PMT	HQ	not P	No significant biodegradation in 301C and D tests, but nearly complete biodegradation in 302B testimated Therefore, the substance is assessed not to be persistent. (Berger et al. 2018)	vM	exp min. log Dow/Kow = -2.9 (ionizable cmpd.)	T	STOTRE_2	Z (det.)	
104-15-4, 6192-52-5	Toluene-4-sulphonic acid	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	read-across min. log Dow/Kow = -5.9 (ionizable cmpd.)	T	Rep_1b	Z (det.)	HOT-L
3039-83-6	Sodium ethylenesul-phonate	very high	Y	Not PMT	HQ	not P	inherently biodeg: 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	exp min. log Doc/Koc = 1.4 (single_anion cmpd.)	Pot. T	Cramer Class III	Z (det.)	

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
497-18-7	Carbonohydrazide	very high	Y	Not PMT	HQ	not P	The substance shows significant biodegradation above the threshold in a OECD 306 sea water testimated The threhold is reached in an early stage of the test, Therefore, it can be expected that the substance would also degrade in fresh-water. Used QSAR not applicable - substance is out of its application domain. Therefore, the substance is assessed not to be persistent. (Ber-ger et al. 2018)	vM	exp min. log Doc/Koc = 1.3 (ioniz-able cmpd.)	Pot. T	Cramer Class III	Z (det.)	HOT-L
51410-72-1	(3-methacrylami-dopropyl)trime-thylammonium chlo-ride	very high	Y	Not PMT	HQ	not P	Results from enhanced ready test enable the conclusion that the substance is not persistent in water. (Berger et al. 2018)	vM	QSAR min. log Dow/Kow = -2.1 (single_cation cmpd.)	Pot. T	Cramer Class III	Z (det.)	DK-study
5205-93-6	N-[3-(dimethyla-mino)propyl]methac-rylamide	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. log Doc/Koc = 1.4 (ioniz-able cmpd.)	Pot. T	Cramer Class III	Z (det.)	
53-16-7	Estrone	very high	Y	Not PMT	HQ	not P	inherently biodeg: 301 B (Ready Biodegradabil-ity: CO2 Evolution Test)	M	exp min. log Dow/Kow = 2.6 (ne-utral cmpd.)	T	Carc_1a Carc_1b Carc_2 Lact Rep_1a Rep_1b Rep_2_Sus pected ED	A; D (GW: 0.045)	
84-74-2, 93952-11-5	Dibutyl phthalate	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I))	M	exp min. log Doc/Koc = 3.1 (neu-tral cmpd.)	T	SVHC	N (DW: 2.7)	SVHC
95-63-6	1,2,4-trimethylben-zene	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I))	M	exp min. log Doc/Koc = 3.0 (neu-tral cmpd.)	T	STOTRE_1	H;O (DW&GW: 3)	
84-65-1	Anthraquinone	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I))	M	exp min. log Doc/Koc = 3.2 (neu-tral cmpd.)	T	Carc_2	H (DW: 0.1)	DK-study
63-05-8	Androst-4-ene-3,17-dione	very high	Y	Not PMT	HQ	not P	readily biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. log Dow/Kow = 2.7 (ne-utral cmpd.)	T	Carc_1b Carc_2 Lact	B;H (DW&GW: 0.1)	DK-study

CAS Number	Name	REACH Emission Likeli-hood	PBT/ vPvB req.	PMT/ vPvM	Quality	P	Rationale	M	Rationale	T	Rationale	DW/GW study (max conc. µg/L)	Comments
											Rep_1a_Suspected ED		
50-28-2, 35380-71-3	Estradiol	medium	N	**Not PMT**	HQ	**not P**	readily biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test)	**Pot. M**	QSAR min. log Dow/Kow = 3.9 (neutral cmpd.)	**T**	ecotox Carc_1a, 1b, 2, Lact Rep_1a,1b,2 STOTRE_1&2, ED	D;H (DW&GW: 0.1)	
85-68-7	Benzyl butyl phthalate	very high	Y	**Not PMT**	HQ	**not P**	inherently biodeg: 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	**not M**	exp min. log Dow/Kow = 4.8 (neutral cmpd.)	**T**	SVHC	N (DW: 0.9)	SVHC

