TECHNICAL NOTE

Preliminary assessment of substances registered under REACH that could fulfil the proposed PMT/vPvM criteria

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Preliminary assessment of substances registered under REACH that could fulfil the proposed PMT/vPvM criteria

Contents

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Disclaimer

This report is a preliminary assessment of REACH registered substances that could be considered PMT/vPvM substances. This report and its conclusions were prepared by the Norwegian Geotechnical Institute, as part of a research project commissioned the Federal Ministry for the Environment, Nature Conservation, Building and Nuclear Safety of Germany. It does not present an official list of substances that the German Environment Agency (UBA) or any other authority consider as PMT/vPvM substances. The primary purpose of this report is to make an initial survey to stimulate further, public discussions and feedback on the finalization and implementation of the proposed PMT/vPvM criteria and assessment procedure by the UBA. To this end this document was prepared specifically as a background document to the workshop:

> "PMT and vPvM substances under REACH. Voluntary measures and regulatory options to protect the sources of drinking water"
> March 13'th-March 14'th. Held at the Bundespresseamt, Berlin, Germany

1 Introduction

The German Environment Agency (UBA) has proposed criteria and an assessment procedure for identifying Persistent, Mobile and Toxic (PMT) substances and very Persistent, very Mobile (vPvM) substances registered under REACH. The underlying purpose of this initiative is to protect "sources of drinking water" from REACH registered substances that pose a hazard, if they are used without appropriate risk mitigation measures. The phrase “sources of 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. (Neumann and Schliebner, 2017)

An initial guidance document for conducting a PMT hazard assessment was prepared in 2014 by Kalberlah et al. (2014) (document UFOPLAN: FKZ 371265416). Based on discussions and feedback at various arenas, such as meetings organized by ECHA (Risk Management Expert meetings, PBT expert group meetings, etc.), public workshops, and invitations to the public to provide comments, the initially proposed criteria has continuously been updated to reflect the feedback received. It may now considered to be approaching a general consensus and finalization.

The most recent criteria and assessment procedure was presented in a position paper by UBA in October 2017 (Neumann and Schliebner, 2017), entitled " Protecting the sources of our drinking water: A revised proposal for implementing criteria and an assessment procedure to identify Persistent, Mobile and Toxic (PMT) and very Persistent, very Mobile (vPvM) substances registered under REACH". In addition to proposing PMT criteria, this newest revision also introduced the vPvM criteria. This position paper serves as the basis for the assessment conducted in this report.

The purpose of this document is to present a preview of a preliminary assessment of the number and identity of substances registered under REACH that could be considered to fulfil the current revision of the criteria and assessment procedure for PMT and vPvM substances. The intent being that the outcome of this preliminary assessment is used as a background document for discussions related to the finalization of the PMT/vPvM criteria and assessment procedure.

2 Assessment Procedure

The general outline for the assessment procedure is presented in Figure 1.

