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# Protecting the sources of our drinking water: The criteria for identifying persistent, mobile and toxic (PMT) substances and very persistent and very mobile (vPvM) substances under EU Regulation REACH (EC) No 1907/2006

For our Environment

Umwelt Bundesamt

TEXTE 127/2019

# Protecting the sources of our drinking water: The criteria for identifying persistent, mobile and toxic (PMT) substances and very persistent and very mobile (vPvM) substances under EU Regulation REACH (EC) No 1907/2006

by

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# Table of Contents

## List of figures

## List of tables

# 1 Summary

Substances with a specific combination of intrinsic substance properties pose a hazard to the sources of our drinking water, including substances that are very persistent (vP) in the environment and very mobile (vM) in the aquatic environment as well as substances that are persistent (P), mobile (M), and toxic (T). To identify such substances the German Environment Agency (UBA) since 2010 has funded research projects and since 2017 has performed two written consultations and several workshops. This document presents the result of this scientific and technical development of the PMT/vPvM criteria under EU REACH Regulation (EC) No 1907/2006. The German authorities propose to name such substances in the regulatory context of REACH "PMT substances" or "vPvM substances" (Neumann et al., 2015; Neumann, 2017; Neumann and Schliebner, 2017a, b).

The combination of the two intrinsic substance properties P (persistence) and M (mobility) increase the chances for substances to pass natural barriers like river banks and artificial barriers in water treatment facilities. Consequently, a contamination potentially becomes irreparable. A partial removal only up to 80% in additional water treatment facilities for the approximately 5.2 billion m$^3$ of wastewater produced every year in Germany would cost 0.8 to 1.5 billion € per year. Complete removal of persistent and mobile substances is neither economically nor technologically feasible.

Substantial analytical challenges exist related to the detection and quantification of mobile (polar) substances in water samples. Conventional methods using gas chromatography (GC) and reverse-phase liquid chromatography (RPLC) are not able to detect and quantify the most mobile (polar) substances. As such, waiting for monitoring data before minimising emissions of persistent and mobile substances into the environment is irresponsible.

The PMT/vPvM criteria are based on scientific and regulatory considerations under REACH. The scientific justifications include (1) monitoring data, (2) simulation and model studies and (3) impact considerations. The basis of the regulatory justification is integration with existing data and assessment requirements of the REACH registration process to allow for the least possible additional workload for registrants.

A literature review of 25 studies, comprising data between 2000 and 2018, was performed. 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. REACH registered substances comprise 113 (46%) of the 246 total drinking water contaminants and 75 (40%) of the 187 total groundwater contaminants. 58% of the detected REACH registered substances exceed the 0.1 µg/L limit value of the EU´s drinking water directive. Therefore, a substantial portion of drinking water and groundwater contaminants are substances registered under REACH.

The PMT/vPvM assessment will benefit chemical industry and downstream users by providing clarity regarding which substances require scrutiny in chemical risk assessment for posing a hazard to the sources of our drinking water. It can be considered a ready-to-use tool for industry to identify PMT/vPvM substances. Risk mitigation measures to minimise emissions would only apply to a limited and clearly defined number of substances. It may be concluded that under REACH fewer substances fulfil the PMT/vPvM criteria than the PBT/vPvB criteria and that the implementation of the PMT/vPvM assessment would have a relatively small impact on the European chemical industry as a whole.

More careful and transparent use of identified PMT/vPvM substances will result in less, more specific chemical monitoring and if needed treatment technologies, leading to overall less water management costs.

# 1 Zusammenfassung

Stoffe mit einer spezifischen Kombination von intrinsischen Stoffeigenschaften stellen eine Gefahr für die Ressourcen unserer Trinkwässer dar. Dies schließt Stoffe ein, die sehr persistent (vP) in der Umwelt und sehr mobil (vM) in der aquatischen Umwelt sind, sowie solche, die persistent (P), mobil (M) und toxisch (T) sind. Zur Identifizierung dieser Stoffe fördert das Umweltbundesamt (UBA) seit 2010 Forschungsprojekte und führte seit 2017 zwei schriftliche Konsultationen sowie mehrere Workshops durch. Dieses Dokument stellt das Ergebnis dieser wissenschaftlichen und technischen Entwicklung der PMT/vPvM-Kriterien unter der EU-Chemikalienverordnung REACH (EG) Nr. 1907/2006 dar. Die deutschen Behörden schlagen vor, solche Stoffe unter REACH als "PMT-Stoffe" oder "vPvM-Stoffe" zu bezeichnen (Neumann et al., 2015; Neumann, 2017; Neumann und Schliebner, 2017a, b).

Die Kombination der beiden intrinsischen Stoffeigenschaften P (Persistenz) und M (Mobilität) erhöht die Chancen für Chemikalien natürliche Barrieren wie Uferfiltrationsstrecken und künstliche Barrieren in der Wasseraufbereitung zu überwinden. Infolgedessen ist eine Kontamination möglicherweise irreparabel. Bereits eine nur teilweise Entfernung bis zu 80% in zusätzlicher Wasseraufbereitung für die jährlich rund 5,2 Milliarden m$^3$ Abwasser in Deutschland würde 0,8 bis 1,5 Milliarden € pro Jahr kosten. Die vollständige Entfernung von persistenten und mobilen Stoffen ist weder wirtschaftlich noch technologisch realisierbar.

Erhebliche analytische Herausforderungen bestehen mit dem Nachweis und der Quantifizierung mobiler (polarer) Stoffe in Wasserproben. Herkömmliche Verfahren mit Gaschromatographie (GC) und Umkehrphasen-Flüssigkeitschromatographie (RPLC) sind nicht in der Lage, die mobilsten (polarsten) Substanzen zu erkennen und zu quantifizieren. Auf Monitoringdaten zu warten bevor Emissionen von persistenten und mobilen Stoffen in die Umwelt minimiert werden ist daher unverantwortlich.

Die PMT/vPvM-Kriterien basieren auf wissenschaftlichen und regulatorischen Überlegungen unter REACH. Die wissenschaftlichen Begründungen umfassen (1) Monitoringdaten, (2) Simulations- und Modellierungsstudien und (3) Folgenabschätzungen. Grundlage der regulatorischen Überlegungen ist die Integration mit den bereits bestehenden Daten- und Bewertungsanforderungen im REACH-Registrierungsprozess, um so für Registranten einen möglichst geringen zusätzlichen Arbeitsaufwand zu verursachen.

Durch eine Literaturrecherche mit 25 Studien zwischen 2000 und 2018 wurden 333 Chemikalien identifiziert, von denen 246 im Trinkwasser und 187 im Grundwasser nachgewiesen wurden, davon 100 in beiden. REACH-registrierte Stoffe machen 113 (46%) der 246 Trinkwasser- und 75 (40%) der 187 Grundwasserkontaminanten aus. 58% der nachgewiesenen REACH-registrierten Stoffe überschreiten den Grenzwert von 0,1 µg/L. Ein signifikanter Anteil der Kontaminanten in Trink- und Grundwasser ist unter REACH registriert.

Die PMT/vPvM-Bewertung schafft für die Chemieindustrie und den nachgeschalteten Anwendern Klarheit darüber, welche Stoffe einer Prüfung bedürfen, um eine Gefahr für die Ressourcen unserer Trinkwässer auszuschließen. Es ist ein einsatzbereites Werkzeug für die Chemieindustrie zur Identifizierung von PMT/vPvM-Stoffen. Risikominderungsmaßnahmen zur Minimierung der Emissionen sind für eine begrenzte und klar definierte Anzahl von Stoffen notwendig. Unter REACH erfüllen weniger Stoffe die PMT/vPvM-Kriterien als die PBT/vPvB-Kriterien und die Umsetzung hätte relativ geringe Auswirkungen auf die Chemieindustrie.

Eine sorgfältigere und transparentere Verwendung der identifizierten PMT/vPvM-Stoffe wird zu geringerem Monitoring und Wasseraufbereitung führen, was insgesamt zu geringeren Kosten für die Wasserwirtschaft führt.

# 2 The technical development of PMT/vPvM criteria under REACH

The hazard posed by persistent chemicals that are mobile in the aquatic environment has been well known since decades (Schröder, 1991; Knepper et al., 1999). Such chemicals have previously been named in the scientific literature as Polar Persistent Organic Pollutants (PPOPs) (Giger et al. 2005), Persistent Polar Pollutants (PPPs, P3 substances) (Steinhäuser & Richter 2006) or Persistent and Mobile Organic Contaminants (PMOCs) (Reemtsma et al. 2016). The German authorities in May 2017 proposed criteria for identifying such chemicals in the regulatory context of EU REACH Regulation (EC) No 1907/2006. Substances meeting these criteria are referred to as either persistent, mobile and toxic (PMT) or very persistent and very mobile (vPvM) substances (Neumann et al., 2015; Neumann, 2017; Neumann and Schliebner, 2017a, b).

Under REACH, industry must demonstrate in their registration dossier the safe use of substances over their entire life cycle. For substances with intrinsic 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 it is not possible to determine a threshold, 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. Unfortunately, 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. For this purpose, the German Environment Agency (UBA) deemed it necessary to scientifically and technically develop PMT/vPvM criteria under REACH.

Since 2010 the German Environment Agency (UBA) has funded research projects to develop PMT/vPvM criteria under REACH. 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). Since 2016 a research project has further developed and justified the PMT/vPvM criteria and assessed all REACH registered substances as of May 2017 (Arp and Hale, 2019 - FKZ 371 667 4160).

The German authorities had submitted a first proposal (Neumann and Schliebner, 2017a) for the criteria persistence in the environment ("P"), mobility in the aquatic environment ("M") and toxicity to humans ("T") to the Risk Management Expert Meeting (RiME-2/2017) on the 17th-18th of May 2017 in Łódź, Poland and to the 15th meeting of the European Chemicals Agency's (ECHA) PBT expert group (PBT EG) on the 23rd-24th of May 2017 for comments and suggested revisions. The comments were further discussed during a WEBEX-Meeting on the 16th of August 2017 with the members of the PBT EG and have been summarised in a Response to Comment (RCOM) document.

The proposal was then revised by the German authorities, and the second version of the proposal (Neumann and Schliebner, 2017b) was submitted to the 16th meeting of ECHA's PBT expert group (PBT EG) on 28rd-29th of September 2017 and to the Risk Management Expert Meeting (RiME-3/2017) on 4th-5th of October 2017 in Tallinn, Estonia for a second round of comments and suggested revisions. In addition to these two written consultations the proposal was repeatedly presented and discussed, e.g. at the SETAC Europe Conferences 2015, 2016, 2017 and 2018; the first UBA workshop "REACH in der Praxis: PMT-Stoffe erkennen und ihre Emissionen vermeiden" ("REACH in practice: Identifying PMT substances and avoiding their emissions") held by the German Environment Agency (UBA) for industry on 4th of May 2017 in Berlin, Germany, the Centre for Environmental Research (UFZ) European stakeholder workshop "Persistent and mobile organic chemicals in the water cycle: Linking science, technology and regulation to protect drinking water quality" on 23rd-24th of November 2017 in Leipzig, Germany and finally at the second UBA workshop "PMT/vPvM substances under REACH. Voluntary measures and regulatory options to protect the sources of drinking water" on 13th-14th of March 2018 in Berlin, Germany.

Through these meetings and consultations, the scientific and technical descriptive comments received as well as the feedback and suggestions have been, as far as possible, accommodated in this third version. Consequently, this document presents the result of the scientifically and technical development under REACH of the PMT/vPvM criteria.

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# 3 Preamble

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*".

Two of the UN's Sustainable Development Goals (2015) for the next 15 years specifically address the need to protect water resources from the use of chemicals: Goal No 6 "*Ensure availability and sustainable management of water and sanitation for all*”, and Goal No 12 "*Ensure sustainable consumption and production patterns*". Further, water quality is central to Goal No 3 "*Ensure healthy lives and promote well-being for all at all ages*". Targets within and related to these goals include "*by 2030 to improve water quality by reducing pollution, eliminating dumping and minimizing release of hazardous chemicals and materials…*" (Target 6.3), "*by 2020 to achieve the environmentally sound management of chemicals and all wastes throughout their life cycle, in accordance with agreed international frameworks, and significantly reduce their release to air, water and soil in order to minimize their adverse impacts on human health and the environment*" (Target 12.4), "*by 2030 substantially reduce the number of deaths and illnesses from hazardous chemicals and air, water, and soil pollution and contamination"* (Target 3.9); and "*by 2020 ensure conservation, restoration and sustainable use of terrestrial and inland freshwater ecosystems and their services*" (Target 15.1).

A desire to enact these goals can be seen on a local scale in Europe. The ‘Memorandum regarding the protection of European rivers and watercourses in order to protect the provision of drinking water’ (ERM, 2013) prepared by 170 European water companies across 17 countries expresses the vision that "*water must be protected for its own sake. Nobody has a right to pollute water bodies*". A desire to enact these goals can also be found on a regional scale in Europe. The European Commission's 7th Environment Action Programme strategy for a non-toxic environment (EC, 2017a) has the goal to "*create and maintain a non-toxic environment that is free of exposures to minimise and eliminate all exposures to hazardous substances*".

These directives, goals and vision statements collectively address a growing threat to the sources of Europe's drinking water and freshwater environments. This threat is the increasing number and volume of chemical substances that contribute to the concern of planetary boundary threats from persistent substances (MacLeod et al., 2014; Diamond et al., 2015). Persistent and mobile substances emitted into the aquatic environment could, over long time frames, not only impact the taste, odour and colour of drinking water, but also public health, ecosystem services and human rights leading to substantial costs for society.

Implementing the PMT/vPvM criteria under EU REACH Regulation (EC) No 1907/2006 is a pollution prevention strategy and will help ensuring protection of Europe's drinking water and freshwater environments for future generations.

# 4 The presence of chemicals in drinking water and groundwater

To illustrate which chemicals have recently been detected in drinking water and groundwater, a literature review of 25 studies, comprising data between 2000 and 2018, was performed (Arp and Hale, 2019). The list of these studies can be found in Appendix Table A1. 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 may 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. These chemicals are presented in Table 1. The 191 chemicals not registered under REACH (as of May 2017), with several pharmaceuticals and their metabolites (74) as well as pesticides and their metabolites (62) and 55 chemicals belonging to other use categories, are presented in the Appendix Table B1. The REACH registered substances in Table 1 comprise 113 (46%) of the 246 total drinking water contaminants and 75 (40%) of the 187 total groundwater contaminants. It can therefore be considered factual that a substantial portion of drinking water and groundwater contaminants are substances registered under REACH.

**Table 1 REACH registered substances (as of May 2017) detected in drinking water (DW) and/or groundwater (GW).**

The CAS numbers partly correspond to the registered salts of unregistered free acids. The column example usage present uses inside or outside the scope of the REACH registrations. The study ID refers to appendix Table A1. Source: Arp and Hale (2019).

| CAS No | Name | Example Usage | max. conc. (ng/L) in DW | max. conc. (ng/L) in GW | Study ID |
|---|---|---|---|---|---|
| 139-13-9 | NTA | chelating agent | | detected | H |
| 140-01-2 | Pentasodium pentetate | chelating agent | detected | | E |
| 60-00-4 | EDTA | chelating agent | 13600 | >10000 | B; E; S |
| 67-43-6 | DTPA acid | chelating agent | 9000 | >3000 | B; S; E |
| 77-93-0 | Triethyl citrate | cosmetic | 82 | | H; J |
| 121-82-4 | RDX | explosive | 1100 | | H |
| 85-98-3 | 1,3-Diethyl-1,3-diphenylurea | explosive | detected | | X |
| 126-73-8 | TBP | flame ret. | 180 | | J |
| 13674-84-5 | TCPP | flame retardant | 510 | | E; F; K |
| 128-44-9 | Saccharin | food additive | detected | | F |
| 76-22-2 | Camphor | food additive | 17 | | H; J |
| 1634-04-4 | MTBE | fuel oxygenate | 57800 | >10000 | E; H; O; S |
| 637-92-3 | ETBE | fuel oxygenate | | detected | H |
| 994-05-8 | Tert-amyl methyl ether | fuel oxygenate | | 200-500 | O |
| 108-20-3 | Diisopropyl ether | fuel oxygenate | | >10000 | O |
| 74-83-9 | Bromomethane | fumigant | | 200-500 | O |
| 106-46-7 | 1,4-Dichlorobenzene | fumigant | | >10000 | O |
| 78-87-5 | 1,2-Dichloropropane | fumigant | 1710 | 5000-10000 | H; O |
| 106-93-4 | Ethylene dibromide | fumigant | | 200-500 | O |

| CAS No | Name | Example Usage | max. conc. (ng/L) in DW | max. conc. (ng/L) in GW | Study ID |
|---|---|---|---|---|---|
| 96-18-4 | 1,2,3-Trichloropropane | fumigant | | 1000-5000 | O |
| 95-16-9 | Benzothiazole | metabolite | 10 | | S |
| 1222-05-5 | Galaxolide | musk | 82 | 23000 | D; H; Q |
| 21145-77-7 | AHTN | musk | 68 | | J |
| 98-86-2 | Acetophenone | musk | 490 | | H |
| 1506-02-1 | Acetylhexamethyltetrahydronaphtalin | musk | detected | | H |
| 120-12-7 | Anthracene | PAH | | detected | H |
| 129-00-0 | Pyrene | PAH | | detected | H |
| 83-32-9 | Acenaphthene | PAH | | detected | H |
| 29420-49-3 | PFBS | PFAS | 19 | 25 | A; H; I; L; M |
| 56773-42-3 | PFOS | PFAS | 20 | 135 | A; E; H; I; L; S |
| 62037-80-3 | GenX | PFAS | 11 | | M |
| 137862-53-4 | Valsartan acid | pharm. | detected | | E |
| 15307-86-5 | Diclofenac | pharm. | 35 | 590 | A; B; D; H; R |
| 50-78-2 | Acetylsalicylic acid | pharm. | 120 | >100 | B; S |
| 80-08-0 | Dapsone | pharm. | detected | | F |
| 103-90-2 | Paracetamol | pharm. | 210.1 | 120000 | B; C; D; H; J; Q; R |
| 114-07-8 | Erythromycin | pharm. | | >1000 | B |
| 117-96-4 | Diatrizoic acid | pharm. | 1200 | >1000 | B; S; R |
| 15687-27-1 | Ibuprofen | pharm. | 1350 | 12000 | A; B; C; D; N; R |
| 22204-53-1 | Naproxen | pharm. | detected | detected | H |
| 3380-34-5 | Triclosan | pharm. | 734 | 2110 | A; D; K; N; R |
| 50-28-2 | 17b-Estradiol | pharm. | 1 | 120 | D; H |
| 57-41-0 | Phenytoin | pharm. | 19 | | H; K; R |
| 57-68-1 | Sulfamethazine | pharm. | | 616 | C; D; H; Q |
| 57-83-0 | Progesterone | pharm. | 0.57 | >100 | B; H; K |
| 58-08-2 | Caffeine | pharm. | 119 | 110000 | A; B; C; D; H; J; L; Q; R |
| 60-80-0 | Phenazone | pharm. | 400 | 3950 | B; D; H; R; S |
| 68-35-9 | Sulfadiazine | pharm. | | >100 | B; H; Q |
| 69-72-7 | Salicylic acid | pharm. | | 1225 | D; H |
| 826-36-8 | Vincubine | pharm. | detected | | E |
| 53-16-7 | Estrone | pharm. | | 45 | A; D |
| 63-05-8 | Androstenedione | pharm. | detected | >100 | B; H |
| 152459-95-5 | Imatinib | pharm. | | >100 | B |
| 76-74-4 | Pentobarbital | pharm. | | >1000 | B |
| 93413-69-5 | Venlafaxine | pharm. | 1.1 | | L |
| 144-83-2 | Sulfapyridine | pharm. | | 104 | Q |
| 18559-94-9 | Salbutamol | pharm. | | 9 | Q |
| 50-48-6 | Amitryptilline | pharm. | 1.4 | | R |
| 66108-95-0 | Iohexol | pharm. | 11050 | | H; S |
| 131-57-7 | Oxybezon | pharm. | detected | | H |
| 83905-01-5 | Azithromycin | pharm. | detected | | X |
| 139481-59-7 | Candesartan | pharm. | detected | | X |
| 144689-24-7 | Olmesartan | pharm. | detected | | X |
| 13674-87-8 | TDIP | plasticizer | 510 | | H; J |