Explanation of columns and selected terms in Table A1:

"REACH Emission Likelihood": the REACH Emission Likelihood category (see Table 5);

"PBT/vPvB required": if the substance is mandated for a PBT/vPvB assessment based on Article 14 (i.e. non-intermediate uses and volumes over 10 tonnes/year), with Y referring to yes and N referring to no;

"Quality": quality level of the PMT/vPvM assessment (high quality = HQ, medium quality = MQ, low quality = LQ);

"DW/GW (max conc. µg/L)": if the substance has been monitored in drinking water or groundwater, referring to the study ID presented in Table A2 and the maximum concentration across all studies reported in µg/L;

"Comments": this column provides additional information about the substance in certain cases. Key terms used here are:

"HOT-H"/"HOT-L": refers to substances considered relevant to drinking water using the "Hot-Target" approach (Nödler et al., 2019) mentioned in section 9.1, with "HOT-H" referring to substances that were prioritized for follow up and "HOT-L" referring to substances meeting the "Hot-Target" criteria but ultimately removed from the "Hot-Target" list due to additional considerations ;

"DK-study": refers to substances considered PMT/vPvM by at least one QSAR modelling approach in Danish study (Holmberg et al., 2019) presented in section 9.1.

"SVHC": refers to the substances of very high concern (SVHC) for authorisation under REACH

"WFD": indicates a priority substance under the Water Frame Work Directive (2013/39 EU)

"DWD": indicates the substance is included in water quality recommendations via the Drinking Water Directive (98/83/EC)

Table A2: List of references used in the review of substances in drinking water and groundwater. Data for REACH registered substances is presented in Table A1 in the column for drinking water/groundwater (DW/GW) using the Study ID.

STUDY ID	TYPE OF MEDIA	CHEMICAL TYPE TARGETED	AREA	REFERENCE
A	GW	Various	Europe	(Loos et al., 2010)
B	GW	Pharmaceuticals	Europe	(EC, 2016)
C	GW	Pharmaceuticals	USA	(Barnes et al., 2008)
D	GW	Various	International	(Lapworth et al., 2012)
E	DW	Various	Europe	(EurEau, 2017)
F	DW	Industrial	Europe	(Berger et al., 2017)
G	DW	Solvents	Europe	EU Regulation 98/83/EC
H	DW&GW	Various	Europe	(Kuhlmann et al., 2010)
I	DW	PFAS	International	(Kaboré et al., 2018)
J	DW	Various	USA	(Stackelberg et al., 2007)
K	DW	Various	USA	(Benotti et al., 2008)
L	DW	Various	Europe	(Tröger et al., 2018)
M	DW	PFAS	Europe	(Gebbink et al., 2017)
N	DW	Various	USA	(Loraine and Pettigrove, 2006)
O	GW	Solvents	USA	(Zogorski et al., 2006)
P	DW	Solvents	Europe	(Kavcar et al., 2006)
Q	GW	Various	Europe	(Jurado et al., 2012)
R	DW	Pharmaceuticals	International	(Mompelat et al., 2009)
S	DW	Various	International	(Schriks et al., 2010)
T	DW	1,4-dioxane	Europe	(Stepien et al., 2014)
U	DW	TFAA	International	(Boutonnet et al., 1999)
V	GW	disinfection by-products	Europe	(Berg et al., 2000)
W	DW	disinfection by-products	Europe	(Zahn et al., 2016)
X	DW	Various	Europe	(Umweltbundesamt, 2018)
Z [A)]	DW, GW & SW	Various	Europe	(Schulze et al., 2019) [A)]

A) Not used in the critical review, but only in the impact assessment, and in Table A1.

Table A3: List of substances detected in drinking water and groundwater that are not REACH registered substances (as of May 2017). The study ID refers to Annex Table A2.