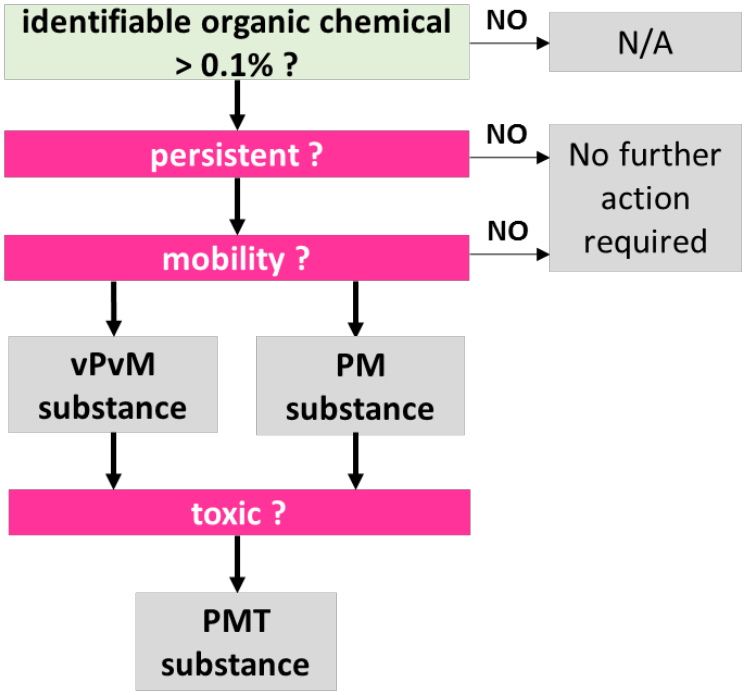

Figure 1: Overview of the proposed assessment procedure to identify PMT/vPvM substances registered under REACH.

Herein this assessment was initiated for the 15469 substances registered under REACH as of May 2017. After a thorough search of structural and composition information, 9741 contained an identifiable organic constituent in concentrations > 0.1% (w/w). Only these are considered "assessable" substances, as the remainder are either inorganic or complex mixtures, such as UVCB substances[1], with no workable structural information.

[1] UVCB refer to substances are defined as "substances of Unknown or Variable composition, Complex reaction products or Biological material" for which the number of constituents is high, or the composition is to a significant extent unknown, or the variability of composition is large or unpredictable.

3 Persistency

Threshold values for Persistent (P) and very persistent (vP) in the proposed PMT/vPvM criteria (Neumann and Schliebner, 2017) are consistent with that in Annex XIII of REACH for the PBT/vPvB assessment. These criteria are presented in Box 1.

Box 1. P/vP criteria set out in Annex XIII of Regulation REACH and in Guidance on Information Requirements and Chemical Safety Assessment Chapter R.11: PBT/vPvB assessment (June 2017)

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 and pH 4-9 is higher than 40 days;

(c) the degradation half-life in marine sediment at 9 °C is higher than 180 days;

(d) the degradation half-life in fresh or estuarine water sediment at 12 °C and pH 4-9 is higher than 120 days;

(e) the degradation half-life in soil at 12 °C and pH 4-9 is higher than 120 days.

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

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

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

(c) the degradation half-life in soil (12 °C and pH 4-9) is higher than is higher than 180 days.

These criteria are based on first order half-lives of a substance in different environmental compartments. Relevant half-live data to evaluate persistence is, for most substances, not available. Reliable half-lives, such as from following the standardized methods OECD 307 (soil), OECD 308 (sediment) and OECD 309 (water), requires more monetary investment than alternative methods that can be used to infer that the persistency criteria is not met. Data that is mentioned in the PBT guideline (European Chemicals Agency, 2017) as suitable for reaching a conclusion of not persistent or potentially persistent based on a weight-of-evidence approach include 1) evidence of ready biodegradation (e.g. OECD 301; OECD 310); 2) inherent biodegradation test data (e.g. OECD 302b; OECD 302c) and 3) enhanced screening tests. In addition, QSARs to predict persistency, pure culture data, evidence of anaereobic degradation, abiotic degradation data, field studies and monitoring data can be used collectively to amass a conclusion of P, vP or not P based on weight-of-evidence and expert assessment.

In this assessment, 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 classifications based on

weight-of-evidence assessments from 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 (European Chemicals Agency, 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 "ProS.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 not considered, as these were found to vary widely in their reliability, and across multiple dossier entries for a specific substance.

The breakdown of preliminary persistency (P or vP) conclusions for the 9741 substances is presented in Figure 2.