| CAS No | Name | Example Usage | max. conc. (ng/L) in DW | max. conc. (ng/L) in GW | Study ID |
|---|---|---|---|---|---|
| 80-05-7 | Bisphenol A | plasticizer | 420 | 9300 | A; B; D; H; J; K; Q |
| 80-09-1 | Bisphenol S | plasticizer | detected | | F |
| 3622-84-2 | n-Butylbenzenesulphonamide | plasticizer | 50 | | S |
| 139-40-2 | Propazine | pesticide | 0 | 25 | A; H; Q |
| 1912-24-9 | Atrazine | pesticide | 1900 | 3450 | A; E; H; K; Q |
| 330-54-1 | Diuron | pesticide | 2100 | 178 | A; E; H; Q; S |
| 834-12-8 | Ametryn | pesticide | detected | detected | H |
| 7085-19-0 | Mecoprop | pesticide | detected | 785 | A; E |
| 128-37-0 | butylhydroxytoluol | preservative | 26 | | K; H |
| 75-71-8 | Dichlorodifluoromethane | refrigerant | | 5000-10000 | O |
| 79-01-6 | Trichloroethene | solvent | 21600 | >10000 | G; H; O; S |
| 123-91-1 | 1,4-dioxane | solvent | 600 | | E; S; T |
| 127-18-4 | Tetrachloroethene | solvent | 180000 | | G; H; J |
| 143-24-8 | Tetraglyme | solvent | detected | | E |
| 67-66-3 | Chloroform | solvent | 34580 | >10000 | H; O; P |
| 71-55-6 | 1,1,1-Trichlorethane | solvent | detected | >10000 | O |
| 71-43-2 | Benzene | solvent | 25770 | >10000 | H; O; S |
| 100-41-4 | Ethylbenzene | solvent | detected | >10000 | H; O |
| 98-82-8 | Isopropylbenzene | solvent | 110 | 1000-5000 | H; O |
| 108-88-3 | Toluene | solvent | 63120 | >10000 | H; O; P |
| 95-63-6 | 1,2,4-Trimethylbenzene | solvent | 130 | 1000-5000 | H; O |
| 1330-20-7 | total Xylenes | solvent | 16470 | >10000 | H; O |
| 56-23-5 | Carbon tetrachloride | solvent | 2240 | 1000-5000 | H; O |
| 108-90-7 | Chlorobenzene | solvent | | 5000-10000 | O |
| 75-00-3 | Chloroethane | solvent | | 1000-5000 | O |
| 74-87-3 | Chloromethane | solvent | | >10000 | O |
| 95-50-1 | 1,2-Dichlorobenzene | solvent | 10 | >10000 | H; O |
| 107-06-2 | 1,2-Dichloroethane | solvent | 81900 | 1000-5000 | H; O |
| 156-60-5 | trans-1,2-Dichloroethene | solvent | | >10000 | O |
| 127-18-4 | Perchloroethene | solvent | | >10000 | O |
| 111-96-6 | Diethylene glycol dimethyl ether | solvent | 150 | | S |
| 75-09-2 | Dichloromethane | solvent | 531 | | H |
| 87-61-6 | 1,2,3-Trichlorbenzene | solvent | 160 | | H |
| 120-82-1 | 1,2,4-Trichlorbenzene | solvent | 920 | | H |
| 79-00-5 | 1,1,2-Trichlorethane | solvent | 100 | | H |
| 107-07-3 | 2-Chlorethanol | solvent | detected | | X |
| 104-40-5 | Nonylphenol | surfactant | 1100 | 84000 | A; D; H; J; K; Q |
| 140-66-9 | tert-Octylphenol | surfactant | | 1800 | A; Q |
| 131-11-3 | Dimethyl phthalate | surfactant | 540 | | N |
| 84-66-2 | Diethyl phthalate | surfactant | 2470 | 1115 | N; Q; S |
| 84-74-2 | Dibutyl phthalate | surfactant | 2730 | | N |
| 85-68-7 | Butyl benzyl phthalate | surfactant | 911 | | N |
| 117-81-7 | DEHP | surfactant | 2680 | 5661 | N; Q |
| 126-86-3 | Surfynol 104 | surfactant | 240 | | N |
| 78-51-3 | (2-Butoxyethyl)phosphate | surfactant | 350 | | H |
| 74-95-3 | Dibromomethane | various | 740 | | H |
| 76-05-1 | Trifluoroacetate | various | 150 | 123 | E; U; V |
| 108-78-1 | Melamine | various | detected | | E; F |

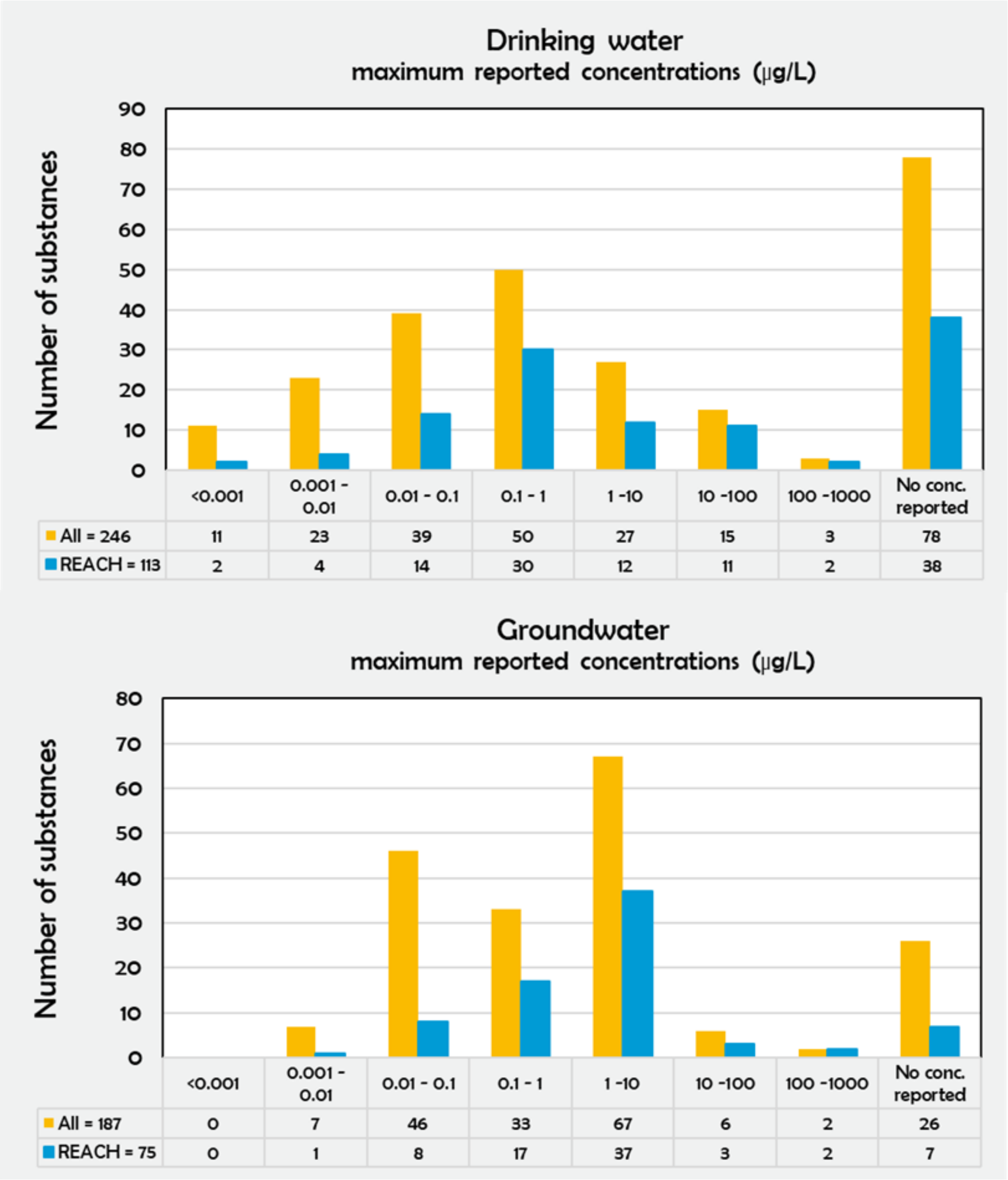
| CAS No | Name | Example Usage | max. conc. (ng/L) in DW | max. conc. (ng/L) in GW | Study ID |
|---|---|---|---|---|---|
| 288-13-1 | Pyrazole | various | detected | | E |
| 461-58-5 | Cyanoguanidine | various | detected | | F |
| 100-02-7 | Nitrophenol | various | | 122 | A |
| 102-06-7 | 1,3-Diphenylguanidine | various | detected | | F |
| 102-76-1 | Triacetin | various | detected | | E |
| 105-60-2 | e-Caprolactam | various | detected | | F |
| 108-80-5 | Cyanuric acid | various | detected | | F |
| 115-96-8 | TCEP | various | 470 | 740 | D; E; J; K |
| 120-18-3 | Naphthalenesulfonic acid | various | detected | | F |
| 121-57-3 | Sulfanilic acid | various | detected | | F |
| 1493-13-6 | Trifluoromethansulfonic acid | various | 1000 | | F; W |
| 15214-89-8 | 2-Acrylamido-2-methylpropanesulphonic acid | various | detected | | F |
| 25321-41-9 | Dimethylbenzene sulfonic acid | various | detected | | F |
| 288-88-0 | 1,2,4-Triazole | various | detected | | E |
| 51-28-5 | 2,4-Dinitrophenol | various | 333000 | 122 | A; H |
| 532-02-5 | Sodium naphthalene-2-sulphonate | various | detected | | E |
| 56-93-9 | Benzyltrimethyl ammonium | various | detected | | F |
| 95-14-7 | Benzotriazoles | various | 200 | 1548 | A; B; E; S |
| 97-39-2 | 1,3-Di-o-tolylguanidine | various | detected | | F |
| 119-61-9 | Benzophenone | various | 260 | | N |
| 91-20-3 | Naphthalene | various | 900 | 1000-5000 | H; O; P |
| 75-35-4 | 1,1-Dichloroethene | various | | >10000 | O |
| 75-01-4 | Vinyl chloride | various | 250 | 5000-10000 | H; O |
| 791-28-6 | Triphenyl phosphorus oxide | various | 130 | | S |
| 84-65-1 | Anthraquinone | various | 72 | | H |
| 541-73-1 | 1,3-Dichlorbenzene | various | 100 | | H |
| 98-95-3 | Nitrobenzene | various | 100000 | | H |
| 100-42-5 | Styrene | various | 46400 | | H |
| 96-76-4 | 2,4-Di-tert-butylphenol | various | detected | | X |
| 70-55-3 | 4-Methylbenzolsulfonamide | various | detected | | X |

For many substances in Table 1 and in Appendix Table B1 it was only reported whether they were detected or not, due to elevated limits of quantification, missing quantification standards or absence of concentration data in the references. If available from the studies listed in Appendix Table A1, 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 histograms in Figure 1 of the total number of substances and of the REACH registered substances only.

Chemicals contaminating drinking water and groundwater may cause a wide variety of problems, depending on their concentration and toxicity, including possible mixture effects with other chemicals (Schriks et al., 2010). These problems can range from 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 chemicals it must be noted that also a contamination with less toxic substances can become biologically relevant.

**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**

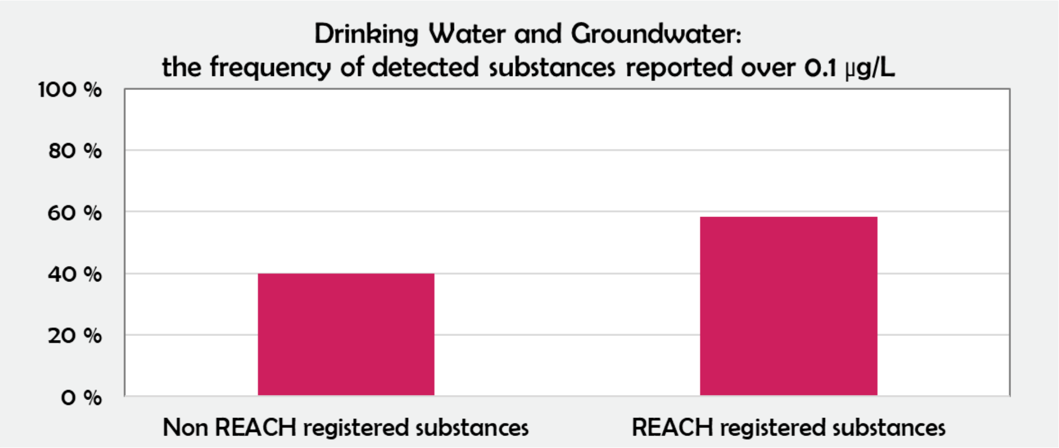
The data are presented for all detected substances reported in the review of monitoring studies (yellow bars) and just for REACH registered substances as of May 2017 (blue bars).



Source: Arp and Hale (2019)

On the other hand this random collection of analytic data indicates that REACH registered substance are detected with higher concentrations. While the portion of REACH registered substances from all detected substances is 43% (142 of 333) the portion from those substances exceeding 0.1 µg/L (e.g. cut-off value of the drinking water directive (EU Regulation 98/83/EC) for pesticides) is 52% (83 of 159). 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 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: Arp and Hale (2019)

A substance may contaminate drinking water and groundwater because of its emissions into the environment in combination with the intrinsic substance properties to be persistent in the environment and mobile in the aquatic environment. Consequently, here we use the intrinsic substance properties of the substances registered under REACH already detected in drinking water and groundwater in chapter 11 to scientifically justify the cut-off values for the PMT/vPvM criteria. As a consequence, intrinsic substance properties alone can be used to identify potential drinking water and groundwater contaminants.

# 5 Aims of this initiative

With this initiative, the German authorities has set out to achieve three major aims:

The first aim is to seek consensus on the need to prevent undue emissions into the environment by substances, registered under EU REACH Regulation (EC) No 1907/2006, which have the intrinsic substance properties that indicate a hazard to the sources of our drinking water. 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.

The second aim is to establish under REACH the persistency, mobility and toxicity (PMT) criteria as well as the very persistent and very mobile (vPvM) criteria for the identification of those substances that potentially pose a hazard to the sources of our drinking water. Beyond the T criteria set out in Annex XIII, 1.1.3 of REACH this also includes other hazardous properties posing a risk to human health and the environment. With these criteria, registrants are able to assess the intrinsic substance properties of their substances. Identified PMT/vPvM substances should be particularly considered in monitoring and in the minimisation of emissions.

The third aim is to actually minimise emissions of PMT/vPvM substances into the aquatic environment. Depending on their uses and emissions, registrants should implement risk mitigation measures to prevent pollutions precautionarily. Proper management of PMT/vPvM substances and chemical safety over the complete life-cycle can be achieved by chemical stewardship programs. If necessary, authorities must implement regulatory measures to minimize emissions and to protect the valuable water resources for future generations.

# 6 Benefits from this initiative

The German authorities are convinced that all stakeholders affected by this initiative will benefit.

Chemical industry, including downstream users, will obtain clarity regarding which substances require minimising emissions into the environment. The PMT/vPvM criteria as well as the assessment procedure are strongly rooted in existing obligations and requirements under the REACH registration process (see chapter 11). Thus, they can be considered a ready-to-use tool not causing additional testing other than already required by existing obligations. This reduces the additional costs for industry to identify their PMT/vPvM substances. Risk mitigation measures to minimise emissions consequently apply to a limited and clearly defined number of substances. Innovation and substitution towards sustainability will provide competitive advantages to the more proactive companies. Overall, this initiative will benefit registrants in fulfilling their existing responsibility of guaranteeing the safe use of their REACH registered substances and to protect the sources of our drinking water.

Authorities and regulators, including member states (MS), the European Chemical Agency (ECHA) and the European Commission (COM) will benefit by focusing regulatory actions under REACH on those substances and their uses that give rise to a high concern to contaminate the sources of our drinking water. Implementing the PMT/vPvM criteria under EU REACH Regulation (EC) No 1907/2006 will allow regulatory actions to be justified and implemented precautionarily before an irreparable contamination has happened or has been proven by monitoring data.

Drinking water suppliers will be able to ensure clean and safe water using natural treatment methods or conventional technologies, rather than implementing costly advanced water treatment technologies at drinking water production facilities. A future list of PMT/vPvM substances registered under REACH will result in less, but instead more specified chemical monitoring and if needed less remediation, leading to overall more efficient use of financial resources. This initiative may also stimulate joint strategies between industry, enforcement authorities and drinking water suppliers to develop prevention strategies, proactively.

European Society as a whole will benefit by avoiding contamination to the sources of our drinking water, and the negative financial, health and social consequences thereof. If all stakeholders act voluntarily, society can develop sustainably while managing to avoid one of the most important threats to the sources of our drinking water.

# 7 What intrinsic substance properties make a substance a hazard to the sources of our drinking water?

For a chemical substance emitted into the environment to pose a threat to the sources of our drinking water, it must be transported from the point of emission through soil layers, riverbanks, aquifers, and other natural or even artificial barriers. The time scales for this can vary from a few days in the case of surface water sources, to one or two weeks for riverbank filtration, or few years for remote groundwater extraction wells. Important factors are the scale of environmental emissions, and whether the substance, or its transformation products, are sufficiently *persistent in the environment* and enough *mobile in the aquatic environment* to survive such a journey. Inherently through these definitions, they accumulate with emissions, potentially being irreversibly present (Plumlee et al., 2008; Reemtsma et al., 2016).

Therefore, substances that have the *intrinsic substance properties* of being persistent (P) in the environment, mobile (M) in the aquatic environment and toxic (T) are the ones we must handle with care, monitor and – if necessary – regulate. Beyond the T criteria set out in Annex XIII, 1.1.3 of REACH this also includes other hazardous properties posing a risk to human health and the environment. An accumulating presence in the sources of our drinking water could eventually lead to a serious threat to both ecosystem and human health, particularly if they are considered toxic at low concentrations or are present at concentrations that exceed ecological thresholds (Liu et al., 2015).