CAS	Name	Common Usage	Max. conc. (ng/L) in DW	Max. conc. (ng/L) in GW	Study ID
75-27-4	Bromodichloromethane	by-product	27450	>10000	O; P
124-48-1	Dibromochloromethane	by-product	17930	>10000	O; P
13078-36-9	Trisodium dihydrogen -N,N-[bis[2-[bis(carboxylatomethyl)amino]ethyl]]glycinate	chelating agent	detected		E
603-52-1	Ethyl N,N-diphenylcarbamate	explosive	detected		Y
140-08-9	(2-Chlorethyl)phosphate	flame retardant	470		H
33665-90-6	Acesulfame	food additive	detected		F
56038-13-2	Sucralose	food additive	2400	2400	L; Y
501-52-0	Hydrocinnamic acid	food additive	20100		N
25013-16-5	Butylated hydroxyanisole	food additive	3450		N
1996-12-08	Dibromochloropropane	Fumigant	140	1000-5000	H; O
76-99-3	Molinate	insecticide		5	Q
56070-16-7	Terbufos-sulfon	insecticide	420		H
108-60-1	Bis(2-chloroisopropyl)ether	metabolite	1900		S
62-75-9	n-Nitrosodimethylamine	metabolite	630		H; S
2706-90-3	PFPeA	PFAS	5.7		I; M
27619-97-2	6:2FTSA	PFAS	6.3		I
307-24-4	PFHxA	PFAS	5.3		I; L; M
335-67-1	PFOA	PFAS	520	39	A; E; H; I; L; M; S
335-76-2	PFDA	PFAS	1	11	A; I; L; M
375-22-4	PFBA	PFAS	13		I; M
375-85-9	PFHpA	PFAS	3.2		I; L; M
375-95-1	PFNA	PFAS	4.5	10	A; I; L; M
3871-99-6	PFHxS	PFAS	1	19	A; I; L; M
67906-42-7	PFDS	PFAS	1.5		I; M
914637-49-3	5:3FTCA	PFAS	39		I
754-91-6	FOSA	PFAS	0.3		L
307-55-1	PFDoDA	PFAS	1.6		L
2058-94-8	PFUnDA	PFAS	0.12		L
375-92-8	PFHpS	PFAS	0.03		M
2706-91-4	PFPeS	PFAS	detected		Y
106266-06-2	Risperidone	pharm.	2.9		K
125-33-7	Primidone	pharm.	40	12000	B; D; E; R
1401-69-0	Tylosin	pharm.	detected		H
14698-29-4	Oxolinic acid	pharm.	detected	>100	B; H
154-21-2	Lincomycin	pharm.		320	C; D
1672-58-8	4-Formylaminoantipyrine	pharm.	detected		E
22071-15-4	Ketoprofen	pharm.	8	2886	A; B; D; H; Q; R
2465-59-0	Oxipurinol	pharm.	detected		E
25812-30-0	Gemfibrozil	pharm.	70	574	H; K; Q; R
29122-68-7	Atenolol	pharm.	18	106	H; K; L; Q
298-46-4	Carbamazepine	pharm.	258	99194	A; B; D; E; H; J; K; L; Q; R; S
37350-58-6	Metoprolol	pharm.	2100	56.3	E; H; L; Q; S
3930-20-9	Sotalol	pharm.	3.6	16	H; L; Q
42399-41-7	Diltiazem	pharm.		28	C
443-48-1	Metronidazol	pharm.		>100	B; H
479-92-5	Propyphenazone	pharm.	240	1250	B; D; Q; R
486-56-6	Cotinine	pharm.	20	400	B; C; D; H; J; L
525-66-6	Propranolol	pharm.		62	H; Q
57-53-4	Meprobamate	pharm.	42		H; K; R
59333-67-4	Fluoxetine	pharm.	8.71		H; K
60142-96-3	Gabapentin	pharm.	detected	>10000	B; E
60166-93-0	Iopamidol	pharm.	100	2400	B; D; H; S