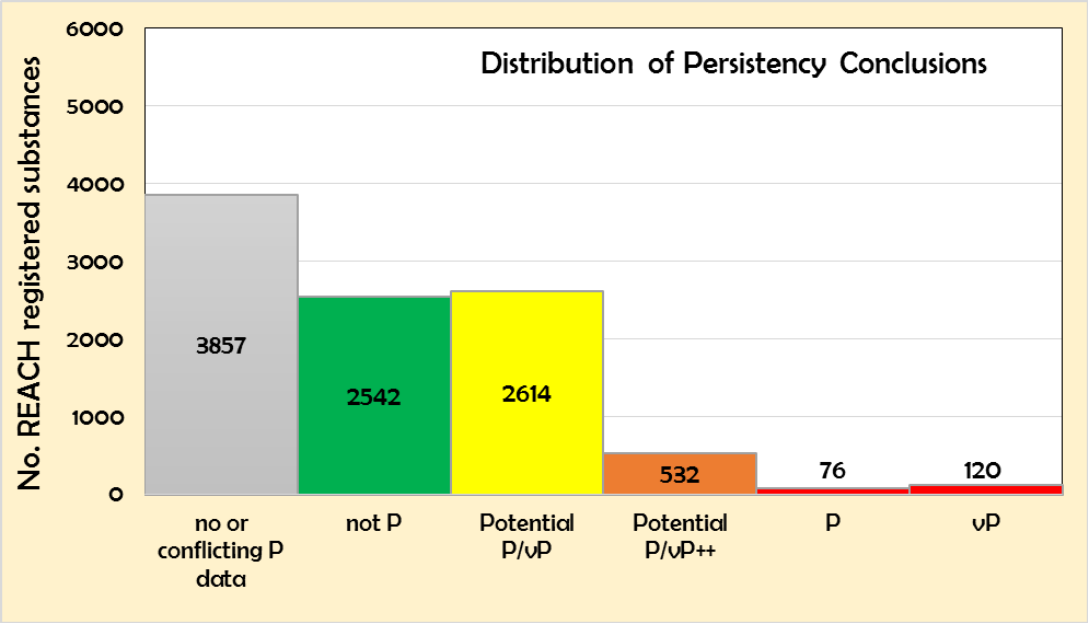

Figure 2. Distribution of persistency (P or vP) conclusions.

A description of the persistency (P or vP) conclusions presented in Figure 2 is as follows:

vP (120 substances): meets the criteria for vP and P based on experimental half-life data or a substantial weight-of-evidence;

P (76 substances): meets the criteria for P but not vP, based on experimental half-life data or a substantial weight-of-evidence;

Potential P/vP++ (532 substances): experimental half-life data for all media is lacking, but all available weight-of-evidence strongly leans towards a conclusion of P or vP;

Potential P/vP (2614 substances): experimental half-life data lacking, but initial information cannot yet rule out possibility of persistence;

not P (2542 substances): experimental data indicates not persistent, or the weight-of-evidence strongly indicates not persistent;

no or conflicting P data (3857 substances): no information about P available, except for QSARs, which gave conflicting or low quality conclusions.

Following the general assessment procedure in Figure 1, only the 728 substances assessed as vP, P and Potential vP/P++ are evaluated for mobility.

4 Mobility

The mobility criterion in Box 2 are a unique criterion in the PMT/vPvM assessment.

Box 2. M/vM criteria used in this assessment

A substance that fulfils the P or vP criterion also fulfils the mobility criterion (M) in any of the following situations:

(a) the lowest log K_{OC} is ≤ 4.0 over the environmentally relevant pH range of 4-9

(b) in the absence of log K_{OC} data, the lowest log D_{OW} is ≤ 4.0 over the environmentally relevant pH range of 4-9.

A substance that fulfils the P or vP criterion also fulfils the "very mobile" criterion (vM) in any of the following situations:

(a) the lowest log K_{OC} is ≤ 3.0 over the environmentally relevant pH range of 4-9

(b) in the absence of log K_{OC} data, the lowest log D_{OW} is ≤ 3.0 at environmentally relevant pH range of 4-9.