Analogously, substances that are considered very persistent in the environment (vP) and very mobile in the aquatic environment (vM), regardless of their toxicity, must also be considered due to their enhanced potential to transport to remote areas or irreversibly be present within the water cycle, even for a long time after emissions have ceased. This is reflected in the European Commission's study on very persistent (vP) chemicals: "*[vP chemicals] may remain in the natural and man-made environments for an indefinite time and eventually reach levels leading to the same type of continuous exposure as occurs with bioaccumulation and to harmful effects to health, environment and natural resources. Such contamination may be poorly reversible or even irreversible, and could render natural resources such as soil and water unusable far into the future*" (EC, 2017b).

The German authorities propose to name such substances in the regulatory context of REACH persistent, mobile and toxic (PMT) substances or very persistent and very mobile (vPvM) substances (Neumann et al., 2015; Neumann, 2017; Neumann and Schliebner, 2017a, b).

## 7.1 Challenges related to water treatment

Once raw water used for drinking water production is contaminated with persistent and mobile substances, the general population is placed at risk of exposure and must also bear the cost of cleaning and purifying the contaminated water. A survey from 2014 found that 59% of Europe used either non-treated drinking water or drinking water treated with natural treatment methods and conventional technologies (van der Hoek et al., 2014). Only 41% used advanced water treatment technologies, such as granular-activated-carbon (GAC) filtration, ultra-filtration, advanced oxidation processes (like ozonation) and reverse osmosis. However, even these costly treatments are not completely effective for all persistent and mobile substances. A study on 113 organic compounds found that even after clarification, disinfection (chlorination) and GAC filtration, many mobile substances were not effectively removed, such as DEET (35% removal), nonylphenol (73% removal), camphor (25% removal) and bisphenol A (76% removal) (Stackelberg et al., 2007). A study on the treatment of wastewater in the Netherlands (Mulder et al., 2015) reported that 12 out of 28 substances they monitored have a removal rate of less than

40% in wastewater, and even if extra units were added to remove these pollutants, such as ozonolysis followed by sand filtration, GAC and powder activated carbon (PAC), there were still various persistent and mobile substances with poor removal rate, such as iopromid, atrazine and perfluorinated substances. Similar results were also seen for mobile compounds going through a large scale powder activated carbon facility, particularly those with small molecular size, low hydrophobicity and negative charges (Mailler et al., 2015). It was further commented on in the Dutch study that some of these treatments, like ozonolysis, could form persistent and mobile by-products (Mulder et al., 2015).

Thus, the same intrinsic substance properties that lead to persistence in the environment and mobility in the aquatic environment lead to breakthrough in drinking water treatment facilities. If emissions are continuous or increasing, the concentration of such persistent and mobile substances in the wastewater-drinking water cycle will increase over time (Steinhäuser and Richter, 2006), potentially becoming irreversible. Studies have indicated that persistent and mobile substances can be recirculated in this way (Plumlee et al., 2008; Filipovic and Berger, 2015).

An idea of direct economic costs of this advanced water treatment technology can be obtained by considering the following theoretical example: If Germany mandated the treatment of the approximately 5.2 billion $m^3$ of wastewater produced every year (Umweltbundesamt, 2014), how much would this cost? The aforementioned Dutch study (Mulder et al., 2015) estimated costs to remove between 30 – 80% of micropollutants (depending on the micropollutant) using different technologies. The cheapest technology (ozonation plus sand filtration) would cost 0.16 €/$m^3$ for a system set up for 300 000 person equivalents at 150 g/$m^3$ total oxygen demand, and the most expensive method would cost 0.29 €/$m^3$ for GAC filtration at 20 000 person equivalents at 150 g/$m^3$ total oxygen demand. This would correspond to 0.8 to 1.5 billion € per year in treatment for this partial removal for Germany only. Complete removal of persistent and mobile substances like certain perfluorinated substances is neither economically nor technologically feasible. At best, wastewater treatment facilities can be designed to reach target effluent levels. Remediation of persistent and mobile substances in wastewaters is costly; reducing concentrations to drinking water standards would be even more so.

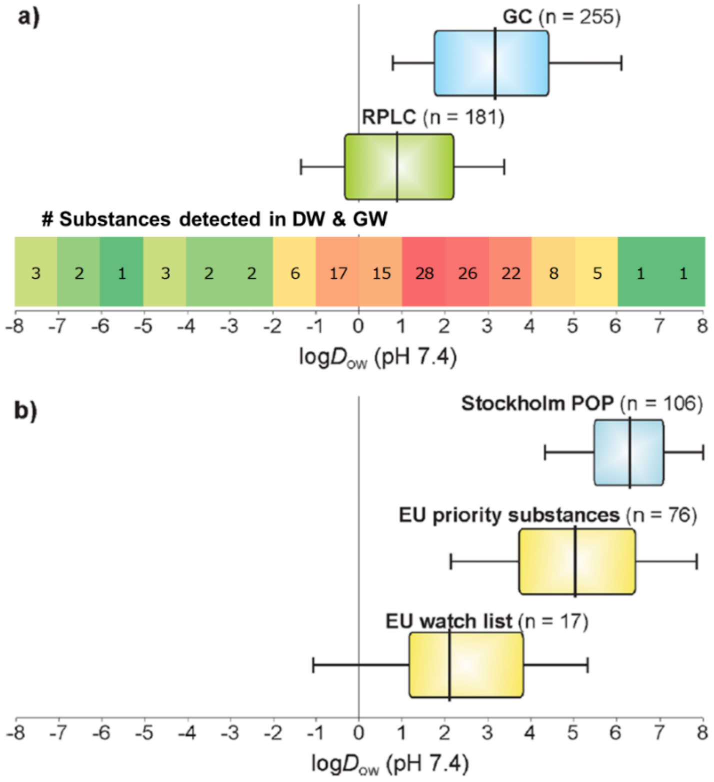
Therefore, relying on retrospective and costly advanced water treatment technology to protect or remediate drinking water is no sustainable solution, particularly because even costly treatments are not completely effective in removing persistent and mobile substances.

## 7.2 Challenges related to the analysis of water samples

A substantial analytical challenge exists related to the detection and quantification of mobile substance in water samples. Conventional methods using gas-chromatography (GC) and reverse-phase liquid chromatography (RPLC) are not able to detect and quantify the most mobile substances, such as those that are very polar, ionisable or ionic, resulting in high water solubility and low octanol-water partition coefficients ($K_{ow}$), or low pH-dependant octanol-water distribution coefficients ($D_{ow}$). This has recently been described as the analytical and monitoring gap (Reemtsma et al., 2016), and is illustrated in Figure 3. The log $D_{ow}$ value of those substances already regulated (presented under b) overlay the range of log $D_{ow}$ easily detectable by GC and RPLC (presented under a). The most mobile substances, with a log $D_{ow}$ value less than -1, require dedicated analytic methods and cannot easily be identified by standard analytic methods or non-target approaches. These cannot be measured without dedicated methods, and thus they remain invisible unless they are being specifically looked for. This implies that due to the lack of existing analytical techniques there are potentially several mobile substances in the aquatic environment that remain undetected, unmonitored and consequently unregulated.

**Figure 3 Box and Whisker plots of calculated log $D_{ow}$ values at ph 7.4 (chemaxon)**

of: (a) chemicals in water analysed by either GC-MS or RPLC, and (b) contaminants regulated by the Stockholm convention, the list of priority substances according to the water framework directive (WFD) and the so-called watch list of the WFD. The Whiskers point to the 10th and 90th percentile. The coloured numbers show the distribution of the REACH registered substances detected in drinking water (DW) and groundwater (GW) presented in chapter 4 (Table 1), which have been identified in the literature review.



Source: Adapted with permission from (Reemtsma et al., 2016).

The number of REACH registered substances detected in drinking water and groundwater presented in Table 1 are given as a function of their log $D_{ow}$ in Figure 3. This illustrates that there are several chemicals of concern falling within the analytical gap, which require dedicated methods. Examples of some of these which have only recently been detected for the first time in drinking water (Schulze et al., 2019) using state-of-the-art analytical techniques include 1,3-di-o-tolylquanidine (log $D_{ow}$ -3.0), Benzyltrimethyl ammonium (log $D_{ow}$ -1.0), Dimethylbenzene sulfonic acid (log $D_{ow}$ -6.0), 2-acrylamido-2-methylpropanesulphonic acid, ((log $D_{ow}$ -3.7).

REACH Annex IX and X sections 10 requires from every registrant to provide methods for detection and analysis for substances manufactured or imported in quantities of 100 tonnes or more on request only (Annex IX and X, sections 10 of REACH). Therefore, it must be assumed that for many mobile substances under REACH dedicated analytical methods are not available and consequently the extent of an already existing contamination of the sources of our drinking water is unknown.

# 8 Comparing PMT/vPvM substances to PBT/vPvB substances

For the 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, 2017), it can be demonstrated that this applies equivalently to PMT/vPvM substances.

The intrinsic substance property of bioaccumulation is on its own insufficient to imply a hazard to the food chain; therefore, within REACH it is substances that are persistent and bioaccumulative that are considered substances of very high concern (Brown and Wania, 2008, Matthies et al. 2016). Analogously, the intrinsic substance property of mobility in the aquatic environment is on its own insufficient to imply a hazard due to enrichment in the source of drinking water; rather, it is substances that are persistent and mobile which are potential substances of very high concern. The first can potentially bioaccumulate in biota to levels that cause harmful effects; the latter can potentially accumulate in the sources of our drinking water to levels that cause adverse effects through chronic exposure.

For persistent and mobile substances, as with persistent and bioaccumulative substances, "*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 persistence, 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, 2017a).

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 they can enrich in edible crops (Blaine et al., 2013; Felizeter et al., 2014).

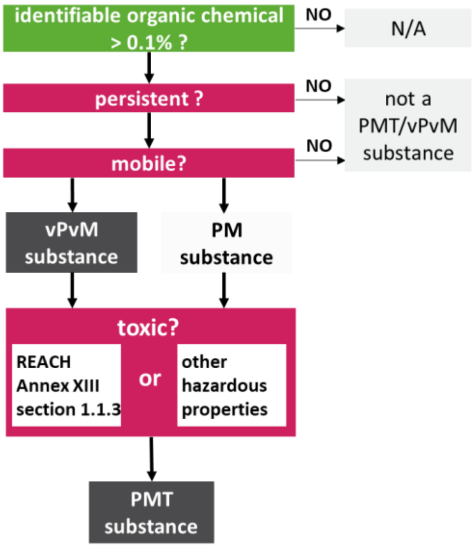
ECHA's PBT/vPvB guidance concludes that "*a "safe" concentration in the environment cannot be established using the methods currently available with sufficient reliability for an acceptable risk to be determined in a quantitative way*". This also applies to persistent and mobile substances, particularly in view of the water treatment and analytical challenges presented in chapter 7. For both persistent and bioaccumulative and persistent and mobile substances there are several exposure pathways, and no general removal pathway which could mitigate the contamination unless done at the point of emissions.

# 9 The assessment procedure for PMT/vPvM substances

The assessment procedure for identifying PMT/vPvM substances is presented in Figure 4. The first step is identical to the assessment of PBT/vPvB substances, and that is to identify if and what organic and organometallic chemical constituents, including impurities, additives, and transformation product precursors, are present in a substance at greater than 0.1% abundance. Although conducting a PMT/vPvM assessment is most straightforward for substances with single constituents, the intention is that it can also be used to assess relevant organic constituents, impurities, additives and transformation/degradation products or metabolites of each substance registered under REACH.

It is not always easy to identify all constituents, for instance for substances of "unknown or variable composition, complex reaction products or biological material" (so-called UVCB substances). For these substances, an identification of all constituents that may be present over 0.1% is recommended, as is done as part of the PBT/vPvB assessment (ECHA, 2017). Regarding transformation products, particular attention should be paid to the ones that are most persistent in the environment, particularly if the pathway to such persistent transformation products and their yields are known. Purely inorganic substances are exempted from this assessment. A formalized definition of organic and inorganic constituents, and an approach to identify transformation products was recently suggested (Arp et al., 2017; Arp and Hale, 2019).

**Figure 4: Overview of the assessment procedure to identify PMT/vPvM substances registered under REACH**



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Once the list of relevant constituents has been established, they are assessed for P/vP properties as described herein, and if any of them meet this criteria, they are assessed for M/vM properties, as also described herein. If a substance contains no organic constituent that fulfils the criteria for P/vP or M/vM, no further action is required within this assessment procedure for identifying PMT/vPvM substances. 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, it is assessed for T properties, as also described herein 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). Note that some substances may meet the criteria for both vPvM and PMT. Further guidelines is given in Arp and Hale (2019).

# 10 The criteria for identifying PMT/vPvM substances

## 10.1 PMT substances

A substance that fulfils the persistence, mobility and toxicity criteria of sections 10.1.1, 10.1.2 and 10.1.3 shall be considered to be a PMT substance.

### 10.1.1 Persistence

A substance fulfils the persistence 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 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 is higher than 120 days;

e) the degradation half-life in soil at 12 °C is higher than 120 days.

### 10.1.2 Mobility

A substance fulfils the mobility 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

### 10.1.3 Toxicity

A substance fulfils the toxicity criterion (T) in any of the following situations. Point (a) to (c) are already set out in Annex XIII, 1.1.3 of REACH:

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;

Beyond these T criteria already now set out in Annex XIII, 1.1.3 of REACH there might be cases, where it is necessary to identify persistent and mobile substances with other hazardous properties posing a risk to human health and the environment. These substances will be addressed as a separate category. In such cases it is proposed to demonstrate according to Art. 57 (f) an overall concern which is equivalent to Art. 57 (a) - (e). Aspects to be considered are comparable to the SVHC-identification for respiratory sensitizers:

- 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, societal concern.

Evidence (so called indicators) for significant risk to human health and the environment for persistent and mobile substances may arise in any of the following situations and need assessment to demonstrate fulfilling the equivalent level of concern of Art. 57 (f). These indicators are:

d) the substance meets the criteria for classification as carcinogenic (category 2), or germ cell mutagenic (category 2) according to 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 following Annex I;

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

## 10.2 vPvM Substances

A substance that fulfils the persistence and mobility criteria of sections 10.2.1 and 10.2.2 shall be considered to be a vPvM substance.

### 10.2.1 Persistence

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) is higher than 60 days;

b) the degradation half-life in marine (9 °C) fresh or estuarine water sediment (12 °C) is higher than 180 days;

c) the degradation half-life in soil (12 °C) is higher than is higher than 180 days.

### 10.2.2 Mobility

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

a) the lowest organic carbon-water coefficient log $K_{oc}$ over the pH range of 4-9 is less than 3.0.

## 10.3 Information relevant for the screening of P, vP, M, vM, and T Properties.

The following information shall be considered for screening for P, vP, M, vM and T properties.

### 10.3.1 Indication of P and vP properties

a) Results from tests on ready biodegradation in accordance with Section 9.2.1.1 of Annex VII of REACH;

b) Results from other screening tests (e.g. enhanced ready test, tests on inherent biodegradability);

c) Results obtained from biodegradation (Q)SAR models in accordance with Section 1.3 of Annex XI of REACH;

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

### 10.3.2 Indication of M and vM properties

a) For ionisable substances, the lowest pH dependant octanol-water distribution coefficient ($D_{ow}$) experimentally determined between pH 4-9 in accordance with Section 7.8 of Annex VII of REACH and the dissociation constant in accordance with Section 7.16 of Annex IX 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.

### 10.3.3 Indication of T properties

a) Short-term aquatic toxicity in accordance with Section 9.1 of Annex VII of REACH and Section 9.1.3 of Annex VIII of REACH;

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

## 10.4 Information relevant for the assessment of P, vP, M, vM, and T Properties.

The following information shall be considered for assessment for P, vP, M, vM and T properties.

### 10.4.1 Assessment of P or vP properties

a) Results from simulation testing on degradation in surface water; though if not available:

b) Results from simulation testing on degradation in soil;

c) Results from simulation testing on degradation in sediment;

d) Other information, such as information from field studies or monitoring studies, provided that its suitability and reliability can be reasonably demonstrated.

### 10.4.2 Assessment of M or vM properties

a) The partitioning between soil-water, sediment-water or sludge-water, expressed as log $K_{oc}$ within or across the pH range of 4-9 for neutral and dissociating species, respectively experimentally determined by partitioning studies in accordance with Section 9.3.1 of Annex VIII of REACH or estimated by (Q)SAR in accordance with Section 1.3 of Annex XI of REACH.

b) Other information, such as information from field studies or monitoring studies, provided that its suitability and reliability can be reasonably demonstrated.

c) Other information on the mobility in the aquatic environment provided that its suitability and reliability can be reasonably demonstrated on a weight-of-evidence basis, such as:

- Soil column leaching studies
- Lysimeter studies
- Field observations
- Water treatment breakthrough studies
- modelling studies

### 10.4.3 Assessment of T properties

a) Results from long-term toxicity testing on invertebrates as set out in Section 9.1.5 of Annex IX of REACH;

b) Results from long-term toxicity testing on fish as set out in Section 9.1.6 of Annex IX of REACH;

c) Results from growth inhibition study on aquatic plants as set out in in Section 9.1.2 of Annex VII of REACH;

d) The substance meeting the criteria for classification as carcinogenic in Category 1A, 1B or 2 (assigned hazard phrases: H350, H350i or H351), germ cell mutagenic in Category 1A, 1B or 2 (assigned hazard phrase: H340 or H341), toxic for reproduction in Category 1A, 1B and/or 2 (assigned hazard phrases: H360, H360F, H360D, H360FD, H360Fd, H360fD, H361, H361f, H361d or H361fd), specific target organ toxic after repeated dose in Category 1 or 2 (assigned hazard phrase: H372 or H373), additional category for "effects on or via lactation" (assigned hazard phrase: H362), according to Regulation EC No 1272/2008;

e) Results from long-term or reproductive toxicity testing with birds as set out in Section 9.6.1 of Annex X of REACH;

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

g) Results from in silico, in vitro and in vivo studies or results from (Q)SAR models that give evidence for endocrine properties of the substance in humans and/or wildlife species. Guidance on how to interpret results from various assays providing endocrine relevant endpoint information is given by the OECD Guidance Document 150 and by the EFSA/ECHA guidance document (Andersson et al., 2018)

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

# 11 Regulatory and Scientific Justification

The PMT/vPvM criteria are based on regulatory and scientific justifications. The basis of the regulatory justification is integration with existing data and assessment requirements of the REACH registration process. This is done to allow for the least possible additional workload for REACH registrants. The basis of the scientific justification was the identification and validation of what intrinsic properties make substances a threat to the sources of our drinking water, as evident from (1) monitoring data (Arp and Hale, 2019), (2) simulation and model studies (Arp and Hale, 2019; Kalberlah et al., 2014) and (3) impact considerations (Arp and Hale, 2019).

The PMT/vPvM criteria have been adjusted based on consultations and scientific research, as outlined in chapter 2. As a result of this process, the best balance between the regulatory and scientific justifications was sought to develop criteria and an assessment procedure that meets an appropriate level of precaution to protect the sources of our drinking water. The decisions presented within these final criteria have been discussed during various consultations and workshops and the pro and contra have been evaluated with care.