CAS	Name	Common Usage	Max. conc. (ng/L) in DW	Max. conc. (ng/L) in GW	Study ID
604-75-1	Oxazepam	pharm.	2	detected	H; L
611-59-6	1,7-Dimethylxanthine	pharm.		57	C
62-73-7	Diazepam	pharm.	23.5	19.4	H; K; Q; R
6493-05-6	Pentoxifylline	pharm.		>100	B
657-24-9	Metformin	pharm.		>100	B
723-46-6	Sulfamethoxazole	pharm.	30	7300	A; B; C; D; E; K; Q; S
73334-07-3	Iopromide	pharm.	86		E; H; R; S
738-70-5	Trimethoprim	pharm.		>100	B; H
81103-11-9	Clarithromycin	pharm.		detected	H
83-07-8	4-Aminoantipyrine	pharm.	detected		E
882-09-7	Clofibric acid	pharm.	270	>100	B; D; H; R; S
28721-07-5	Oxcarbazepine	pharm.		>100	B
551-92-8	Dimetridazole	pharm.		>100	B
74-11-3	4-Chlorobenzoic acid	pharm.		>100	B
15935-54-3	Carboxyibuprofen	pharm.		>100	B
83-15-8	n-Acetyl-4-aminoantipyrin	pharm.		>100	B
483-63-6	Crotamiton	pharm.		>3000	B
125-40-6	Butabarbital	pharm.		>1000	B
72-44-6	Methaqualone	pharm.		>100	B
2078-54-8	Propofol	pharm.		>1000	B
54-31-9	Furosemide	pharm.		>100	B
2206-57-1	Fenofibric acid	pharm.	210	>100	B; H
137-58-6	Lidocaine	pharm.	1.2	>10000	B; L
70288-86-7	Ivermectine	pharm.		>100	B
27203-92-5	Tramadol	pharm.	3.6	>100	B; L
28179-44-4	Ioxithalamic acid	pharm.		>100	B
58-93-5	Hydrochlorothiazide	pharm.		2548	B; Q
50-36-2	Cocaine	pharm.		>100	B; Q
90357-06-5	Bicalutamide	pharm.	0.61		L
84057-84-1	Lamotrigine	pharm.	9.5		L
22083-74-5	Nicotine	pharm.	0.24	144	L; Q
72-14-0	Sulfathiazole	pharm.	detected	16.8	H; Q
122-11-2	Sulfadimethoxine	pharm.		91.5	Q
144-82-1	Sulfamethizole	pharm.		9.3	Q
127-79-7	Sulfamerazine	pharm.		744.7	Q
80-35-3	Sulfamethoxypyridazine	pharm.		68.7	Q
127-69-5	Sulfisoxazole	pharm.		17.1	Q
100-90-3	N4-acetylsulfamethazine	pharm.		57	Q
76-57-3	Codeine	pharm.	30	348.3	H; Q; R
61-68-7	Mefenamic acid	pharm.		32.5	Q
57-27-2	Morphine	pharm.		27.2	Q
519-09-5	Benzoylecgonine	pharm.		19.6	Q
41859-67-0	Bezafibrate	pharm.	27		H; R
78649-41-9	Iomeprol (iomeron)	pharm.	10		H; S
57-63-6	Ethinylestradiol	pharm.	23		H
59277-89-3	Aciclovir	pharm.	detected		Y
519-65-3	AMDOPH	pharm.	detected		Y
479-92-5	4-Isopropylantipyrine	pharm.	detected		Y
58955-94-5	10,11-Dihydroxy-10,11–dihydrocarbamazepine	pharm.	detected		Y
141-83-3	Guanylurea	pharm.	detected		Y
50-06-6	Phenobarbital	pharm.	detected		Y
61566-34-5	Ibuprofen methyl ester	pharm.-metabolite	4950		N
1014-69-3	Desmetryn	pesticide		detected	H
1071-83-6	Glyphosate	pesticide	460		E; S
116-06-3	Aldicarb	pesticide		detected	H
118-74-1	Hexachlorobenzene	pesticide	detected		E; H
120-36-5	Dichlorprop	pesticide	detected	3199	A; E; S