There are some changes to the M/vM criterion in Box 2, compared to the most recent proposal (Neumann and Schliebner, 2017), based on the most recent feedback received. These changes are:

1) the water solubility criterion of 0.15 mg/L was removed for simplification, as these substances typically have a log K_{OC} / log D > 4.0; and the data availability for solubility is similar to log K_{OC} / log D.

2) the temperature requirement of 12 °C was removed, as the influence of temperature between 12 °C and room temperature on K_{OW} values for polar compounds, as well as the influence on water solubility, is generally minimal (i.e. usually within a factor 3) (Schwarzenbach et al. 2017).

Unlike half-life data, experimental data for log K_{OC} and log D_{OW} are available for many REACH substances, and further, QSARs for most neutral and ionizable substances perform fairly robustly (within an order of magnitude) (Arp et al., 2017).. However, robust QSARs for ionic substances have yet to be developed (Arp et al., 2017).

Experimental data was given highest priority in this assessment. The main sources were 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. (2017) and the eChemPortal database (accessed November 2017). When no experimental data was available, QSAR predictions for log D_{OW} were performed using ADMET Predictor 7.1 software by Simulations-plus[2] primarily, and ChemAxon[3] (October 2017 version) as a backup. The distribution of best available M related data is presented in Figure 3.

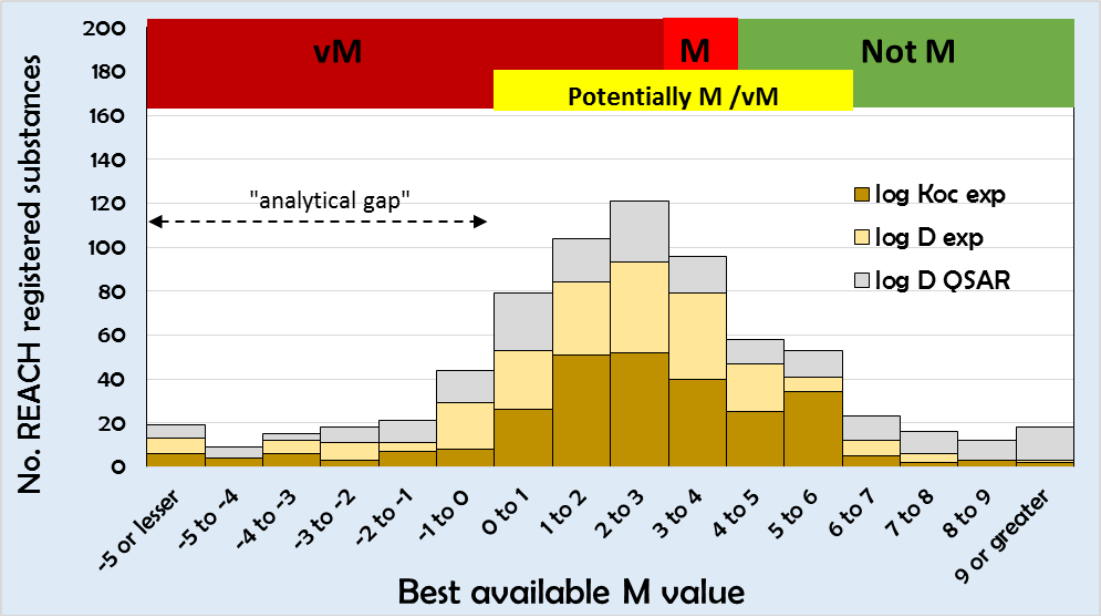

Figure 3. Distribution of best available and minimum log Koc (experimental), log Dow (experimental and QSAR) values over a pH range of 4-9 for substances where the Potential P/vP++, P or vP criterion is met. Also shown is the "analytical gap", where analysis is difficult (Reemtsma et al. 2016)

The distribution of preliminary mobility (M or vM) conclusions for the 728 substances that had the highest potential of meeting the P criteria (that is vP, P and Potential vP/P++) is presented in Figure 4.