As the PMT/vPvM criteria are essentially hazard criteria, the appropriate level of precaution is primarily evaluated in terms of avoiding *false negatives*. Herein, false negatives refer to substances that have been shown to cause a risk to the sources of drinking water, but would not be identified by the PMT/vPvM criteria. False negative analysis requires simply analytical data for substances already in the sources of our drinking water as well as the intrinsic substance properties for those substances. If too many false negatives are found, this would imply the PMT/vPvM criteria are not sufficiently protective and the appropriate level of precaution is not met.

Whether the criteria are over-protective can best be evaluated by considering *false positives*. Herein, this would refer to substances that meet the PMT/vPvM criteria but do not threaten the sources of our drinking water, despite being emitted into the environment at a sufficiently large scale. Analysing for false positives is inherently more challenging than analysing of false negatives. There are many potential reasons why a substance cannot be identified in monitoring samples. False positive analysis requires detailed information of use and emission patterns (which is outside the scope of the PMT/vPvM criteria), in addition to the intrinsic substance properties, available analytical techniques and monitoring data.

This chapter 11 presents the regulatory and scientific justifications of P/vP, M/vM and T criteria, individually. Chapter 12 assesses, through analysis of false negatives and false positives, the level of precaution for the entire PMT/vPvM criteria and assessment concept. Chapter 13 presents an impact assessment of implementing these criteria within REACH.

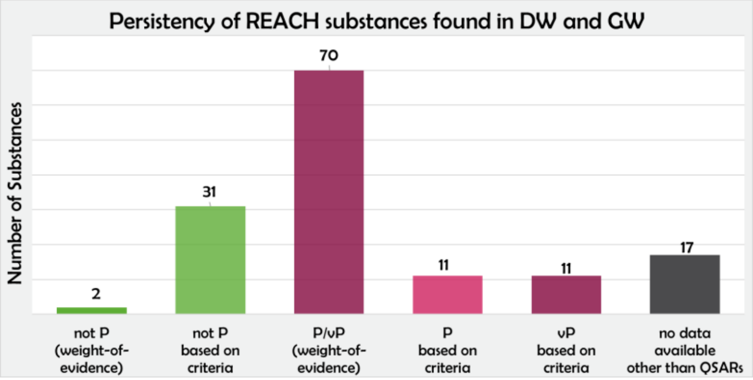
## 11.1 Justification of the P/vP criteria

The persistence criterion (P) and very persistent criterion (vP) are taken directly from Annex XIII of REACH. The main advantage is that it is consistent with existing regulatory definitions of P and vP. This means that no additional workload is caused for registrants by the PMT/vPvM assessment since an assessment of P and vP within the PBT/vPvB assessment has to be performed for any registration above 10 t/a. The ECHA guidance on the PBT/vPvB assessment (ECHA, 2017) already now recommends in general to first asses the persistence in the freshwater compartment with the OECD TG 309, which is also recommended in 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 soil and freshwater sediments. For surface water transport, the freshwater half-life would be the most relevant. It has been argued during consultations that the marine water and marine water sediments are irrelevant for the PMT/vPvM criteria, as the focus is on freshwater systems; however, no exception is being proposed to eliminate these criteria because marine water data is considered a suitable proxy for freshwater data, particularly when no freshwater data exists. Also, in practice marine water half-life studies are quite rare compared to freshwater studies.

Arp and Hale (2019) state, that in regard to whether the half-life cut-off values themselves provide the appropriate level of precaution to protect the sources of our drinking water, the concept of persistence would be most relevant in the context of the travel time required for a substance to leave a point of emission to the sources of our drinking water. If a substance was not persistent enough to survive this travel time, it would not pose a threat. An extreme case here is when emissions are occurring directly into a source for drinking water, where there is no barrier and travel time could be negligible, and a P criterion would be irrelevant. A more realistic situation in most of Europe is allowing water to first pass through the banks of river or lake, a process referred to as bank filtration. 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 a river bank. A substance that meets the P criterion of 120 days in soil and travels through a river bank at or near the speed of water would easily breakthrough 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) which would correspond to 27 to 2700 m over 180 days (vP criteria for fresh or estuarine water sediment at 12 °C). Considering that still 50% of a chemical is present 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 amounts. In river water, where velocities are orders of magnitude faster than in groundwater, transport distances over the freshwater P half-life time of 40 days can be thousands of kilometres. An example would be 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. 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 the water cycles.

**Figure 5** **Categories of P evaluations for 142 REACH registered substances detected in drinking water and/or groundwater**



Source: Original figure

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 can be kept in mind that highly volatile substances are likely removed during water treatment through aeration; however, this is not applicable for untreated groundwater.

In chapter 4, the monitoring data of 142 REACH registered substances (as of May 2017) that were measured in drinking water or groundwater were presented. An evaluation of whether these 142 substances meet the P/vP criterion is presented in Figure 5, with information about the P assessment for individual substances in the Appendix Table C1.

A clear outcome of this evaluation is that empirical data to make a definitive P/vP assessment is largely lacking. Good quality half-life data is rare, because of the cost and expense (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). Here, half-life data or experimental screening test data that indicated P, vP or not P was only available for 53 substances. For the other 89 substances there was no definitive P/vP evaluation data available even after a thorough search. However, for 72 a weight-of-evidence evaluation could be made based on available data, such as enhanced ready tests and QSARs (Arp et al., 2017; Berger et al., 2018; Arp and Hale, 2019). In summary, 92 substances (65%) met or were suspected of meeting the P/vP criterion, 33 (23%) substances did not meet or are suspected not to meet the P criteria, and for 17 substances no conclusion could be made on P/vP. From this analysis, the P criteria on its own is not overprotective of substances reported in drinking water and groundwater; with 23 % false negatives from this analysis, referring to contaminants measured in drinking water that are not P. Two potential explanations are 1) high emissions and 2) local contamination. As an indicator that high emissions is a plausible explanation, Appendix Table D1 presents the publicly available tonnages of these false negatives, showing that many of these substances are indeed high volume substances. A possible instance of false negatives due to local contamination are reports of phthalate plasticizers in drinking water, which are used in water pipes (Amiridou and Voutsa, 2011). Though it could be argued that the P criteria should be more protective, the regulatory considerations presented above justify this level of protection. Another consideration is that substances that are in drinking water and are not persistent would disappear after emissions cease. Substances that do meet the P criteria, however, would be less reversible, and inherently travel farther and be more problematic after emissions cease (see chapter 8).

## 11.2 Justification of the M/vM criteria

The following justification of the M/vM criteria is presented in Arp and Hale (2019):

REACH defines in Annex II section 12.4 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 $K_{oc}$ as the central intrinsic substance property to describe mobility. This has a long history, as since the 1980s persistence and $K_{oc}$ in combination were used to describe mobility (Gustafson, 1989). More recently a modelling exercise by Kalberlah et al. (2014) demonstrated that for persistent substances, $K_{oc}$ was the parameter that correlate best with modelled amounts of breakthrough fractions from wastewater treatment, more so than other mobility descriptors. The use of the lowest organic carbon-water coefficient log $K_{oc}$ over the pH range of 4-9 as the assessment parameter to describe mobility has been widely supported in the consultations, scientific discussions and internal review listed in chapter 2.

There have been two major changes during the development of the M/vM criteria compared to previous versions. (1) Water solubility is considered neither a suitable property to set a threshold for the assessment of mobility, nor for the screening, and was removed from the criteria in chapter 10. While it was already shown that water solubility is not correlated with mobility (Kalberlah et al., 2014), its necessity was further recently questioned through a Quantitative structure–activity relationship (QSAR) model assessment (Holmberg et al., 2019). Other central reasons were difficulties when applying this parameter for ionic and ionisable substances, in which water solubility is dependent on counter ions, and some concerns related to data quality for this parameter. (2) The log $D_{ow}$ is no longer an assessment criterion, but now the main indication (screening) criterion for mobility. Here the main reasons are the compatibility to the screening for B and vB properties and to thereby reduce the work load for registrants, as will be described below.

During consultations, there were some discussions on the role of clays and minerals in reducing mobility in soils. In specific situations, particularly for ionic substances and clay rich environments, clays and minerals can measurably reduce mobility (Droge and Goss, 2013). However, these specific cases are difficult to generalize. Clays and minerals can have widely differing available surface areas and capacities for ion-exchange across different soils, which makes their influence on mobility extremely site specific. Therefore, it is extremely challenging to include a generic parameter to account for clay and mineral sorption as part of a hazard criterion. It is acknowledged that basing the assessment for mobility strictly on $K_{oc}$ may be conservative for specific, local, and substance specific case studies, in which minerals may further reduce mobility (Droge and Goss, 2013). However, for developing a hazard criterion, there is an argument for being conservative, and that is to reduce the number of false negatives.

The pH range of 4-9 is included to account for how variations within this environmentally relevant range can influence the $K_{oc}$ value. This influence is most noticeable for ionisable substances that can be cationic (e.g. bases) or anionic (e.g. acids) within this pH range. Because soils are generally anionically charged, the more the substance is present in a cationic form, the larger its $K_{oc}$ value is. Therefore, 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 zwitterions and some soil types, such as those with 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 this initiative was commenced there has long been an apparent consensus within the scientific community that a log $K_{oc}$ cut-off of ca 3.0 is a suitable cut-off for the protection of groundwater of 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 following metric to assess subsurface mobility:

► $$GUS = \log DT_{50soil} (4 - \log K_{oc}) \qquad (M1)$$

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. mobile), below 1.8 a "non-leacher" (i.e. non-mobile), and those in between in the "transition zone" and capable of leaching (i.e. potentially mobile). Considering the vPvM criteria from this initiative, specifically 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 a value that can be considered protective of groundwater. A cut-off value log $K_{oc}$ of 2.7 would correspond to a "leacher" and would not been protective for groundwater.

The cut-off value of the assessment criterion for vM (log $K_{oc}$ value of 3.0 or smaller) is harmonised with the Groundwater Watch List coordinated by the EU Common Implementation Strategy Working Group Groundwater (EC, 2016), which also uses a log $K_{oc}$ cut-off of 3.0 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 of 4.0 or smaller) is scientifically justified for the protection against bank filtration breakthrough. In the first version an even higher cut-off value was originally proposed based on the research project by Kalberlah et al. (2014), wherein a simulation of sewage treatment plant outlet concentration was conducted using ECETOC TRA software (http://www.ecetoc.org/TRA). As a result, the authors proposed a log $K_{oc}$ cut-off value of 4.5 or smaller for mobility. The same cut-off value was also used in the JPI Promote project (www.ufz.de/promote/) to successfully identify several high emission PM substances in different stages of drinking water production, many of which for the first time (Schulze et al., 2019). In another independent research project, a log $D_{ow}$ cut-off value of 4.5 or smaller was used successfully to prioritize substances relevant for water supply companies (Nödler et al., 2019). Further, a recent evaluation of mobility within the Stockholm Convention concluded that very persistent substances meeting a log $K_{oc}$ value up to 5.0 may reach remote environments (Crookes and Fisk, 2018). However, despite the success of these cut-off values in these recently completed projects, the log $K_{oc}$ cut-off value of 4.5 or smaller for mobility was criticised during the consultations and scientific discussions as outlined in chapter 2 as being too high and too protective. Motivated by this feedback, a thorough re-evaluation of the cut-off value for mobility was done based on further scientific considerations, and more importantly based on real monitoring data (chapter 4). A summary of this evaluation is presented here.

Regarding theoretical considerations, the breakthrough time of substance in bank filtrate $t_{substance}$ compared to the flow rate of the water, $t_{water}$ is:

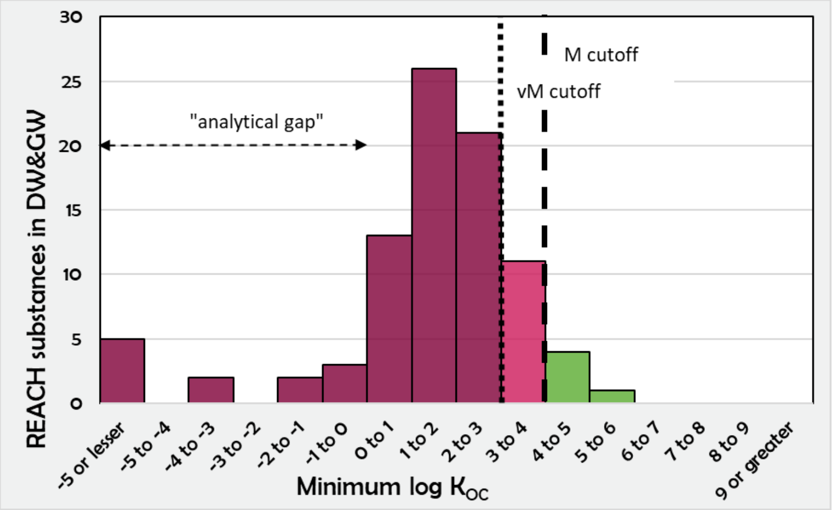
► $$t_{substance} = t_{water}\,(1 + (\rho/\Theta)K_{oc}foc) \qquad \text{(M2)}$$

which includes the fraction of organic carbon (foc), bulk density, ρ, and the porosity, Θ, which are typically 1.7 kg/L and 0.4, respectively, in Europe (ECHA, 2016). The foc for an agricultural soil is typically 0.02 (ECHA, 2016), in less organic rich environments such as sands it is 0.002 (Hale et al., 2017). With these parameters, the breakthrough time of substances relative to the flow rate of the water during bank filtration can be considered as a function of $K_{oc}$. In an extreme case, the bank filtration $t_{water}$ can be considered 5 days, with a log $K_{oc}$ of 4.0 and considering equation M2, it would take 4255 days in an agricultural soil and 430 days in a sandy soil for the breakthrough of the substance. Both of these breakthrough times are larger than the P criteria for soil of 120 days; however, considering the general equation for exponential decay as a function of half-life (equation M3), some contaminant will still remain after breakthrough:

► $$\text{fraction of substance remaining} = 0.5^{\text{time / DT50}} \qquad \text{(M3)}$$

In the example just presented, 8% of contaminant 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 a log $K_{oc}$ of 4.0 appears as a suitable maximum cut-off for the mobility threshold, for protection against substances that are permeable to bank filtration. However, the ultimate test for the suitability of this cut-off would be an assessment of log $K_{oc}$ values of substances found in the sources of our drinking water. Such an assessment is presented in Figure 6 for the REACH registered substances detected in drinking water and groundwater in Table 1 from the analytical studies in Appendix Table A1; wherein the number of substances reported is plotted as a function of their $K_{oc}$ range.

**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: Arp and Hale (2019)

Figure 6 shows the distribution of the 90 out of 142 substances for which experimental $K_{oc}$ data was available, ranging from -6.0 to 5.4. The "analytical gap" as discussed in section 7.2, is also presented in this chart. This highlights that there may be more substances detected if more analytical methods were available for highly polar substances. There were 11 substances with a log $K_{oc}$ between 3.0 and 4.0 (or 12% of considered substances), implying they meet the M criterion but not vM, and a further 5 (or 6% of 90 substances) ranging from 4.0 to 5.4, implying these are false negatives (substances in drinking water not meeting the M criteria). Thus, lowering the vM and M criteria further would increase the number of false negatives, which is considered insufficiently conservative.

Regarding substances for which log $K_{oc}$ data are not available, the use of the lowest pH dependant octanol-water distribution coefficient ($D_{ow}$) for ionisable substances, is recommended as an indication criterion for mobility. Consequently, the screening criterion for the mobility assessment is:

*the lowest pH-dependant octanol-water distribution coefficient log $D_{ow}$ over the pH range of 4-9 is less than 4.5*

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:

- $D_{ow} = (1/(1+10^{pH - pKa}))K_{ow}$ (for monoprotic acids) (M5)
- $D_{ow} = (1 - 1/(1+10^{pH - pKa}))K_{ow}$ (for monoprotic bases) (M6)

For neutral and non-ionisable substances over a specified pH range the $D_{ow}$ has the same value as the octanol-water partition coefficient ($K_{ow}$). Determining the pKa is required under Section 7.16 of Annex IX of REACH when volumes are over 100 tonnes per year. $K_{ow}$ 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 in Section 7.7 - 7.8 of Annex VII of

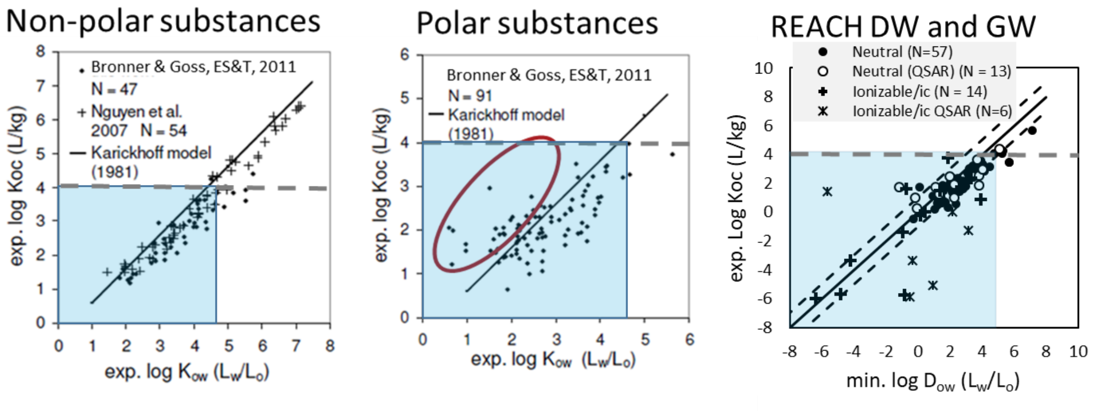
REACH. Furthermore, $K_{ow}$ is already used as an indicator for the bioaccumulation (B) assessment. Specifically, substances with a log $K_{ow}$ larger than 4.5 should be evaluated for B either through direct measurement of bioconcentration factors (BCF) or alternatively a weight-of-evidence approach (ECHA, 2017). If this data is not available, QSAR models for $K_{ow}$ and pKa need to be used. Further guidance to address this is presented in Arp and Hale (2019).

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, 2017). However, this sharp cut-off between screening for B and screening for M is only expected for neutral, weakly to non-polar molecules. Correlations between $K_{oc}$ and $D_{ow}$ for polar, ionisable or ionic compounds are scattered; similar to correlations between B and $D_{ow}$. Consequently, some polar, ionisable or ionic substances, are 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 a threshold for prioritizing whether to screen for B and 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, such as 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 $K_{ow}$ are generally slightly larger than log $K_{oc}$ 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 middle panel of Figure 7. Therefore, for polar compounds in particular, the lowest log $D_{ow}$ over the pH range of 4-9 is the recommended indicator for mobility. In the right panel of Figure 7, REACH registered substances with experimental log $K_{oc}$ available are plotted against the minimum log $D_{ow}$ or log $K_{ow}$. Here it is also evident 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.