CAS	Name	Common Usage	Max. conc. (ng/L) in DW	Max. conc. (ng/L) in GW	Study ID
122-34-9	Simazine	pesticide	190	1690	A; E; H; Q; S
15545-48-9	Chlortoluron	pesticide	detected	1700	A; H; Q
1563-66-2	Carbofuran	pesticide		detected	H
15972-60-8	Alachlor	pesticide	17	9950	A; H; Q
1610-17-9	Atraton	pesticide	detected	detected	H
18691-97-9	Methabenzthiazuron	pesticide		516	A
25057-89-0	Bentazone	pesticide	280	10550	A; E; L; S
298-00-0	Parathion-methyl	pesticide		detected	H
3060-89-7	Metobromuron	pesticide		detected	H
309-00-2	Aldrin	pesticide	detected	detected	H
330-55-2	Linuron	pesticide	6.2	1010	A; H; K; Q
333-41-5	Diazinon	pesticide		300	A; Q
34123-59-6	Isoproturon	pesticide	20	100	A; E; H; Q; S
470-90-6	Chlorfenvinphos	pesticide	detected	2500	H; Q
51218-45-2	Metolachlor	pesticide	2700	5370	A; E; H; K; Q
51235-04-2	Hexazinone	pesticide	detected	589	A; H
58-89-9	Lindane	pesticide	detected	detected	E; H
5915-41-3	Terbuthylazine	pesticide	detected	1270	A; E; Q
60-57-1	Dieldrin	pesticide		detected	H
6190-65-4	Desethylatrazine	pesticide	320	1980	A; H; Q
67129-08-2	Metazachlor	pesticide	detected	detected	H
67564-91-4	Fenpropimorph	pesticide		detected	H
72-20-8	Endrin	pesticide		detected	H
7287-19-6	Prometryn	pesticide		detected	H
841-06-5	Methoprotryn	pesticide		detected	H
93-72-1	2,4,5-TP (Fenoprop)	pesticide		detected	H
93-76-5	2,4,5-T	pesticide	detected	3.7	A; E
94-74-6	MCPA	pesticide		36	A; H
94-75-7	2,4 D (2,4-Dichlorophenoxyacetic acid)	pesticide	110	12	A; E; S
94-82-6	2,4-DB (4-(2,4-dichlorophenoxy)butyric acid)	pesticide	detected		H
131341-86-1	Fludioxonil	pesticide	0.01		L
60207-90-1	Propiconazole	pesticide	0.23		L
886-50-0	Terbutryn	pesticide		180	Q
1007-28-9	Desisopropylatrazine (DIA)	pesticide	75	790	H; Q
21725-46-2	Cyanazine	pesticide	12	3.9	H; Q
60-51-5	Dimethoate	pesticide		2277	Q
122-14-5	Fenitrothion	pesticide		550	Q
1582-09-8	Trifluralin	pesticide		2.4	Q
121-75-5	Malathion	pesticide		3500	Q
34256-82-1	Acetochlor	pesticide	500		H
542-75-6	cis-1,3-Dichlorpropene	pesticide	3910		H
542-75-6	trans-1,3-Dichlorpropene	pesticide	11140		H
83164-33-4	Diflufenican	pesticide	0		H
87674-68-8	Dimethenamide	pesticide	67		H
2212-67-1	Molinat	pesticide	5700		H
14797-73-0	Prometon	pesticide	96		H
2008-58-4	2,6-Dichlorobenzamide	pesticide-metabolite	230		S
77521-29-0	AMPA	pesticide-metabolite	1100		S
187022-11-3	acetochlor ESA	pesticide-metabolite	1100		H
194992-44-4	acetochlor OA	pesticide-metabolite	550		H
142363-53-9	alachlor ESA	pesticide-metabolite	1200		H
171262-17-2	alachlor OA	pesticide-metabolite	140		H
1861-32-1	DCPA mono/di-acid degradate	pesticide-	190000		H