[2] http://www.simulationsplus.com
[3] https://www.chemaxon.com

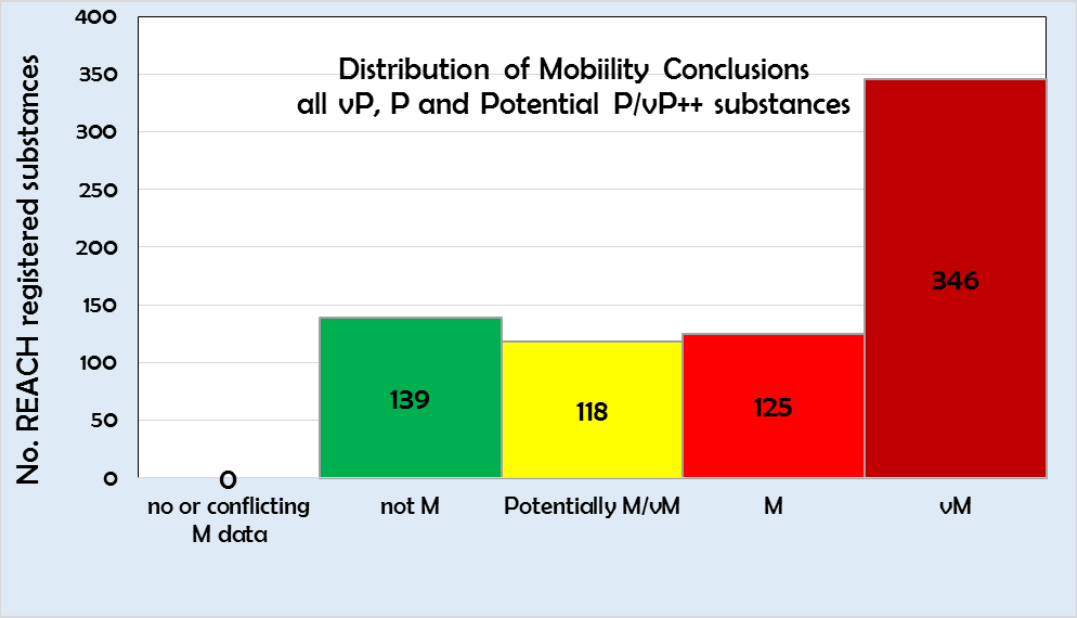

Figure 4. Distribution of mobility (M or vM) conclusions for substances that met or had high potential to meet the P/vP criteria.

A description of the mobility (M or vM) conclusions presented in Figure 4 is as follows:

vM (346 P substances): met the M and vM criteria based on experimental data or sufficiently reliable QSARs

M (125 P substances): met the criteria for M, but not vM, based on experimental data or sufficiently reliable QSARs.

Potential M/vM (118 P substances): no experimental data available, and uncertainty of available QSARs overlap with the threshold cut-offs.

Not M (139 P substances): did not meet the M criteria based on experimental data or sufficiently reliable QSARs.

No or conflicting M data (0 substances): a preliminary M conclusion could not be made, due to lack of sufficiently reliable QSAR data.

Following the general assessment procedure in Figure 1, the substances with the conclusions "Potential M/vM" and "Not M" do not need to be considered further. The remaining 471 substances that are considered can be separated into the categories vPvM (53 substances), PM (but not vPvM, 79 substances) and Potential PM/vPvM (339 substances).

5 Toxicity

Threshold values for Toxicity in the proposed PMT/vPvM criteria (Neumann and Schliebner, 2017) contain elements consistent with that in Annex XIII of Regulation

REACH for the PBT/vPvB assessment, though with extra criteria to reflect chronic human exposure (Box 3).