**Figure 7: The log-log correlation between experimental $K_{OC}$ and $K_{OW}$/$D_{OW}$**

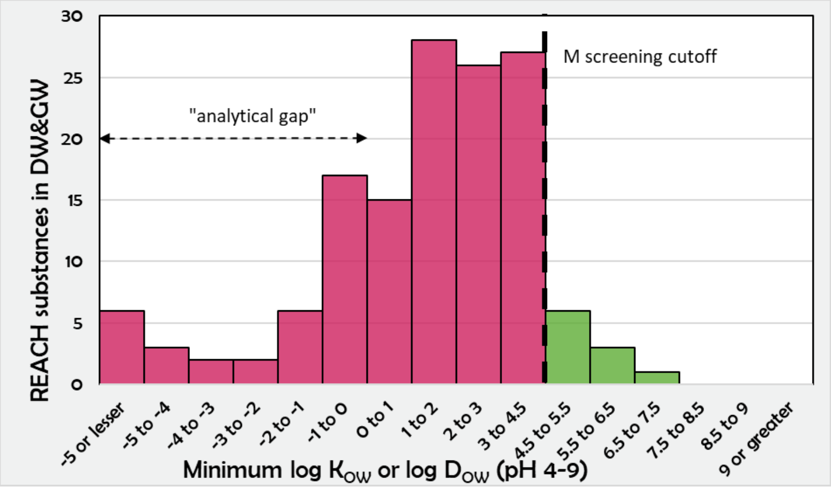
for: left, non-polar substances (defined as having a mass fraction of oxygen + nitrogen atoms in the molecule ≤ 12%); middle, polar substances; right, REACH registered substances detected in drinking water (DW) and groundwater (GW)



Source: Arp and Hale (2019)

The substances meeting the M criteria of log $K_{oc}$ less than 4.0 and screening criterion of the minimum log $D_{ow}$ of 4.5 in the pH range of 4-5 is outlined within 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. Thus, the screening criterion captures most M substances but not all. However, 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. Though it should be kept in mind by registrants that a subset of substances with a log $D_{ow}$ near 4.5 may ultimately meet the criteria for both B and M.

**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: Arp and Hale (2019)

In Figure 8 the 142 REACH substances detected in drinking water and groundwater are categorized by their $K_{ow}$ or lowest $D_{ow}$ (pH 4-9), along with the mobility screening criterion. This screening criterion captures 132 (93%), further indicating its suitability.

An evaluation of whether the 142 detected substances meet the M/vM criterion or M-screening criteria is presented in Appendix Table D2. There were only 8 (5.6%) false negatives for the M criteria, 5 based on experimental $K_{oc}$ values and 3 based on screening using $K_{ow}$. These are DEHP, galaxolide, butylhydroxytoluene (BHT), tert-octylphenol, nonylphenol, pyrene, 2,4-di-tertiary-butylphenol and butyl benzyl phthalate, all of which are high volume chemicals. Galaxolide is a musk, BHT and 2,4-di-tertiary-butylphenol are widely used as antioxidants, and the remainder are plasticizers associated with leaking from plastic pipes (Junk et al., 1974; Cheng et al., 2016), epoxy-coatings (Rajasärkkä et al., 2016) and bottles (Zaki and Shoeib, 2018). The tonnages of false negatives are presented in Appendix Table D1 and D2. Similar with the false negatives with the P criteria, the false negatives of the M criteria may be due to 1) high emissions and 2) local contamination. Nevertheless, obtaining only 8 of 142 detected REACH registered substances as false negatives is considered in good agreement with the theoretical considerations, and to provide the appropriate level of precaution.

## 11.3 Justification of the T criteria

In general, the German authorities consider substances which fulfil both persistence and mobility criteria as priority candidates for further hazard assessment. One of the main concerns over persistent and mobile substances is that they could build up over time in source of our drinking water to levels that may eventually cause hazardous effects, either alone or as mixtures. Further, they can remain there for some time after emissions have ceased. Therefore, considering that human populations and remote environments will be exposed to such substances over long time scales, it is relevant to take a hazard-based approach to their identification. REACH considers exposure to the general human populations, including pregnant women, children and the elderly. The T criterion within the PMT/vPvM assessment reflects this and takes chronic exposure via drinking water into account. 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 "*particular effects, such as [...] strong odour and tainting*" to drinking water should be avoided.

Beyond the T criteria set out in Annex XIII, 1.1.3 of REACH there might be cases, where it is necessary to identify persistent and mobile substances with other hazardous properties posing a risk to human health and the environment. Aspects to be considered are defined in section 10.1.3, including e.g. carcinogenic and cell mutagenic category 2, and endocrine disrupting properties. These additional criteria need assessment to demonstrate fulfilling the equivalent level of concern of Art. 57 (f). Some of these criteria were previously included in an earlier version of the PBT assessment, before Annex XIII was established (Matthies et al., 2016).

Considering these additional criteria for persistent and mobile substances is straightforward from a REACH registration point-of-view. Carcinogenic category 2, cell mutagenic category 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. There is also requirements for reporting DNEL values in REACH, following Annex I. The DNEL cut-off within the PMT/vPvM assessment was proposed and 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). In summary, for substances registered with volumes of 10 t/y and fulfilling the criteria for classification in any of the hazard classes or categories listed in Article 14(4) of REACH as amended from 1 December 2010 by Article 58(1) of Regulation (EC) No 1272/2008 (CLP Regulation), the DNEL of the most predominant exposure pathway has to be reported, with key exceptions being intermediates and substances where it is not technically possible to derive DNELs (ECHA, 2012).

Persistent and mobile substances are strongly recommended to be prioritized for the assessment of endocrine disruptor properties. The first step is to assess whether the substance 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 by the OECD Guidance Document 150 and by the EFSA/ECHA guidance document (Andersson et al., 2018). Persistent and mobile substances that fulfil the WHO/IPCS definition of an endocrine disruptor meet the criteria set out in section 10.1.3.

However, substances with ED concern should have been identified as SVHC based on the endocrine disrupting properties. Substances with ED concern that have not yet been identified as ED under REACH, should additionally be proposed as SVHC following the WHO/IPCS definition of an endocrine disruptor and the equivalent level of concern of Art. 57 (f).

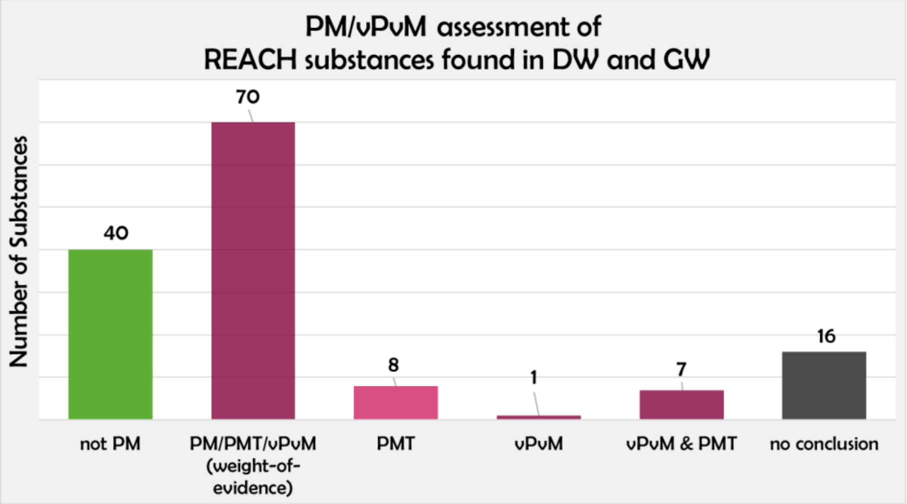
A comparison of all REACH registered substances (as of May 2017) that meet the T criterion for the PBT/vPvB assessment defined in the Annex XIII of REACH with those, that meet the criteria set out in section 10.1.3 of this document, has been performed recently. This study found an increase from 28.5% (2774 of 9741) to 34.6% (3370 of 9741) Arp and Hale (2019).

In chapter 4, the monitoring data of 142 REACH registered substances (as of May 2017) that were measured in drinking water or groundwater were presented. An evaluation of whether these 142 substances meet the T criterion is presented in Appendix Table C1. In total, 113 of these substances were considered T (or 80%). This percentage is much higher than the 34.6% of the total REACH registered substances (as of May 2017) considered T; this may be due to selection bias, as drinking water and groundwater monitoring studies often target toxic substances.

# 12 Validation of the PMT/vPvM criteria

The PMT/vPvM criteria were validated in terms false negatives using the 142 REACH registered substances (as of May 2017) that were measured in drinking water or groundwater (chapter 4). The false negatives refer to substances detected in these media that were considered to not meet the PM criteria (regardless of toxicity). The results of the PMT/vPvM assessment for these substances are presented in Figure 9, with details of the assessment of individual substances in Appendix Table C1.

**Figure 9** **Validation of the PMT/vPvM criteria via comparison to 142 REACH registered substances detected in drinking water and/or groundwater.**



Source: Original figure

The occurrence of false negatives is 28% (40 out of 142). This arguably high number is mainly attributed to the P criteria, which is responsible for 33 of the false negatives, respectively, as previously discussed. This may be interpreted as the cut-off for the P criterion being too high and that already shorter half-lives should be considered. The remaining 7 false negatives were due to the M criteria. Only one substance did not meet the P and M criteria (butyl benzyl phthalate). The T criterion was not considered in this analysis, as it is not relevant in the context of drinking water presence; however, there are 19 substances not meeting the T criteria that are PM, but not vPvM. Therefore, the number of these monitored substances fulfilling the PMT/vPvM criteria is 67, or 47%. It should be pointed out that this fraction could rise up to 83 (or 58%) considering the substances where no conclusion was possible. These substances should be urgently tested for persistence. To conclude regarding false negatives, even if a substance is detected in drinking water or groundwater, there is only a roughly 50% chance this substance would meet the PMT/vPvM criteria and therefore be considered a substantial threat to the sources of our drinking water long after emissions have ceased.

To evaluate for false positives of the PMT/vPvM criteria, referring to substances that would be evaluated as meeting these criteria but are not present in the sources of our drinking water, despite substantial environmental emissions, the 142 REACH substances considered in Figure 9 and chapter 4 are not appropriate as they are in drinking water or groundwater. Recently, however, the JPI Water research project PROMOTE (http://www.ufz.de/promote/) completed a multi-year study that can be used for an analysis of false positives. Within this project, substances that met persistency and mobility criteria very similar to this initiative (Arp et al., 2017) were ranked according to an "Emission Score", which was derived using REACH registration data regarding tonnages and REACH information related to usage (Schulze et al., 2018). The PROMOTE project ultimately chose 64 substances to screen for in water samples from various stages of drinking water production in Spain, Germany, France and the Netherlands, based on their persistence, mobility and emission profile. For this, new analytical methods needed to be developed, and the project was able to develop analytical methods for 57 of these substances. Ultimately, the PROMOTE project was able to identify 43 of the 57 PM substances selected in the samples. Among these, 23 have never been detected previously in environmental water samples (Schulze et al., 2019). It may be inferred from these results that slightly more conservative PM criteria in combination with emission data generate approximately 25% (14 out of 57) or fewer false positives. This is roughly similar to the amount of false negatives in this study for PM/vPvM substances, 28%.

This, in aggregate, is considered as strong validation of relevance and practical utility of the PM/vPvM assessment criteria, as it strikes a good balance between false negatives and false positives; in other words, it can be used to both describe the intrinsic substance properties of the majority of substances found in the sources of our drinking water (with only 28% false negatives), and can be used to correctly predict if substances with substantial environmental emissions will occur in the sources of our drinking water (with only 25% false positives).

# 13 Impact Assessment of the PMT/vPvM criteria

The German Environment Agency (UBA) funded recently a research project to assess all REACH registered substances (as of May 2017) (Arp, 2018; Arp and Hale, 2019). In 2018 the project presented a preliminary assessment of how many REACH registered substances would meet the PMT/vPvM criteria as presented here (Arp, 2018). Out of the 15469 substances registered under REACH (as of May 2017), 9741 substances contained an identifiable organic constituent in concentrations > 0.1% (w/w). Impurities and transformation products were not considered in this assessment.

Several limitations related to data availability were evident that prevented a complete assessment of all substances. The largest data limitation is the lack of high-quality half-life data needed for the persistency assessment, similar to that which occurred for the assessment of monitored substances in this report. This is a general shortcoming for conducting P assessments (UNEP, 2013; Goldenman et al., 2017), as mentioned in section 11.1.

Another, more minor but important limitation for the assessments was the lack of experimental $K_{oc}$ data for ionic and ionisable substances, considering the influence of pH (Nödler et al. 2019). This is due in part to the analytical difficulty in measuring highly polar substances (Reemtsma et al., 2016). Other limitations mentioned above is lack of DNEL (long term, oral, general population) and endocrine disruption assessments. Under this assessment (Arp, 2018), it was noted that for 3857 substances there was insufficient data to make a weight-of-evidence based assessment on their persistency. The remainder were divided into the following categories: vP (120 substances), P (76 substances), not P (2542 substances), substances where half-life data is lacking but the weight-of-evidence points strongly to a P/vP conclusion (532), and substances where half-life data is lacking but the initial data cannot rule out a P/vP conclusion (2614). From this pool, the 728 substances that met the vP, P or where weight-of-evidence pointed strongly to a P/vP conclusion were considered further for the M assessment.

After assessing M for the 728 P/vP substances, substances were separated in four categories: vPvM (53 substances), PM (79 substances), potential PM/vPvM based on weight-of-evidence (339 substances), not PM (139 substances), and not enough data to make a weight-of-evidence conclusion on PM (118 substances).

Finally, after the toxicity assessment there were 240 substances of the original 9714 substances that are considered with sufficient weight-of-evidence to fulfil the PMT/vPvM criteria. These included:

- vPvM and not T: 30 substances
- vPvM and PMT: 23 substances
- PMT (but not vPvM): 35 substances
- High Potential to be either PMT/vPvM: 152 substances

Therefore, the impacts of the PMT/vPvM criteria as presented here on the total number of REACH registered substances with organic constituents is 2.5% (240 out of 9741), or 1.6% of all REACH substances (240 of 15469). Further, when emissions and risk assessment is taken into account, the number of substances that are of concern would drop even further. In the update of the preliminary assessment by , only 122 REACH registered substances that were PMT/vPvM were prioritized for follow up based on emission considerations, duplicate chemical structure entries within REACH, and substances that were already being regulated (Arp and Hale, 2019). It may be concluded that fewer REACH registered substances fulfil the PMT/vPvM criteria than the PBT/vPvB criteria.

The Danish Environmental Protection Agency conducted a separate impact assessment in 2019 (Holmberg et al., 2019), based primarily on QSARs from the Danish QSAR database (http://qsar.food.dtu.dk). This assessment was based on primary organic constituents, and not on transformation products and impurities. The Danish impact assessment considered: 1) different levels of strictness on the QSARs used to evaluate P; 2) a sensitivity analysis on different $D_{ow}$ values for the M criterion; and 3) only mono-constituent substances with volumes at 10 tpa per manufacturer or importer, for which a CAS number or structural information could be found (by June 2017). This analysis yielded a total of 2073 substances. Using the PMT/vPvM criteria as presented here, of the 2073 investigated substances a range of 16 to 96 substances were considered to meet the vPvM criteria and a range of 37 to 166 to meet the PMT criteria, depending on the QSAR approach used. Considering all the QSAR approaches tested, 268 substances were identified as either PMT or vPvM in at least one of the approaches. Therefore, here again, a relatively minor portfolio of chemicals were considered to meet the PMT/vPvM criteria, in the order of max 13% of those organic substances registered above 10 tonnes per annum when relying only on QSAR data.

It is concluded that the introduction of the PMT/vPvM criteria will only impact a minor portfolio of REACH registered substances, and would have a relatively small impact on the European chemical industry as a whole.

# 14 Risk Management Options for PMT/vPvM substances

Removing persistent and mobile substances from raw water for drinking water production is costly, complex and in most cases ineffective (see chapter 7.1). Preventing persistent and mobile substances from contaminating the sources of our drinking water is the best solution providing benefits to all stakeholders and society (see chapter 6). Legislation aimed at ensuring European water quality, including the Water Framework Directive (2000/60/EC), Drinking Water Directive (98/83/EC) and Groundwater Directive (Directive 2006/118/EC), do not implicitly contain any pollution prevention regulation. Consequently, REACH is most suitable for this. Identifying PMT/vPvM substances under REACH is the first step. The second step is an exposure assessment and to ensure that PMT/vPvM substances in commerce under REACH are used in a way resulting in a minimum of emissions.

Demonstration of the safe use of chemicals is a key component of REACH. It serves the purpose to "*ensure a high level of protection of human health and the environment*" (Article 1,1) and is "*underpinned by the precautionary principle*" (Article 1,3). REACH, in its aim and scope, states that "*it is for manufacturers, importers and downstream users to ensure that they manufacture, place on the market or use such substances that do not adversely affect human health or the environment*" (Article 1,3). Through REACH, it becomes the responsibility of the registrants to characterize the intrinsic hazard of the substances and the risk of each of their uses over the complete life cycle. This inherently includes ensuring that their registered substances do not contaminate the sources of our drinking water. This is mentioned in Annex 1, section 0.10 of REACH: "*In relation to particular effects, such as […] strong odour and tainting, […] the risks associated with such effects shall be assessed on a case-by-case basis and the manufacturer or importer shall include a full description and justification of such assessments in the chemical safety report and summarised in the safety data sheet*".

Herein, recommendations are provided as to how diverse sectors can create solutions for the sustainable management of persistent and mobile substances, through the criteria and assessment procedure presented herein, alongside the REACH registration process.

## 14.1 Manufacturers, importers and downstream users

Registrants are already now able to use the criteria presented in chapter 10 to perform voluntarily a PMT/vPvM assessment in the context of their chemical safety report (CSR). This will allow the identification of PMT/vPvM substances during REACH registration, or already during product development. If the data that is currently available for a PMT/vPvM assessment is of low quality, manufacturers, importers and downstream users should strive to obtain data of better quality in order to carry out a more accurate assessment. When PMT/vPvM substances are identified, manufacturers, importers and downstream users can immediately act to reduce or prevent emissions. For instance, safer alternatives could be considered or risk management measures (RMM) could be put into place to minimize emissions into the environment during the whole life cycle of the substance. This would assist industry in fulfilling their obligation under REACH to guarantee safe use of their registered substances. The German authorities strongly recommend that PMT/vPvM properties should be communicated during the scope of registration and throughout the supply chain the same way as PBT/vPvB properties, i.e. via the Chemical Safety Report and/or the Safety Data Sheet. This should also include recommendations for the minimisation of emissions during the supported use.

An important part of this is to develop and share analytical methods for their mobile substances. It is essential for persistent and mobile substances to ensure appropriate analytical techniques are available. This is of importance, especially with regard to the challenges related to the analysis of mobile substances presented in section 7.2. Registrants should take the lead in developing analytical methods for mobile substances and include them in their registration dossier.