CAS	Name	Common Usage	Max. conc. (ng/L) in DW	Max. conc. (ng/L) in GW	Study ID
30125-63-4	Desethylterbutylazine	metabolite pesticide-metabolite	detected		H
56681-55-1	Hydroxyalachlor	pesticide-metabolite	44		H
171118-09-5	metolachlor ESA	pesticide-metabolite	4000		H
152019-73-3	metolachlor OA	pesticide-metabolite	3500		H
75-69-4	Trichlorofluoromethane	refrigerant		>10000	O
76-13-1	Trichlorotrifluoroethane	refrigerant		1000-5000	O
134-62-3	DEET	repellent	97	6500	A; D; H; J; K; S
124-48-1	Dibromochlormethane	solvent	detected	detected	H
75-25-2	Tribrommethane	solvent	4190	5000-10000	H; O; P
75-27-4	Bromdichlormethane	solvent	detected		H
104-51-8	n-Butylbenzene	solvent		200-500	O
75-34-3	1,1-Dichloroethane	solvent	6000	5000-10000	H; O
156-59-2	cis-1,2-Dichloroethene	solvent		1000-5000	O
103-65-1	n-Propylbenzene	solvent		1000-5000	O
79-34-5	1,1,2,2-Tetrachlorethane	solvent	10		H
108-70-3	1,3,5-Trimethylbenzene	solvent	410		H
26636-32-8	Diethoxyoctylphenol	surfactant	0		H
59-89-2	NMOR - N-Nitrosomorpholine	tobacco component		detected	H
332927-03-4	Acridin-9-carbonsäure	unknown	detected		Y
5466-77-3	Octyl methoxy cinnamate	UV filter	450		N
130-14-3	Sodium Naphthalene-1-sulphonate	various	detected		E
18467-77-1	Diprogulic acid	various	detected		E
924-16-3	N-nitrosodibutylamine	various	21		H
55-18-5	N-nitrosodiethylamine	various	85		H
10595-95-6	N-nitrosomethylethylamine	various	5		H
930-55-2	N-nitrosopyrrolidine	various	24		H
1066-42-8	Dimethylsilandiol (DMSD)	various	detected		Y
142-68-7	Tetrahydropyran	various	detected		Y
126-54-5	2,4,8,10-Tetraoxaspiro[5.5]undecan (TOSU)	various	detected		Y

Annex 2. Data sources used in the PMT/vPvM assessment

In this annex the databases, literature sources and QSAR tools for the P, M and T assessments are presented. These were selected based on data quality and compatibility with REACH. These are not included as part of the guidelines above for Persistence (Section 5.2), Mobility (Section 6.2) or Toxicity (Section 7.2), as it is intended that users of this guideline document can also utilize additional or alternative experimental data, databases and QSARs than those used in this report. The purpose of this annex is mainly to present the data sources used in this study for transparency, and to briefly discuss the data quality issues of these sources and how these quality considerations were integrated into the traffic light system for data quality.

Persistence

The approach and priority of persistency evaluations is presented in Section 5.2 and Figure 4.

Priority 1: High quality P/vP assessments.

For each REACH registered substance, an initial check was carried out to see if the substance was on the Candidate List of substances of very high concern (SVHC) because it met PBT/vPvB criteria, or if it was on the Stockholm Convention's list of Persistent Organic Pollutants (i.e. present on annex I of the Regulation EC 850/200). If so, the P or vP status from this assessment was used for the PMT/vPvM assessment. In a recent UBA report supporting a EU funded research project, Berger et al. (2018) conducted a thorough review of available aquatic persistency data for a set of 167 selected REACH registered substances, considering both dossier data and external data sources. Assessments presented by Berger et al. (2018) were largely accepted in this work, unless additional experimental data was found that Berger et al. (2018) did not consider and that would change the conclusion. Berger et al. (2018) only considered aquatic persistency, and not soil or sediment persistency, as in the present study. The third source for experimental data was the EChemPortal database (www.echemportal.org), accessed November 10, 2017), and the complete database of half-lives in surface water (e.g. OECD 309), sediment (OECD 308), and soil (e.g. OECD 307) were extracted, at all levels of reliability and suitable test methodologies. In addition, experimental half-lives reported in Kuhlmann et al. (2010) and Skark et al. (2011) were added to the database. In cases where multiple half-life tests were carried out for the same substance and same medium, the minimum half-life of these tests was chosen, provided they were conducted at the appropriate temperature (near 9 to 12°C depending on the half-life). If the P or the vP criteria in any exposure medium was met, the compound would obtain a P or vP conclusion as appropriate. A conclusion of "not P" would only be made based on this data if experimental half-lives for water (fresh or marine), soil and sediment (fresh or marine) were below the cut-offs in box 1; however, only 17 substances achieved "not P" status in this manner, due to the relative infrequency of reported half-lives.

Priority 2: P screening tests

As recommended by the PBT guideline (ECHA, 2017a), screening approaches are available that can differentiate between substances that are "Not P" and "Potentially P or vP", in particular, ready biodegradability tests (OECD 301; OECD 310), enhanced screening tests and inherent biodegradability tests (OECD 302b and 302c). The sources of the inherent, ready and enhanced screening test data were the EChemPortal database (accessed November 10, 2017). If all the tests performed indicated inherent, ready or enhanced biodegradability, a conclusion of "Not P" was made. If there was one test that indicated potential persistency (i.e. no biodegradation observed), or if there was no data, a Priority 3 screening was carried out.