Box 3. T criterion used in this assessment

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

(a) the long-term no-observed effect concentration (NOEC) or EC10 for marine or freshwater organisms is less than 0.01 mg/l;

(b) the substance meets the criteria for classification as carcinogenic (category 1A, 1B or 2), germ cell mutagenic (category 1A, 1B or 2), or toxic for reproduction (category 1A, 1B, or 2) according to Regulation EC No 1272/2008;

(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;

(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);

(g) the substance acts as an endocrine disruptor in humans and/or wildlife species according to the WHO/IPCS definition of an endocrine disruptor. This is always the case if a substance can be identified as an endocrine disruptor for human health and/or the environment according to the criteria laid down in the draft of COMMISSION REGULATION (EU) …/… of XXX for setting out scientific criteria for the determination of endocrine disrupting properties and amending Annex II to Regulation (EC) 1107/2009.

The hazard categories specific for chronic human exposure that are not in the PBT assessment, but are in the PMT assessment are: carcinogenic category 2; germ cell mutagenic category 2; toxic for reproduction category 2; effects on or via lactation; DNEL ≤ 9 µg/kg/d (oral, long term, general population); and, endocrine disruption. To illustrate how much influence these additional criteria have on a T evaluation, a comparison of T conclusions for the 9714 REACH substances identified to contain an identifiable organic constituent in concentration > 0.1% (w/w), with and without these categories, are presented in Figure 5.

The data sources for most of the toxicity criteria was the C&L registry[4], with the exception for NOEC/EC10 values (obtained from the eChemPortal database, November 9'th, 2017), DNEL (obtained directly from REACH registration dossiers, as accessed via IUCLID 6, January 11'th, 2017), and *suspected* endocrine disruption (obtained from a 2014 evaluation from ECHA, "Pro.S.P. 2014"). When multiple NOEC/EC10 or DNEL values were found for one substance, the lowest was chosen by default.

[4] Note that the C&L inventory is often based on self-classifications from the companies and not harmonized ones; here the updated list as of October 06, 2017 was used, as published on https://echa.europa.eu/information-on-chemicals/cl-inventory-database.

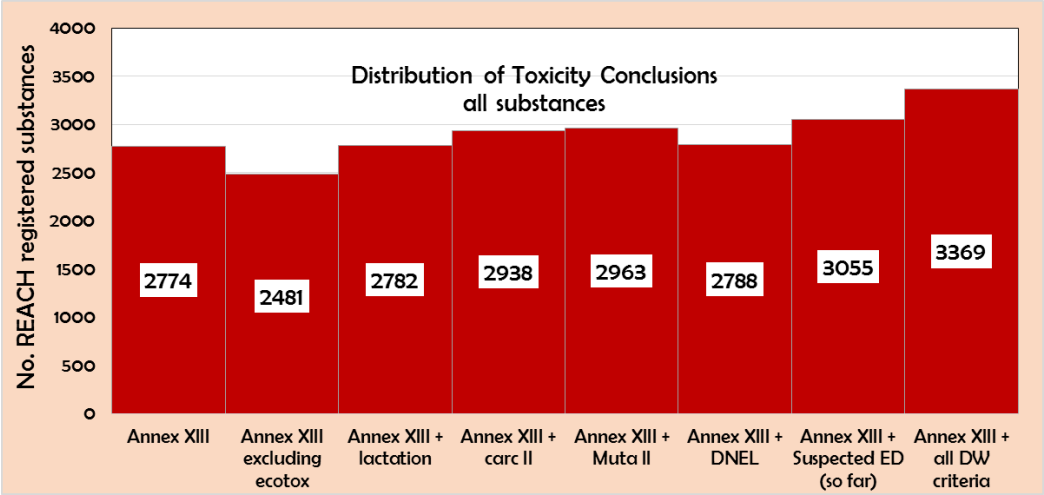

Figure 5. Distribution of substances fulfilling different combinations of T-criteria

From Figure 5, it is evident that the additional T-criteria in the PMT assessment, as compared to the criteria in Annex XIII, only result in a moderate increase in REACH substances that fulfil the T criterion from 2774 to 3369 substances (out of 9741). For the most part, this is due to including carcinogenic II, mutagenic II and suspected endocrine disruptors. Removing the criterion for ecotoxicity reduced the number of substances meeting the T criterion from 2774 to 2481.