Registrants should follow a similar assessment procedure for PMT/vPvM substances, as for PBT/vPvB substances and substances meeting the hazard classes in Article 14(4) of REACH. This assessment procedure is comprised of the following steps as outlined in Annex I section 4.0.2 of REACH:

- Step 1: Comparison with the Criteria
- Step 2: Emission Characterization

For PMT/vPvM substances, "Step 1: Comparison with the Criteria", the criteria in chapter 10 herein is to be used. In essence, "Step 2: Emission Characterization" for PMT/vPvM substances can follow a similar procedure as already in place for 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, 2017). The key step is the exposure assessment following Annex I, Section 5 of REACH, which includes recommendations for risk management measures (RMM) to minimise emissions. Analogously to other hazardous substances under REACH, regulatory measures for PMT/vPvM substances may only need to be considered by authorities, if registrants and downstream users do not put the necessary RMM into place.

## 14.2 Local authorities and water suppliers

Local authorities, water suppliers and producers of drinking water, as well as researchers are invited to consider identified PMT/vPvM substances registered under REACH for their water monitoring programs. That being said, many mobile substances are currently difficult to monitor in the aquatic environment because of a "gap" in suitable analytical methods (Reemtsma et al., 2016); therefore, a future list of PMT/vPvM substances registered under REACH would be of relevance to develop analytical methods (Arp et al., 2017; Arp, 2018; Berger et al., 2018; Schulze et al., 2018; Holmberg et al., 2019; Schulze et al., 2019).

Local authorities could use such a substance list to improve collaborations with local industry in developing strategies to minimize emissions into the environment and to ensure their effectivity. In this way, more economically feasible costs of pollution prevention can be carried out upstream, ideally covered by the potential polluter. This is the preferred approach compared to dealing with non-economically feasible and less effective clean-up costs downstream, far away from the pollution source, where the contributions of various polluters becomes complex to identify from both a forensic and legal perspective. In this way, situations for tax payers clean-up and health-care costs for pollution they did not create are avoided.

However, if contamination of the sources of our drinking water with persistent and mobile substances does occur, enforcement of remediation action from the polluter are necessary. An example of this can be found in Bavaria, in which regulatory authorities are actively monitoring the presence of 1,4-dioxane. Based on the detected contamination, local industry and local authorities developed strategies to ensure the presence in drinking water is reduced (Körner, 2018). However, such collaborations are most effectively undertaken before the contamination takes place, rather than after it has occurred. In this manner, local authorities, water suppliers and producers of drinking water should also attempt to request a PMT/vPvM assessment of those chemicals that are used in their water catchment area or are already detected in the water bodies.

## 14.3 European Commission, ECHA and Member States

European Commission, ECHA and Member States have several regulatory options that could be used in order to protect the sources of our drinking water. The current Drinking Water Directive or Water Framework Directive could be extended in order to include individual PMT/vPvM substances or to set a general concentration limit. Likewise, the voluntary watch list of the Groundwater Directive could be used as a tool to detect PMT/vPvM substances and close the monitoring data gap. However, these types of regulatory tools only apply once a contamination and thus a risk has been established. Therefore, options to encourage pre-emptory, voluntary measures by industry to minimize emissions into the environment to effectively protect the sources of our drinking water should be favoured.

It should be discussed if persistent and mobile substances - if not classifiable as hazardous to the aquatic environment - are a case for a classification as Aquatic Chronic 4, H 413 under the CLP regulation (Regulation (EC) No 1272/2008) which are defined in Annex I as "*cases when data do not allow classification under the above criteria but there are nevertheless some grounds for concern*". This would, even in the absence of other classifiable hazard properties, trigger the obligations for classified substances, e.g. with regard to exposure assessment according to REACH Article 14(4). Further, new hazard classes for P, vP, B, vB, M and vM could be implemented separately in Annex I of the CLP regulation. This would permit the combination of these separate new hazard classes to identify PBT, vPvB, PMT, and vPvM substances in a harmonised and hazard-based fashion.

Under REACH there are many possibilities to implement the PMT/vPvM criteria and to establish a PMT/vPvM assessment. One option would be that Annex I could call for the assessment of PMT/vPvM within the registration dossiers and e.g. the determination of $K_{oc}$ could be required at a low tonnage level. Article 14(4) could also include PMT/vPvM substances and ask for an exposure assessment and a risk characterisation. Further, ECHA's REACH guidance documents could be amended to incorporate a PMT/vPvM assessment.

Another option would be to identify PMT/vPvM substances as substances of very high concern (SVHC) following Article 57. Consequently, Article 57 and Annex XIII could be expanded in order to include the PMT/vPvM criteria. On the other hand, the hazard caused by PBT/vPvB substances is comparable (chapter 8) to the hazard caused by PMT/vPvM substance and they are already now relevant for consideration under Article 57 (f), to demonstrate "*scientific evidence of probable serious effects to human health or the environment which give rise to an equivalent level of concern*".

Restrictions may apply to PMT/vPvM substances without or sequenced to an identification as SVHC. Further, Article 68(2) could be amended to allow fast-track restriction for PMT/vPvM substances for consumer uses.

As reflected in the Preamble, the implementation of the PMT/vPvM criteria is complementary to the underlying principles of REACH and the UN Sustainable Development Goals centred on the realisation of human rights, protection of human health and ensuring a sustainable future.

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# A Studies considered in literature review

**Table A1 Studies considered in this literature review of drinking water (DW) and groundwater (GW) contaminants.**

Source: Arp and Hale (2019)

| 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 | International | 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 byproducts | Europe | Berg et al. (2000) |
| W | DW | disinfection byproducts | Europe | Zahn et al. )2016) |
| X | DW | Various | Europe | Umweltbundesamt (2018) |
| Y | DW&GW | Sucralose | International | Tollefsen et al. (2012) |

# B Other Substances detected in drinking water and groundwater

**Table B1 List of substances detected in drinking water and groundwater that are not REACH registered substances (as of May 2017).**

The Study ID refers to Appendix Table A1. Source: Arp and Hale (2019)

| 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 | | X |
| 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 | | X |
| 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 |

| CAS | Name | Common Usage | Max. conc. (ng/L) in DW | Max. conc. (ng/L) in GW | Study ID |
|---|---|---|---|---|---|
| 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 |
| 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 |

| CAS | Name | Common Usage | Max. conc. (ng/L) in DW | Max. conc. (ng/L) in GW | Study ID |
|---|---|---|---|---|---|
| 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 | | X |
| 519-65-3 | AMDOPH | pharm. | detected | | X |
| 479-92-5 | 4-Isopropylantipyrine | pharm. | detected | | X |
| 58955-94-5 | 10,11-Dihydroxy-10,11–dihydrocarbamazepine | pharm. | detected | | X |
| 141-83-3 | Guanylurea | pharm. | detected | | X |
| 50-06-6 | Phenobarbital | pharm. | detected | | X |
| 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 |
| 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 |

| CAS | Name | Common Usage | Max. conc. (ng/L) in DW | Max. conc. (ng/L) in GW | Study ID |
|---|---|---|---|---|---|
| 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-metabolite | 190000 | | H |
| 30125-63-4 | Desethylterbutylazine | 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 | | X |
| 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 |

| CAS | Name | Common Usage | Max. conc. (ng/L) in DW | Max. conc. (ng/L) in GW | Study ID |
|---|---|---|---|---|---|
| 10595-95-6 | N-nitrosomethylethylamine | various | 5 | | H |
| 930-55-2 | N-nitrosopyrrolidine | various | 24 | | H |
| 1066-42-8 | Dimethylsilandiol (DMSD) | various | detected | | X |
| 142-68-7 | Tetrahydropyran | various | detected | | X |
| 126-54-5 | 2,4,8,10-Tetraoxaspiro[5.5]undecan (TOSU) | various | detected | | X |

# C PMT/vPvM assessment of REACH registered substances detected in drinking water and groundwater

To assess persistency, substances of very high concern (SVHC) that are on the Candidate List because they met the PBT/vPvB criteria, or which are appearing in the Stockholm Convention's list of Persistent Organic Pollutants (i.e. present on annex I of the Regulation EC 850/200), were assigned P or vP, as appropriate. Existing P assessments based on weight-of-evidence assessments from Berger et al. (Berger et al., 2018) were also employed directly. Further weight-of-evidence assessment for remaining substances was performed using available half-life data (OECD 307, 308, 309 or equivalents) and screening tests (OECD 301, 310, 302b+c) available through eChemPortal (https://echemportal.org/. accessed November 20, 2017); and additionally using the following QSARs: the QSAR Toolbox (v4.1) P predictor (www.qsartoolbox.org); the BIOWIN screening approach as recommended in the PBT guideline (ECHA, 2017); the Arnot-BIOWIN approach for estimating half-lives (Arnot et al., 2005); and a recently developed "IFS QSAR" (Arp et al., 2017). Finally, a confidential database on conclusions on P by ECHA (entitled "Pro.S.P. 2014", which has not been updated since 2014) was also considered within the weight-of-evidence assessment. The P conclusions within the REACH dossiers were considered with some scepticism, as these were found to vary widely in their reliability, and across multiple dossier entries for a specific substance; therefore, the half-life data, screening tests, and other relevant information needed to assess P was used to re-evaluate P, rather than simply accepting the conclusions made within the dossiers. The estimated half-lives presented in Appendix Table C1 represent biodegradation rates (Arnot et al., 2005), which are considered accurate within a factor 10 (Arp et al., 2017), therefore outcomes of 4 days can be considered potentially persistent (Arp et al., 2017).

To assess mobility, experimental data was given highest priority in this assessment. The main sources were Arp et al. (Arp et al., 2017) and the eChemPortal database (accessed November 2017). It is noted that assessing the lowest log $D_{ow}$ at environmentally relevant pH range of 4-9 requires both $K_{ow}$ and pKa values; these were also mainly obtained from Arp et al. (Arp et al., 2017) and the eChemPortal database (accessed November 2017).

Sources for the $K_{oc}$ data are REACH registered values from the eChemPortal database available from ECHA and OECD (http://www.echemportal.org), accessed February 2018 as a first priority. Otherwise, values calculated from the use of poly-parameter linear free energy relationships were used, provided experimental sorbent descriptors were available (Bronner and Goss, 2010; Ulrich et al., 2018). For more information see (Arp and Hale, 2019).

When no experimental data was available, QSAR predictions for log $D_{ow}$ were performed using ADMET Predictor 7.1 software by Simulations-plus (http://www.simulationsplus.com) primarily, and ChemAxon (https://www.chemaxon.com) (October 2017 version) as a backup.

To assess toxicity, the C&L registry as of October 06, 2017 was used (https://echa.europa.eu/information-on-chemicals/cl-inventory-database). NOEC/$EC_{10}$ values were obtained from the eChemPortal database (November 9th, 2017), DNEL values were obtained directly from REACH registration dossiers, as accessed via IUCLID 6 (January 11th, 2017), and *suspected* endocrine disruption were obtained from a 2014 evaluation from ECHA (Pro.S.P., 2014) and SIN List provided by ChemSec (January 10'th, 2019). When multiple NOEC/$EC_{10}$ or DNEL values were found for one substance, the lowest was chosen by default.

**Table C1 PMT/vPvM assessment of REACH registered substances (as of May 2017) that have been reported in at least one study as detected in groundwater (GW) or drinking water (DW).**

The Study ID refers to Appendix Table A1. Source: modified from Arp and Hale (2019)