Priority 3. Weight of evidence

In the absence of no or uncertain experimental data, as described above, various other data sets and QSARs were consulted to investigate the possibility of persistency. These were:

1) Conflicting results in inherent, ready or enhanced biodegradability tests, with some tests indicating biodegradability, others not. The number of tests concluding biodegradability verses non-degradability was considered, with the dominant result being considered alongside other information on a case-by-case basis.

2) Substances recently detected in drinking water and raw water, which were analyzed for based on their suspected persistence (Schulze et al., 2019), as well as monitoring data from Chapter 2. Frequent detections of substances was considered an indicator of persistency or high emission likelihood, or both, on a case-by-case basis.

3) Several QSARs were also used. These include:

   i. The PBT-BIOWIN screening approach as recommended in the PBT guideline (ECHA, 2017a) was used to screen for P/vP.

   ii. The QSAR Toolbox P predictor QSAR, conducted November 2017.

   iii. A 2014 database made available to the authors by ECHA, entitled "ProS.P. 2014", where ECHA gave several compounds a T/F if ECHA concluded a substance was persistent (though within the database the reasons for the conclusions were not always clear).

   iv. The Arnot-BIOWIN approach (Arnot et al., 2005), to convert BIOWIN output into to half-lives. All QSARs developed in this approach were used, and the final half-life was the geometric average of these predictions. An important consideration here is that the a comparison of these half-lives in water with experimental data indicated that they were generally accurate within 1 order of magnitude (see Table 5 of Arp et al. (2017)); therefore, any result between 4 days and 400 days was considered "Potential P/vP" (i.e. a factor 10 above and below the threshold for P in water), a result between 400 and 600 days was considered "P" (i.e. between a factor 10 larger than the 40 day and 60 day thresholds for persistency and very persistent in water), and a result larger than 600 days favouring vP; though only in the context of other information.

   v. The IFS QSAR from the PROMOTE (Protecting Water Resources from Mobile Trace Chemicals) project (Arp et al., 2017), which was used for compounds that resulted in errors when using BIOWIN, typically these were permanently charged compounds.

With these data sets and QSAR predictions, the following weight of evidence system was used to draw the following conclusions:

vP: The majority of biodegradability tests from Priority 2 indicated "Potential P and vP", QSAR Toolbox concluded P or vP, the Pro S.P. concluded P, and the Arnot-BIOWIN approach resulted in an estimated half-life of >=600 days. If empirical evidence was available and in addition that the substance was detected in drinking water and raw water, this would favour a vP conclusion in borderline cases.

P: The same as vP, but the estimated Arnot-BIOWIN half-life was >=400 days and <600 days

Potential P/vP++: The weight of evidence leans strongly to a P or vP conclusion, but not enough evidence is available to decide whether P or vP should be the conclusion. The criteria for these are the same as vP and P, but the estimated Arnot-BIOWIN half-life was not included amongst other evidence, other than it must be >=4 days (to reflect that Arnot-BIOWN data may be a factor 10 off from the cut-off value of 40 days); or if Arnot-BIOWIN data was not available (e.g. for ions) the IFS QSAR resulted in P. Frequent observations in recent screening studies in drinking water or raw water were an important weight-of-evidence consideration in concluding Potential P/vP++ on a case-by-case basis, in the context of other information (e.g. frequently

detected substances with low registered volumes were considered more likely to be Potential P/vP++).

Potential P/vP: this indicated there was some evidence of persistence, but not as much as for "Potential P/vP++". This conclusion was drawn when either 1) no ready/enhanced/inherent biodegradability test was conducted, but the BIOWIN QSAR approach conducted according to the PBT guideline (ECHA, 2017a) resulted in "P"; 2) no ready/enhanced/inherent biodegradability test was conducted, but at least two QSARs showed P, with a predicted Arnot-BIOWIN half-life >= 4 days or an IFS QSAR result of P, or 3) the substance was found in recent screening studies in raw water or drinking water (in Chapter 2 or Schulze et al., (2019)), though most available evidence indicates it should not be persistent.