The breakdown of preliminary Toxicity (T) conclusions for the 471 substances that had the highest potential of meeting the PM criteria (that is vPvM, PM and Potential PM/vPvM) is presented in Figure 6.

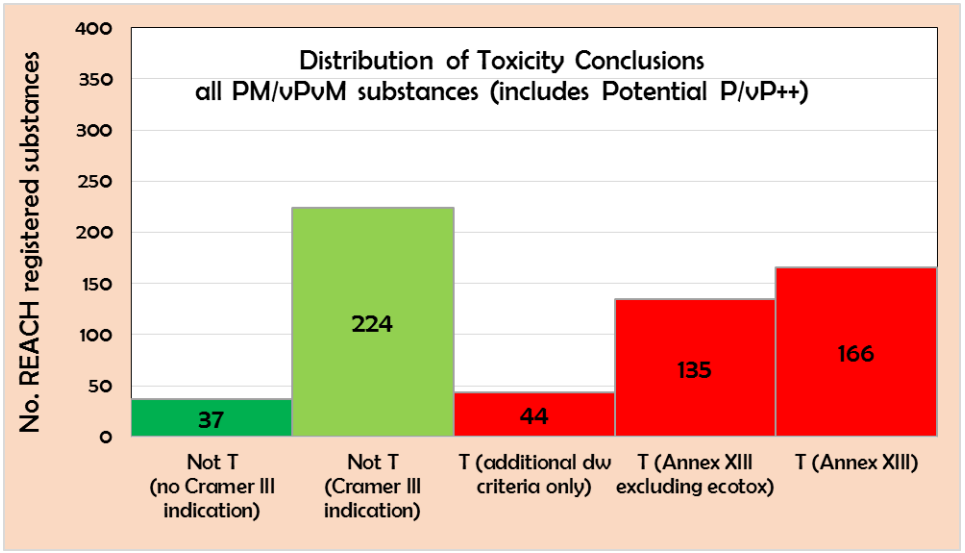

Figure 6. Distribution of toxicity conclusions for the substances that met or had high potential to meet the PM/vPvM criteria.

The distribution of toxicity conclusions in Figure 6 is divided as follows:

T(Annex XIII) (166 substances): Potential PMT/vPvM, PMT and vPvM substances that meet the T criterion according to Annex XIII.

T(Annex XIII excluding ecotox) (135 substances): Potential PMT/vPvM, PMT and vPvM substances that meet the T criterion according to Annex XIII, other than the ecotox criterion. This is added due to discussions on the need to include the ecotox criteria in the PMT/vPvM assessment.

T (additional dw criteria only) (44 substances): Potential PMT/vPvM, PMT and vPvM substances that do not meet the T criteria in Annex XIII, but meet one of the additional chronic human exposure criteria in the PMT/vPvM assessment.

Not T (Cramer III indication) (224 substances): Potential PMT/vPvM, PMT and vPvM substances that do not meet the T criteria in Annex XIII nor additional criteria, but contained a moiety that causes a Cramer III structure alert (i.e. "chemical structures that permit no strong initial impression of safety and may even suggest a significant toxicity" (Cramer et al. 1978).

Not T (37 substances): Potential PMT/vPvM, PMT and vPvM substances that do not meet the T criteria in Annex XIII nor additional criteria.

6 Preliminary list

Based on the currently proposed PMT/vPvM criteria and assessment procedure and available data thus far, there are 240 substances that are considered from this initial, preliminary assessment with sufficient weight-of-evidence to fulfil the PMT and vPvM criteria. These are given in Table 1.