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| vPvM & PMT | 108-78-1 | melamine | 100000 - 1000000 | 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<br>STOTRE_2 | DW | det. | E; F |
| vPvM & PMT | 80-08-0 | Dapsone | 100 - 1000 | 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<br>STOTRE_2<br>Suspected ED | DW | det. | F |
| vPvM & PMT | 127-18-4 | Tetrachloroethene | 100000 - 1000000 | vP | No significant biodegradation in 301 C tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018) | vM | exp min. log Doc/Koc = 2.2 (neutral cmpd.) | T | Carc_1b<br>Carc_2 Rep_2<br>STOTRE_2<br>Suspected ED | DW | 180 | G; H; J |
| vPvM & PMT | 330-54-1 | Diuron | 100 - 1000 | vP | measured half life = 2 241 d (soil) | vM | exp min. log Doc/Koc = 2.1 (neutral cmpd.) | T | ecotox Carc_2<br>STOTRE_2<br>Suspected ED | DW&GW | 2.1 | A; E; H; Q; S |
| vPvM & PMT | 56773-42-3 | PFOS | 0 - 10 | vP | on SVHC list - vPvB substance | vM | exp min. log Doc/Koc = 0.0 (single_anion cmpd.) | T | SVHC | DW&GW | 0.14 | A; E; H; I; L; S |
| vPvM & PMT | 62037-80-3 | GenX | 10 - 100 | vP | All biodegradation results in 301B and 302C imply 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 | DW | 0.011 | M |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| vPvM & PMT | 127-18-4 | Perchloroethene | 100000 - 1000000 | vP | No significant biodegradation in 301 C tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018) | vM | exp min. log Doc/Koc = 2.2 (neutral cmpd.) | T | Carc_1b<br>Carc_2 Rep_2<br>STOTRE_2<br>Suspected ED | GW | 10 | O |
| vPvM | 95-50-1 | 1,2-Dichlorobenzene | 10000 - 100000 | vP | measured half life = 191 d (soil) | vM | exp min. log Doc/Koc = 2.7 (neutral cmpd.) | Tscreen | Cramer Class III | DW&GW | 10 | H; O |
| PMT | 3622-84-2 | n-Butylbenzenesulphonamide | 1000 - 10000 | vP | measured half life = 1 011 d (fresh water) | M/vM | exp min. log Dow/Kow = 2.0, M or vM unclear due to data uncertainty (ionizable cmpd.) | T | STOTRE_2 | DW | 0.1 | S |
| PMT | 79-01-6 | Trichloroethene | 10000 - 100000;<br>0 - 10 | P | No significant biodegradation in 301C and D tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018) | vM | exp min. log Doc/Koc = 2.2 (neutral cmpd.) | T | SVHC | DW&GW | 21.6 | G; H; O; S |
| PMT | 123-91-1 | 1,4-dioxane | 1000+ | P | No significant biodegradation in 301F test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018) | vM | exp min. log Doc/Koc = -0.5 (neutral cmpd.) | T | Carc_2<br>STOTRE_1<br>STOTRE_2 | DW | 0.6 | E; S; T |
| PMT | 288-88-0 | 1,2,4-triazole | 1000 - 10000 | 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 | DW | det. | E |
| PMT | 834-12-8 | Ametryn | 1000 - 10000 | P | measured half life = 143 d (soil) | vM | exp min. log Doc/Koc = 1.8 (ionizable cmpd.) | T | ecotox | DW&GW | det. | H |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PMT | 126-86-3 | Surfynol 104 | 1000+ | 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 | DW | 0.2 | N |
| PMT | 107-06-2 | 1,2-Dichloroethane | 1000000 - 10000000 | P | Due to lack of other information the substance was assessed by PBT assessment in water. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018) | vM | exp min. log Doc/Koc = 1.1 (neutral cmpd.) | T | SVHC | DW&GW | 81.9 | H; O |
| PMT | 120-12-7 | Anthracene | Intermediate Use Only | P | On SVHC list - PBT substance | M | exp min. log Doc/Koc = 3.6 (neutral cmpd.) | T | SVHC | GW | det. | H |
| Pot. PM & vPvM | 13674-84-5 | TCPP | 0 - 10;<br>0 - 10 | 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/vM | QSAR min. log Dow/Kow = 2.9, M or vM unclear due to data uncertainty(neutral cmpd.) | Tscreen | Cramer Class III | DW | 0.5 | E; F; K |
| Pot. PM & vPvM | 76-05-1 | Trifluoroacetatic acid | 1000 - 10000 | P/vP | est. t1/2 = 20d, weight-of-evidence based on 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.) | Tscreen | Cramer Class III | DW | 0.2 | E; U; V |
| Pot. PMT | 137862-53-4 | Valsartan acid | Intermediate Use Only | P/vP | est. 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 products, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test) | M/vM | exp min. log Dow/Kow = 1.2, M or vM unclear due to data uncertainty (ionizable cmpd.) | T | Rep_1a Rep_2 | DW | det. | E |
| Pot. PMT & vPvM | 140-01-2 | Pentasodium (carboxylatomethyl)imi | 10000 - 100000 | P/vP | est. t1/2 = 8d, weight-of-evidence based on QSARs and no biodeg. | vM | QSAR min. log Dow/Kow = -15.6 | T | Rep_1a Rep_2<br>STOTRE_2 | DW | det. | E |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | Detected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | nobis(ethylenenitrilo)tetraacetate | | | observed in majority of biodegradation screen tests e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test),301 B (Ready Biodegradability: CO2 Evolution Test) | | (multiple_anion cmpd.) | | | | | |
| Pot. PMT | 15307-86-5 | Diclofenac | Intermediate Use Only | P/vP | est. t1/2 = 99d, weight-of-evidence based on consistent indications of P across tested QSARs | M | exp min. log Doc/Koc = 3.8 (ionizable cmpd.) | T | Lact Rep_2 STOTRE_1 | DW&GW | 0.6 | A; B; D; H; R |
| Pot. PMT & vPvM | 288-13-1 | Pyrazole | Intermediate Use Only | P/vP | est. t1/2 = 13d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Dow/Kow = 0.3 (ionizable cmpd.) | T | Rep_2 STOTRE_1 | DW | det. | E |
| Pot. PM & vPvM | 461-58-5 | Cyanoguanidine | 10000 - 100000 | 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.) | Tscreen | Cramer Class III | DW | det. | F |
| Pot. PMT & vPvM | 60-00-4 | EDTA | 1000 - 10000 | P/vP | est. t1/2 = 6d, weight-of-evidence based on QSARs and no biodeg. observed in majority of biodegradation 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 | DW&GW | 13.6 | B; E; S |
| Pot. PMT & vPvM | 67-43-6 | N-carboxymethyliminobis(ethylenenitrilo)tetra(acetic acid) | 100 - 1000 | P/vP | est. t1/2 = 8d, weight-of-evidence based on 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 = -8.8 (ionizable cmpd.) | T | Rep_2 STOTRE_2 | DW&GW | 9 | B; S; E |
| Pot. PMT & vPvM | 100-02-7 | Nitrophenol | Intermediate Use Only | P/vP | est. t1/2 = 31d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = -1.4 (ionizable cmpd.) | T | STOTRE_2 Suspected ED | GW | 0.1 | A |
| Pot. PMT | 102-06-7 | 1,3-diphenylguanidine | 1000 - 10000 | P/vP | est. t1/2 = 68d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority | M/vM | exp min. log Dow/Kow = 1.4, M or vM unclear | T | Rep_2 | DW | det. | F |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | of biodegradation screen tests for substance/main transformation products, e.g. 301 D (Ready Biodegradability: Closed Bottle Test) | | due to data uncertainty (ionizable cmpd.) | | | | | |
| Pot. PMT & vPvM | 114-07-8 | Erythromycin | Intermediate Use Only | P/vP | est. t1/2 = 768d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = 0.1 (ionizable cmpd.) | T | Rep_2 | GW | 1 | B |
| Pot. PMT & vPvM | 115-96-8 | TCEP | 0 - 10 | P/vP | est. t1/2 = 35d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 0.7 (neutral cmpd.) | T | SVHC | DW&GW | 0.7 | D; E; J; K |
| Pot. PM & vPvM | 117-96-4 | Diatrizoic acid | Intermediate Use Only | P/vP | est. t1/2 = 797d, weight-of-evidence based on consistent indications of P across tested QSARs | M/vM | QSAR min. log Dow/Kow = 1.1, M or vM unclear due to data uncertainty (ionizable cmpd.) | Tscreen | Cramer Class III | DW&GW | 1.2 | B; S; R |
| Pot. PMT & vPvM | 121-57-3 | Sulfanilic acid | 1000 - 10000 | P/vP | est. t1/2 = 44d, and consistency across all tested QSARs | vM | QSAR min. log Dow/Kow = -1.9 (ionizable cmpd.) | T | Suspected ED | DW | det. | F |
| Pot. PMT | 13674-87-8 | TDIP | 1000 - 10000 | P/vP | est. 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 products, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II)) | M | exp min. log Doc/Koc = 3.7 (neutral cmpd.) | T | Carc_2<br>STOTRE_2 | DW | 0.5 | H:J |
| Pot. PMT & vPvM | 139-40-2 | Propazine | Intermediate Use Only | P/vP | est. t1/2 = 186d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 1.8 (neutral cmpd.) | T | Carc_2<br>Suspected ED | DW&GW | 0 | A; H; Q |
| Pot. PMT & vPvM | 143-24-8 | Tetraglyme | 100+ | P/vP | est. t1/2 = 83d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Dow/Kow = -0.8 (neutral cmpd.) | T | Rep_1b | DW | det. | E |
| Pot. PM & vPvM | 1493-13-6 | Trifluoromethansulfonic acid | 100 - 1000 | P/vP | est. t1/2 = 39d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority | vM | exp min. log Dow/Kow = 0.3 (neutral cmpd.) | Tscreen | Cramer Class III | DW | 1 | F; W |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | Detected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | of biodegradation screen tests for substance/main transformation products, e.g. 301 D (Ready Biodegradability: Closed Bottle Test) | | | | | | | |
| Pot. PM & vPvM | 15214-89-8 | 2-acrylamido-2-methylpropanesulphonic acid | 1000 - 10000 | 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.) | Tscreen | Cramer Class III | DW | det. | F |
| Pot. PMT & vPvM | 15687-27-1 | Ibuprofen | Intermediate Use Only | P/vP | est. t1/2 = 18d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 2.5 (neutral cmpd.) | T | Rep_1b<br>Rep_2<br>STOTRE_2 | DW&GW | 12 | A; B; C; D; N; R |
| Pot. PMT & vPvM | 1634-04-4 | MTBE | 1000000 - 10000000 | 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 (neutral cmpd.) | T | Suspected ED | DW | 57.8 | E; H; O; S |
| Pot. PMT & vPvM | 1912-24-9 | Atrazine | Intermediate Use Only | P/vP | est. t1/2 = 153d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 1.5 (neutral cmpd.) | T | STOTRE_2<br>Suspected ED | DW&GW | 3.5 | A; E; H; K; Q |
| Pot. PM & vPvM | 21145-77-7 | AHTN | 0 - 10 | P/vP | est. t1/2 = 74d, weight-of-evidence based on consistent indications of P across tested QSARs | M | exp min. log Doc/Koc = 3.4 (neutral cmpd.) | Not T | - | DW | 0.1 | J |
| Pot. PMT & vPvM | 3380-34-5 | Triclosan | 10 - 100 | P/vP | The P conclusion of triclosan remains controversial, with P assessment still under development. | vM | exp min. log Doc/Koc = 0.9 (ionizable cmpd.) | T | ecotox<br>Suspected ED | DW&GW | 2.1 | A; D; K; N; R |
| Pot. PMT & vPvM | 51-28-5 | 2,4-Dinitrophenol | 100 - 1000 | 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 evident in monitoring studies (UBA, 2019), there were consistent indications of P across tested QSARs, and this substances was also considered prioritized by Nödler et al. | vM | exp min. log Doc/Koc = -3.4 (ionizable cmpd.) | T | muta_2<br>Rep_2<br>STOTRE_1<br>STOTRE_2<br>DNEL<br>Suspected ED | DW&GW | 333 | A; H |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pot. PMT & vPvM | 56-93-9 | Benzyltrimethyl ammonium | 100 - 1000 | P/vP | est. 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 | DW | det. | F |
| Pot. PMT | 57-83-0 | progesterone | Intermediate Use Only | P/vP | est. t1/2 = 78d, and consistency across all tested QSARs | M | exp min. log Dow/Kow = 3.7 (neutral cmpd.) | T | Carc_1b<br>Carc_2 Lact<br>muta_1b<br>muta_2<br>Rep_1a<br>Rep_1b<br>Rep_2<br>Suspected ED | DW&GW | 0.1 | B; H; K |
| Pot. PMT & vPvM | 67-66-3 | Chloroform | 100000 - 1000000 | P/vP | est. t1/2 = 45d, weight-of-evidence based on 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<br>muta_2<br>Rep_2<br>STOTRE_1<br>STOTRE_2 | DW&GW | 34.6 | H; O; P |
| Pot. PMT & vPvM | 71-55-6 | Trichloroethane, 1,1,1- | Intermediate Use Only | P/vP | est. t1/2 = 65d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 1.7 (neutral cmpd.) | T | Carc_1b<br>Carc_2<br>STOTRE_2 | DW&GW | 10 | O |
| Pot. PMT & vPvM | 80-09-1 | Bisphenol S | 1000 - 10000 | P/vP | The 301C test indicates non readily biodegradable; however, based on readacross with BPA, the likelihood this meets the P requirement are low. | vM | exp min. log Doc/Koc = -0.3 (ionizable cmpd.) | T | Suspected ED | DW | det. | F |
| Pot. PM & vPvM | 826-36-8 | vincubine | Intermediate Use Only | P/vP | est. t1/2 = 32d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = -3.3 (ionizable cmpd.) | Tscreen | Cramer Class III | DW | det. | E |
| Pot. PMT & vPvM | 95-14-7 | benzotriazoles | 1000 - 10000 | P/vP | est. t1/2 = 18d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority | vM | exp min. log Doc/Koc = 1.5 (ionizable cmpd.) | T | muta_2 | DW&GW | 1.5 | A; B; E; S |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | Detected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | of biodegradation screen tests for substance/main transformation products, e.g. 301 D (Ready Biodegradability: Closed Bottle Test) | | | | | | | |
| Pot. PMT & vPvM | 97-39-2 | 1,3-di-o-tolylguanidine | 100 - 1000 | P/vP | est. 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 products, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I)) | vM | exp min. log Dow/Kow = -3.0 (ionizable cmpd.) | T | Carc_1b<br>Rep_2 | DW | det. | F |
| Pot. PM & vPvM | 83-32-9 | Acenaphthene | Intermediate Use Only | P/vP | est. t1/2 = 28d, weight-of-evidence based on consistent indications of P across tested QSARs | M | exp min. log Doc/Koc = 3.3 (neutral cmpd.) | Tscreen | Cramer Class III | GW | det. | H |
| Pot. PM & vPvM | 29420-49-3 | PFBS - Potassium 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulphonate | Intermediate Use Only | P/vP | est. t1/2 = 327d, weight-of-evidence based on 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 | QSAR Dow/Kow = -1.0 (ionizable cmpd.) | Tscreen | Cramer Class III | DW&GW | 0.03 | A; H; I; L; M |
| Pot. PMT & vPvM | 152459-95-5 | Imatinib | Intermediate Use Only | P/vP | est. t1/2 = 881d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = -0.7 (ionizable cmpd.) | T | Carc_2<br>muta_2<br>Rep_1b<br>Rep_2<br>STOTRE_2 | GW | 0.1 | B |
| Pot. PMT | 76-74-4 | Pentobarbital | Intermediate Use Only | P/vP | est. t1/2 = 45d, weight-of-evidence based on consistent indications of P across tested QSARs | M/vM | QSAR min. log Dow/Kow = 1.1, M or vM unclear due to data uncertainty(ionizable cmpd.) | T | Rep_2 | GW | 1 | B |
| Pot. PMT & vPvM | 93413-69-5 | Venlafaxine | Intermediate Use Only | P/vP | est. t1/2 = 83d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = 1.4 (ionizable cmpd.) | T | Lact Rep_1a | DW | 0 | L |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pot. PMT | 119-61-9 | benzophenone | 1000 - 10000 | P/vP | est. 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 C (Ready Biodegradability: Modified MITI Test (I)) | M | exp min. log Doc/Koc = 3.1 (neutral cmpd.) | T | Carc_2<br>STOTRE_2<br>Suspected ED | DW | 0.3 | N |
| Pot. PMT & vPvM | 78-87-5 | 1,2-Dichloropropane | 1000 - 10000 | P/vP | P data for this substance is variable and difficult to conclude; however, its identification in monitoring studies in DW and GW indicates it is persistent enough. | vM | exp min. log Doc/Koc = 1.3 (neutral cmpd.) | T | Carc_1b | DW&GW | 7.5 | H; O |
| Pot. PMT & vPvM | 106-93-4 | Ethylene dibromide | 1000 - 10000 | P/vP | est. t1/2 = 20d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 0.3 (neutral cmpd.) | T | Carc_1a<br>Carc_1b<br>Carc_2<br>Suspected ED | GW | 0.4 | O |
| Pot. PMT & vPvM | 96-18-4 | 1,2,3-Trichloropropane | 1000 - 10000 | P/vP | P data for this substance is variable and difficult to conclude; however, its identification in monitoring studies in DW and GW indicates it is persistent enough. | vM | exp min. log Doc/Koc = 1.9 (neutral cmpd.) | T | SVHC | GW | 3 | O |
| Pot. PMT & vPvM | 98-82-8 | Isopropylbenzene | 1000000 - 10000000 | P/vP | Initial evidnce suggests this si not P under aerobic 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 (neutral cmpd.) | T | STOTRE_1 | DW&GW | 3 | H; O |
| Pot. PMT & vPvM | 91-20-3 | Naphthalene | 100000 - 1000000 | P/vP | Data indicates certain conditions where Naphthalene is persistent, but no definitive conclusion 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 (neutral cmpd.) | T | Carc_2<br>STOTRE_1 | DW&GW | 3 | H; O; P |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pot. PMT & vPvM | 108-20-3 | Diisopropyl ether | 1000 - 10000 | P/vP | est. 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 products, e.g. 301 D (Ready Biodegradability: Closed Bottle Test) | vM | exp min. log Doc/Koc = 0.6 (neutral cmpd.) | T | Rep_2 | GW | 10 | O |
| Pot. PMT & vPvM | 75-35-4 | 1,1-Dichloroethene | 10000 - 100000 | P/vP | est. t1/2 = 28d, weight-of-evidence based on 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 = 1.4 (neutral cmpd.) | T | Carc_1b<br>Carc_2<br>STOTRE_1<br>STOTRE_2 | GW | 10 | O |
| Pot. PM & vPvM | 75-71-8 | Dichlorodifluoromethane | 100 - 1000 | P/vP | est. t1/2 = 44d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 1.0 (neutral cmpd.) | Tscreen | Cramer Class III | GW | 7.5 | O |
| Pot. PMT & vPvM | 56-23-5 | Carbon tetrachloride | 1000 - 10000 | P/vP | est. t1/2 = 97d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 1.9 (neutral cmpd.) | T | Carc_1b<br>Carc_2 Rep_2<br>STOTRE_1<br>STOTRE_2 | DW&GW | 3 | H; O |
| Pot. PMT & vPvM | 108-90-7 | Chlorobenzene | 10000 - 100000 | P/vP | est. t1/2 = 23d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 2.4 (neutral cmpd.) | T | Carc_1a<br>muta_1b<br>Rep_2<br>STOTRE_1 | GW | 7.5 | O |
| Pot. PMT & vPvM | 74-87-3 | Chloromethane | 1000000 - 10000000 | P/vP | est. t1/2 = 16d, weight-of-evidence based on 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 (neutral cmpd.) | T | Carc_2 Rep_2<br>STOTRE_2 | GW | 10 | O |
| Pot. PMT & vPvM | 144-83-2 | Sulfapyridine | Intermediate Use Only | P/vP | est. t1/2 = 88d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = 0.5 (ionizable cmpd.) | T | Rep_2<br>Suspected ED | GW | 0.1 | Q |
| Pot. PMT & vPvM | 18559-94-9 | Salbutamol | Intermediate Use Only | P/vP | est. t1/2 = 13d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority | vM | QSAR min. log Dow/Kow = -0.6 (ionizable cmpd.) | T | Suspected ED | GW | 0.009 | Q |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
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| | | | | | of biodegradation screen tests for substance/main transformation products, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test) | | | | | | | |
| Pot. PMT & vPvM | 50-48-6 | Amitryptilline | Intermediate Use Only | P/vP | est. t1/2 = 100d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = -1.3 (ionizable cmpd.) | T | Rep_2 | DW | 0.001 | R |
| Pot. PMT | 95-16-9 | Benzothiazole | 10 - 100 | P/vP | est. 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 products, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test) (1992) | M/vM | exp min. log Dow/Kow = 2.0 M or vM unclear due to data uncertainty (ionizable cmpd.) | T | STOTRE_2 | DW | 0.010 | S |
| Pot. PMT & vPvM | 111-96-6 | Diethylene glycol dimethyl ether | 100 - 1000 | P/vP | est. 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 products, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test) | vM | exp min. log Dow/Kow = -0.4 (neutral cmpd.) | T | SVHC | DW | 0.2 | S |
| Pot. PM & vPvM | 66108-95-0 | Iohexol | Intermediate Use Only | P/vP | est. t1/2 = 224d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = -2.5 (neutral cmpd.) | Tscreen | Cramer Class III | DW | 11.1 | H; S |
| Pot. PM & vPvM | 791-28-6 | Triphenyl phosphorus oxide | Intermediate Use Only | P/vP | est. t1/2 = 31d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 3.0 (neutral cmpd.) | Tscreen | Cramer Class III | DW | 0.1 | S |
| Pot. PM & vPvM | 1506-02-1 | AHTN | 1000 - 10000 | P/vP | est. t1/2 = 74d, weight-of-evidence based on consistent indications of P across tested QSARs | M | exp min. log Doc/Koc = 3.4 (neutral cmpd.) | Not T | - | DW | 0 | H |
| Pot. PM & vPvM | 74-95-3 | Dibromomethane | Intermediate Use Only | P/vP | est. t1/2 = 20d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 1.3 (neutral cmpd.) | Tscreen | Cramer Class III | DW | 0.7 | H |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pot. PMT & vPvM | 541-73-1 | Dichlorbenzene, 1,3- | 1000 - 10000 | P/vP | est. 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 products, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I)) | vM | exp min. log Doc/Koc = 2.6 (neutral cmpd.) | T | STOTRE_2<br>Suspected ED | DW | 0.1 | H |
| Pot. PMT & vPvM | 98-95-3 | Nitrobenzene | Intermediate Use Only | P/vP | est. 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 products, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test) | vM | exp min. log Doc/Koc = 1.7 (neutral cmpd.) | T | SVHC | DW | 100 | H |
| Pot. PMT | 131-57-7 | Oxybezone | 100 - 1000 | P/vP | est. t1/2 = 16d, weight-of-evidence based on consistent indications of P across tested QSARs | M | exp min. log Dow/Kow = 3.6 (neutral cmpd.) | T | STOTRE_2<br>Suspected ED | DW | det. | H |
| Pot. PMT & vPvM | 121-82-4 | RDX | 1000 - 10000 | P/vP | est. t1/2 = 33d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Dow/Kow = 0.9 (neutral cmpd.) | T | STOTRE_1<br>STOTRE_2 | DW | 1.1 | H |
| Pot. PM & vPvM | 87-61-6 | Trichlorobenzene, 1,2,3- | Intermediate Use Only | P/vP | est. t1/2 = 88d, 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 = 2.9 (neutral cmpd.) | Tscreen | Cramer Class III | DW | 0.2 | H |
| Pot. PMT | 120-82-1 | Trichlorobenzene, 1,2,4- | Intermediate Use Only | P/vP | est. t1/2 = 88d, weight-of-evidence based on consistent indications of P across tested QSARs | M | exp min. log Doc/Koc = 3.4 (neutral cmpd.) | T | Suspected ED | DW | 0.9 | H |
| Pot. PMT & vPvM | 79-00-5 | Trichlorethane, 1,1,2- | Intermediate Use Only | P/vP | est. t1/2 = 47d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 1.7 (neutral cmpd.) | T | Carc_1b<br>Carc_2 | DW | 0.1 | H |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | Detected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pot. PM & vPvM | 78-51-3 | (2-butoxyethyl)phosphate | 1000 - 10000 | P/vP | est. t1/2 = 10d, weight-of-evidence based on QSARs and no biodeg. observed in majority of biodegradation screen tests e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II)) | vM | exp min. log Doc/Koc = 2.5 (neutral cmpd.) | Tscreen | Cramer Class III | DW | 0.4 | H |
| Pot. PM & vPvM | 85-98-3 | 1,3-diethyldiphenylurea | 100 - 1000 | P/vP | est. t1/2 = 31d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 2.5 (neutral cmpd.) | Tscreen | Cramer Class III | DW | det. | X |
| Pot. PM & vPvM | 96-76-4 | 2,4-Di-tertiary-butylphenol | 100 - 1000 | P/vP | est. 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 products, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II)) | not M | exp min. log Dow/Kow = 4.8 (neutral cmpd.) | T | STOTRE_2 Suspected ED | DW | det. | X |
| Pot. PM & vPvM | 144689-24-7 | Olmesartan | Intermediate Use Only | P/vP | est. t1/2 = 112d, weight-of-evidence based on consistent indications of P across tested QSARs | M/vM | QSAR min. log Dow/Kow = 1.5. M or vM unclear due to data uncertainty (ionizable cmpd.) | Tscreen | Cramer Class III | DW | det. | X |
| not PMT | 1222-05-5 | Galaxolide | 1000 - 10000 | vP | measured half life = 203 d (soil) | not M | exp min. log Doc/Koc = 4.3 (neutral cmpd.) | T | Rep_2 | DW&GW | 23 | D; H; Q |
| not PMT | 140-66-9 | tert-Octylphenol | 10000 - 100000 | P | measured half life = 49 d (fresh water) | not M | exp min. log Doc/Koc = 4.0 (neutral cmpd.) | T | SVHC | GW | 1.8 | A; Q |
| not PMT | 80-05-7 | Bisphenol A | 1000000 - 10000000 | not P | inherently biodeg: 302 A (Inherent Biodegradability: Modified SCAS Test) | vM | exp min. log Doc/Koc = 2.3 (ionizable cmpd.) | T | SVHC | DW&GW | 9.3 | A; B; D; H; J; K; Q |
| not PMT | 117-81-7 | DEHP | 10000 - 100000 | P | measured half life = 176 d (soil) | not M | exp min. log Doc/Koc = 5.7 (neutral cmpd.) | T | SVHC | DW&GW | 5.7 | N; Q |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| not PMT | 106-46-7 | 1,4-Dichlorobenzene | 10000 - 100000 | not P | readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test) | vM | exp min. log Doc/Koc = 2.4 (neutral cmpd.) | T | Carc_2 | GW | 10 | O |
| not PMT | 50-78-2 | Acetylsalicylic acid | 100 - 1000 | not P | est. t1/2 = 7d, and consistency across all tested QSARs | vM | exp min. log Doc/Koc = -5.7 (ionizable cmpd.) | T | Rep_1a<br>Rep_1b<br>Rep_2<br>STOTRE_2 | GW | 0.1 | B; S |
| not PMT | 139-13-9 | NTA | 100 - 1000;<br>0 - 10 | 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<br>muta_1b<br>STOTRE_2 | GW | det. | H |
| not PMT | 126-73-8 | TBP | 1000 - 10000;<br>0 - 10 | 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<br>STOTRE_2 | DW | 0.2 | J |
| not PMT | 77-93-0 | Triethyl citrate | 1000 - 10000;<br>100 - 1000 | not P | readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test) | vM | exp min. log Dow/Kow = 0.7 (neutral cmpd.) | T | Carc_1b<br>muta_1b | DW | 0.1 | H; J |
| not PMT | 102-76-1 | Triacetin | 10000 - 100000 | not P | readily biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test) | vM | QSAR min. log Dow/Kow = 0.1 (neutral cmpd.) | Not T | - | DW | det. | E |
| not PMT | 105-60-2 | e-caprolactam | 1000000 - 10000000 | 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 | DW | det. | F |
| not PMT | 120-18-3 | Naphthalenesulfonic acid | 1000 - 10000 | 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 | DW | det. | F |
| not PMT | 128-37-0 | Butylhydroxytoluene | 10000 - 100000 | P/vP | est. 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 products, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I)) | not M | exp min. log Doc/Koc = 4.4 (neutral cmpd.) | T | Carc_1b<br>Carc_2<br>muta_1b<br>muta_2<br>Rep_2<br>STOTRE_2 | DW | 0.03 | K; H |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| not PMT | 128-44-9 | Saccharine | 1000 - 10000 | 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<br>Carc_1b<br>Carc_2 | DW | det. | F |
| not PMT | 129-00-0 | Pyrene | Intermediate Use Only | P/vP | est. t1/2 = 139d, weight-of-evidence based on consistent indications of P across tested QSARs | not M | exp min. log Doc/Koc = 4.1 (neutral cmpd.) | T | ecotox | GW | det. | H |
| not PMT | 25321-41-9 | Dimethylbenzene sulfonic acid | 1000 - 10000 | 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 | - | DW | det. | F |
| not PMT | 50-28-2 | 17b-Estradiol | Intermediate Use Only | not P | readily biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test) | M | QSAR min. log Dow/Kow = 3.9 (neutral cmpd.) | T | ecotox<br>Carc_1a<br>Carc_1b<br>Carc_2 Lact<br>Rep_1a<br>Rep_1b<br>Rep_2<br>STOTRE_1<br>STOTRE_2<br>Suspected ED | DW&GW | 0.1 | D; H |
| not PMT | 58-08-2 | Caffeine | 100 - 1000 | 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 | - | DW&GW | 110 | A; B; C; D; H; J; L; Q; R |
| not PMT | 69-72-7 | Salicylic acid | 10000 - 100000 | 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<br>STOTRE_1 | GW | 1.2 | D; H |
| not PMT | 76-22-2 | Camphor | 100 - 1000 | not P | readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test) | vM | exp min. log Doc/Koc = 2.1 (neutral cmpd.) | T | muta_2<br>Rep_1a<br>STOTRE_2 | DW | 0.02 | H; J |
| not PMT | 53-16-7 | Estrone | 0 - 10;<br>0 - 10 | not P | inherently biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test) | M | exp min. log Dow/Kow = 2.6 (neutral cmpd.) | T | Carc_1a<br>Carc_1b<br>Carc_2 Lact<br>Rep_1a | GW | 0.05 | A; D |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | Rep_1b<br>Rep_2<br>Suspected ED | | | |
| not PMT | 7085-19-0 | Mecoprop | Intermediate Use Only | not P | longest measured half life all media = 50 d (sediment) | vM | exp min. log Dow/Kow = -4.2 (ionizable cmpd.) | Tscreen | Cramer Class III | DW&GW | 0.8 | A; E |
| not PMT | 63-05-8 | Androstenedione | 100 - 1000 | not P | readily biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test) | M | exp min. log Dow/Kow = 2.7 (neutral cmpd.) | T | Carc_1b<br>Carc_2 Lact<br>Rep_1a<br>Suspected ED | DW&GW | 0.1 | B; H |
| not PMT | 131-11-3 | Dimethyl phthalate | 1000 - 10000;<br>0 - 10 | 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<br>Suspected ED | DW | 0.5 | N |
| not PMT | 84-66-2 | Diethyl phthalate | 1000 - 10000;<br>0 - 10 | not P | est. t1/2 = 6d, and consistency across all tested QSARs | vM | exp min. log Doc/Koc = 2.4 (neutral cmpd.) | T | Rep_2<br>STOTRE_2<br>Suspected ED | DW | 2.5 | N; Q; S |
| not PMT | 84-74-2 | Dibutyl phthalate | 1000 - 10000 | not P | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | M | exp min. log Doc/Koc = 3.1 (neutral cmpd.) | T | SVHC | DW | 2.7 | N |
| not PMT | 85-68-7 | Butyl benzyl phthalate | 1000 - 10000 | 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 | DW | 0.9 | N |
| not PMT | 71-43-2 | Benzene | 1000000 - 10000000 | not P | readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test) | vM | exp min. log Doc/Koc = 1.4 (neutral cmpd.) | T | ecotox<br>Carc_1a<br>Carc_1b<br>muta_1a<br>muta_1b<br>STOTRE_1 | DW&GW | 25.8 | H; O; S |
| not PMT | 100-41-4 | Ethylbenzene | 1000000 - 10000000;<br>0 - 10 | 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<br>STOTRE_2 | DW&GW | 10 | H; O |
| not PMT | 108-88-3 | Toluene | 1000000 - 10000000 | 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<br>STOTRE_1<br>STOTRE_2 | DW&GW | 63.1 | H; O; P |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | Detected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| not PMT | 95-63-6 | 1,2,4-Trimethylbenzene | 10000 - 100000 | not P | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | M | exp min. log Doc/Koc = 3.0 (neutral cmpd.) | T | STOTRE_1 | DW&GW | 3 | H; O |
| not PMT | 95-47-6 | Total xylenes | 100000 - 1000000 | not P | readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test) | vM | exp min. log Doc/Koc = 2.7 (neutral cmpd.) | T | Rep_2 | DW&GW | 16.5 | H; O |
| not PMT | 98-86-2 | Acetophenone | 10000 - 100000 | not P | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | vM | exp min. log Doc/Koc = 1.5 (neutral cmpd.) | Not T | - | DW | 0.5 | H |
| not PMT | 84-65-1 | Anthraquinone | 1000 - 10000;<br>0 - 10 | not P | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | M | exp min. log Doc/Koc = 3.2 (neutral cmpd.) | T | Carc_2 | DW | 0.1 | H |
| not PMT | 75-09-2 | Dichloromethane | 100000 - 1000000;<br>0 - 10 | 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<br>muta_1a<br>muta_2<br>Rep_1a<br>STOTRE_1<br>STOTRE_2 | DW | 0.5 | H |
| not PMT | 100-42-5 | Styrene | 1000000 - 10000000;<br>0 - 10;<br>0 - 10 | not P | readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test) | vM | exp min. log Doc/Koc = 2.1 (neutral cmpd.) | T | SVHC | DW | 46.4 | H |
| not PMT | 107-07-3 | 2-Chlorethanol | 10 - 100 | 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<br>muta_1b<br>STOTRE_1 | DW | det. | X |
| not PMT | 70-55-3 | (4-Methylbenzolsulfonamid) | 0 - 10 | not P | readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test) | vM | QSAR min. log Dow/Kow = 0.6 (neutral cmpd.) | T | Rep_2 | DW | det. | X |
| no conclusion | 103-90-2 | Paracetamol | 10 - 100 | no conclusion | est. t1/2 = 11d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 0.0 (ionizable cmpd.) | T | Carc_2<br>muta_2<br>STOTRE_1<br>STOTRE_2 | DW&GW | 120 | B; C; D; H; J; Q; R |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | Detected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| no conclusion | 104-40-5 | Nonylphenol | 0 - 10 | no conclusion | est. t1/2 = 13d, weight-of-evidence based on consistent indications of P across tested QSARs | not M | QSAR min. log Dow/Kow = 6.1 (neutral cmpd.) | T | Rep_2, SVHC Endocrine disrupting properties Article 57f - environment | DW&GW | 84 | A; D; H; J; K; Q |
| no conclusion | 108-80-5 | Cyanuric acid | 10000 - 100000 | no conclusion | est. t1/2 = 20d, found 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 (neutral cmpd.) | Not T | - | DW | det. | F |
| no conclusion | 22204-53-1 | Naproxen | Intermediate Use Only | no conclusion | est. t1/2 = 12d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = -0.2 (ionizable cmpd.) | T | Carc_2 Lact<br>Rep_1b<br>Rep_2<br>STOTRE_2 | DW&GW | det. | H |
| no conclusion | 532-02-5 | Sodium naphthalene-2-sulphonate | 0 - 10 | no conclusion | est. t1/2 = 32d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = -1.5 (single_anion cmpd.) | Tscreen | Cramer Class III | DW | det. | E |
| no conclusion | 57-41-0 | Phenytoin | Intermediate Use Only | no conclusion | est. t1/2 = 43d, weight-of-evidence based on consistent indications of P across tested QSARs | M/vM | QSAR min. log Dow/Kow = 1.1 M or vM unclear due to data uncertainty (ionizable cmpd.) | T | Carc_1a<br>Carc_1b<br>Carc_2<br>muta_1b<br>Rep_1a<br>Rep_1b<br>STOTRE_1 | DW | 0.02 | H; K; R |
| no conclusion | 57-68-1 | Sulfamethazine | Intermediate Use Only | no conclusion | est. t1/2 = 83d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = -0.7 (ionizable cmpd.) | T | Lact Rep_2 | GW | 0.6 | C; D; H; Q |
| no conclusion | 60-80-0 | Phenazone | Intermediate Use Only | no conclusion | est. t1/2 = 24d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = 0.9 (neutral cmpd.) | Not T | - | DW&GW | 4 | B; D; H; R; S |
| no conclusion | 637-92-3 | ETBE | 1000000 - 10000000 | no conc | est. t1/2 = 29d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 0.6 (neutral cmpd.) | Tscreen | Cramer Class III | GW | det. | H |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | lusion | | | | | | | | |
| no conclusion | 68-35-9 | Sulfadiazin | Intermediate Use Only | no conclusion | est. t1/2 = 66d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = -1.7 (ionizable cmpd.) | T | Lact Rep_2 | GW | 0.1 | B; H; Q |
| no conclusion | 74-83-9 | Bromomethane | Intermediate Use Only | no conclusion | est. t1/2 = 14d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 0.7 (neutral cmpd.) | T | muta_2<br>STOTRE_2<br>Suspected ED | GW | 0.4 | O |
| no conclusion | 994-05-8 | tert-Amyl methyl ether | 100000 - 1000000 | no conclusion | est. t1/2 = 29d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 0.7 (neutral cmpd.) | T | Carc_1b | GW | 0.4 | O |
| no conclusion | 75-01-4 | Vinyl chloride | 1000000 - 10000000 ;<br>0 - 10;<br>0 - 10 | no conclusion | est. t1/2 = 17d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 0.8 (neutral cmpd.) | T | Carc_1a<br>muta_2 | DW&GW | 7.5 | H; O |
| no conclusion | 75-00-3 | Chloroethane | 100 - 1000 | no conclusion | est. t1/2 = 17d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | exp min. log Doc/Koc = 0.8 (neutral cmpd.) | T | Carc_2 | GW | 3 | O |
| no conclusion | 156-60-5 | trans-1,2-Dichloroethene | 100 - 1000 | no conclusion | est. t1/2 = 28d, weight-of-evidence based on consistent indications of P across tested QSARs | M/vM | QSAR min. log Dow/Kow = 2.0, M or vM unclear due to data uncertainty (neutral cmpd.) | T | STOTRE_2 | GW | 10 | O |
| no conclusion | 83905-01-5 | Azithromycin | Intermediate Use Only | no conclusion | est. t1/2 = 1 469d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = -0.5 (ionizable cmpd.) | T | STOTRE_2 | DW | det. | X |
| no conclusion | 139481-59-7 | Candesartan | Intermediate Use Only | no conc | est. t1/2 = 48d, weight-of-evidence based on consistent indications of P across tested QSARs | vM | QSAR min. log Dow/Kow = -0.6 (ionizable cmpd.) | T | Rep_2 | DW | det. | X |