Not P: This was assigned if the predicted half-life from the Arnot-BIOWIN approach was < 4 days (or if no Arnot-BIOWIN data was available, the IFS QSAR score concluded not P), and additionally the QSAR Toolbox and ProS.P. 2014 also concluded not P (if available)

No or Conflicting P data: If none of the above resulted in a conclusion, than the conclusion of "no data or conflicting P data" was assigned. This typically was for case when only one QSAR was available, or if multiple QSARs were the only data available, but they resulted in conflicting results.

Mobility

The approach and priority for mobility evaluations is presented in Section 6.2 and Figure 9.

Priority 1. Experimental log K_{OC}

The primary source of experimental K_{oc} data used was a data-set of peer reviewed values presented in Arp et al. (2017). The secondary source of experimental K_{oc} data was the EChemPortal database (accessed November 2017), in which a query was carried out for all K_{oc} data from sediment, soil, sewage sludge, and all test methods. When multiple data for a specific substance was available, the minimum log K_{oc} was always selected by default, unless the data itself is considered suspect.

Priority 2. D_{ow} and K_{ow}

Similar to K_{oc} data, the primary source of experimental values for K_{ow} and pKa was Arp et al. (2017). The secondary source for K_{ow} was the UFZ-LSER database (Ulrich et al., 2018), which was applied using the LSER described in Bronner et al. (2010), though only in cases where experimental LSER coefficients were available. The third source was the EChemPortal database (accessed November 2017), where only experimental or read-across data for K_{ow} or pKa were used. As the fourth source, the QSAR software in ADMET Predictor software by Simulations-plus (http://www.simulationsplus.com/), due to its good comparison with experimental data reported in Arp et al. (2017). For K_{ow} values of a similar priority ranking, the lowest value was always chosen. For pKa values, generally only the most acidic proton (of the acid or base form) was selected.

Toxicity

The approach and priority for toxicity evaluations is presented in Section 7.2 and Figure 12.

Priority 1. CMR, STOT RE, lactation effects, NOEC, DNEL and endocrine disrupting effects

Data for the CMR, STOT RE and "effects of or via lactation" was acquired from the public C&L registry from the ECHA website (https://echa.europa.eu/information-on-chemicals/cl-inventory-database accessed November 2017). It should be noted that the C&L inventory often only have self-classifications

from the companies, not harmonized ones; accordingly, these classifications might lead to different joint entries for the same substance. To err on the side of caution, the most hazardous category was selected per substance. NOEC/EC10 data was obtained from eChemPortal databases for aquatic toxicity for 1) aquatic plants, 2) fish, 3) algae, 4) aquatic invertebrates and 5) other aquatic organisms (all accessed during October 2017). All NOEC/EC10 data was considered, including QSARs (though these were a minority of data). When multiple NOEC/EC10 data were available for a specific chemical, the lowest value was always used. DNEL data - (oral, long term, general population) was obtained from accessing the IUCLID 6 database on January 2018. In case multiple data appeared across different dossiers (which was common), the lowest DNEL was chosen. The assessment of endocrine disruption herein was not conducted according to the most recent guidelines; which were published late in the preparation of this manuscript (Andersson et al., 2018). Instead, endocrine disruption databases were consulted in the following order of priority: 1) substances listed as SVHC because of "Endocrine disrupting properties (Article 57(f) - environment)", as available from the ECHA website (https://echa.europa.eu/information-on-chemicals, accessed January 10'th 2019), 2) the SIN List provided by ChemSec (https://chemsec.org/sin-list/, accessed January 10'th, 2019) and 3) *suspected* endocrine disruption were obtained from a 2014 assessment from ECHA which was used for internal use (entitled "Pro.S.P., 2014") and made available for this study. It should be noted that many of the T assessments are subject to change, pending further, harmonized data.

Priority 2. Cramer Class III

Cramer Class assessments were carried out based on the structure of the primary organic constituent (Chapter 3.3), through the Cramer Class assessment tool in QSAR Toolbox (conducted November 2017). Other organic constituents, impurities and transformation products were not considered.