| PMT & vPvM | CAS | Name | tonnage per annum | P | P rationale | M | M rationale | T | T rationale | De-tected in GW or DW | Max conc. µg/L | Study ID |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | lusion | | 🟥 | | 🟥 | | | | |

# D False Negatives in PMT/vPvM assessment

The identity and publicly available REACH registered tonnage band of these false negatives is presented in Table D1 and D2. As evident, the majority have registered tonnages 1000 tonnes per year or greater, the exceptions are substances that are also used as pharmaceuticals (acetylsalicylic acid, DTPA and caffeine at 100-1000 tpa, estrone at 0-10 tpa, and 17b-Estradiol as an intermediate) or plant protection product (Mecoprop), which have additional emission sources through industrial use. Further, it may be the case that an additional local source of some of the phthalate plasticizers in Table D1 may be plastic piping or from plastic bottles they may have been stored in (Amiridou and Voutsa, 2011).

**Table D1 List of false negatives for the P criterion.**

List of those REACH registered substances presented in Table 1 detected in drinking water and/or groundwater which do not fulfil the P criterion with the publicly available REACH registered tonnage band.

| CAS | Name | Rational for Not P | tonnage per annum |
|---|---|---|---|
| 80-05-7 | Bisphenol A | inherently biodeg: 302 A (Inherent Biodegradability: Modified SCAS Test) | 1000000 - 10000000 |
| 106-46-7 | 1,4-Dichlorobenzene | readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test) | 10000 - 100000 |
| 50-78-2 | Acetylsalicylic acid | est. t1/2 = 7d, and consistency across all tested QSARs | 100 - 1000 |
| 139-13-9 | NTA | readily biodeg: 301 E (Ready biodegradability: Modified OECD Screening Test) | 100 - 1000 |
| 126-73-8 | TBP | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | 1000 - 10000 |
| 77-93-0 | Triethyl citrate | readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test) | 1000 - 10000 |
| 102-76-1 | Triacetin | readily biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test) | 10000 - 100000 |
| 105-60-2 | e-caprolactam | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | 1000000 - 10000000 |
| 120-18-3 | Naphthalenesulfonic acid | OECD tests (301B and E) for surrogate imply no persistence. Therefore the substance is assessed not to be persistent. (Berger et al. 2018) | 1000 - 10000 |
| 128-44-9 | Saccharine | readily biodeg: 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test) | 1000 - 10000 |
| 25321-41-9 | Dimethylbenzene sulfonic acid | Several read-across studies including 301B and D tests imply no | 1000 - 10000 |

| CAS | Name | Rational for Not P | tonnage per annum |
|---|---|---|---|
| | | persistence. Therefore the substance is assessed not to be persistent. (Berger et al. 2018) | |
| 50-28-2 | 17b-Estradiol | readily biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test) | Intermediate Use Only |
| 58-08-2 | Caffeine | readily biodeg: 301 A (new version) (Ready Biodegradability: DOC Die Away Test) | 100 - 1000 |
| 69-72-7 | Salicylic acid | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | 10000 - 100000 |
| 76-22-2 | Camphor | readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test) | 100 - 1000 |
| 53-16-7 | Estrone | inherently biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test) | 0 - 10 |
| 7085-19-0 | Mecoprop | longest measured half life all media = 50 d (sediment) | Intermediate Use Only |
| 63-05-8 | Androstenedione | readily biodeg: 301 B (Ready Biodegradability: CO2 Evolution Test) | 100 - 1000 |
| 131-11-3 | Dimethyl phthalate | readily biodeg: 301 E (Ready biodegradability: Modified OECD Screening Test) | 1000 - 10000 |
| 84-66-2 | Diethyl phthalate | est. t1/2 = 6d, and consistency across all tested QSARs | 1000 - 10000 |
| 84-74-2 | Dibutyl phthalate | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | 1000 - 10000 |
| 85-68-7 | Butyl benzyl phthalate | inherently biodeg: 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test) | 1000 - 10000 |
| 71-43-2 | Benzene | readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test) | 1000000 - 10000000 |
| 100-41-4 | Ethylbenzene | inherently biodeg: 302 C (Inherent Biodegradability: Modified MITI Test (II)) | 1000000 - 10000000 |
| 108-88-3 | Toluene | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | 1000000 - 10000000 |
| 95-63-6 | 1,2,4-Trimethylbenzene | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | 10000 - 100000 |

| CAS | Name | Rational for Not P | tonnage per annum |
|---|---|---|---|
| 95-47-6 | Total xylenes | readily biodeg: 301 F (Ready Biodegradability: Manometric Respirometry Test) | 100000 - 1000000 |
| 98-86-2 | Acetophenone | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | 10000 - 100000 |
| 84-65-1 | Anthraquinone | readily biodeg: 301 C (Ready Biodegradability: Modified MITI Test (I)) | 1000 - 10000 |
| 75-09-2 | Dichloromethane | readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test) | 100000 - 1000000 |
| 100-42-5 | Styrene | readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test) | 1000000 - 10000000 |
| 107-07-3 | 2-Chlorethanol | readily biodeg: 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test),301 F (Ready Biodegradability: Manometric Respirometry Test) | 10 - 100 |
| 70-55-3 | 4-Methylbenzolsulfonamide | readily biodeg: 301 D (Ready Biodegradability: Closed Bottle Test) | 0 - 10 |

### Table D2 List of false negatives for the M criterion.

List of those REACH registered substances presented in Table 1 detected in drinking water and/or groundwater which do not Fulfil the M criterion with the publically available REACH registered tonnage band.

| CAS | Name | Rational for Not M | tonnage per annum |
|---|---|---|---|
| 1222-05-5 | Galaxolide | exp min. log Doc/Koc = 4.3 | 1000 - 10000 |
| 128-37-0 | Butylhydroxytoluene | exp min. log Doc/Koc = 4.4 | 10000 - 100000 |
| 129-00-0 | Pyrene | exp min. log Doc/Koc = 4.1 | Intermediate Use Only* |
| 140-66-9 | tert-Octylphenol | exp min. log Doc/Koc = 4.0 | 10000 - 100000 |
| 117-81-7 | DEHP | exp min. log Doc/Koc = 5.7 | 10000 - 100000 |
| 104-40-5 | Nonylphenol | QSAR min. log Dow/Kow = 6.1 (neutral) | 0 - 10 |
| 96-76-4 | 2,4-Di-tertiary-butylphenol | exp min. log Dow/Kow = 4.8 (neutral) | 100 - 1000 |
| 85-68-7 | Butyl benzyl phthalate | exp min. log Dow/Kow = 4.8 (neutral) | 1000 - 10000 |

*pyrene is also produced by combustion processes (e.g. diesel combustion), and could transport in water via soot particles