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

The compounds considered "high potential to be PMT/vPvM" are those for which no experimental half-life data was available, though expert assessment considered there to be a sufficient weight-of-evidence to indicate a high potential of persistence. Also presented in Table 1 is information about studies in which these substances have been detected in treated drinking water or remote groundwater areas, and the relative emission ranking compared to others substances in Table 1, with the lower the rank the higher the relative emissions, according to the method of Schulze et al. (2018).

Table 1. Preliminary list of the substances that could be considered to meet the PMT or vPvM criteria, or have the highest potential of doing so based on the weight of available evidence. Also presented is if the substances is a known contaminant in treated drinking water (DW) or remote groundwater aquifers (GW), and the relative emission rank (lower the number the more likely emissions occur relative to other substances on this list).

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
201-248-4/ 80-08-0	Dapsone	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 1.8 (neutral)	T	STOTRE_1; STOTRE_2; Susp_ED	DW	F	30
201-861-7/ 88-85-7	Dinoseb	vP	measured half life = 314 d (soil)	vM	exp min. Doc/Koc = -2.3 (ionizable)	T	SVHC			neg. emissions
203-492-7/ 107-46-0	Hexamethyldisiloxane	vP	measured half life = 231 d (soil)	vM	exp min. Doc/Koc = 2.7 (neutral)	T	ecotox; Carc_2			51
203-615-4/ 108-78-1	Melamine	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Dow/Kow = -2.3 (ionizable)	T	Carc_2; STOTRE_2	DW	E; F	2
203-632-7/ 108-95-2	Phenol	vP	measured half life = 68 d (fresh water)	vM	exp min. Doc/Koc = 0.6 (ionizable)	T	Carc_2; muta_1b; muta_2; Rep_1b; STOTRE_1; STOTRE_2			neg. emissions
204-077-3/ 115-27-5	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II)),301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Doc/Koc = 0.9 (neutral)	T	Carc_1a; Carc_2; STOTRE_2			neg. emissions
204-278-6/ 118-79-6	2,4,6-tribromophenol	vP	measured half life = 370 d (soil)	vM	exp min. Doc/Koc = -0.4 (ionizable)	T	Rep_2; STOTRE_2; Susp_ED			54
204-445-3/ 121-03-9	4-nitrotoluene-2-sulphonic acid	vP	expert conclusion (Berger et al. 2018)	vM	QSAR min. Dow/Kow = -0.9 (ionizable)	T	SVHC			neg. emissions
204-825-9/ 127-18-4	Tetrachloroethylene	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 2.2 (neutral)	T	Carc_1b; Carc_2; Rep_2; STOTRE_2; Susp_ED	DW	G; J	11

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
206-354-4/ 330-54-1	Diuron	vP	measured half life = 2,241 d (soil)	vM	exp min. Doc/Koc = 2.1 (neutral)	T	ecotox; Carc_2; STOTRE_2; Susp_ED	DW&GW	E; A	unknown
206-992-3/ 420-04-2	Cyanamide	vP	measured half life = 242 d (soil)	vM	exp min. Dow/Kow = -2.0 (ionizable)	T	Carc_2; Rep_2; STOTRE_2			29
209-218-2/ 561-41-1	4,4'-bis(dimethylamino)-4"-(methylamino)trityl alcohol	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Dow/Kow = -0.6 (ionizable)	T	SVHC			neg. emissions
230-528-9/ 7173-62-8	(Z)-N-9-octadecenylpropane-1,3-diamine	vP	measured half life = 227 d (soil)	vM	exp min. Dow/Kow = -2.8 (ionizable)	T	STOTRE_1			54
247-368-0/ 25956-17-6	Disodium 6-hydroxy-5-[(2-methoxy-4-sulphonato-m-tolyl)azo]naphthalene-2-sulphonate	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Dow/Kow = 0.1 (anionic)	T	SVHC			60
252-156-6/ 34690-00-1	[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methylene)]]tetrakis phosphonic acid	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	QSAR min. Dow/Kow = -11.0 (ionizable)	T	STOTRE_2			54
253-575-7/ 37640-57-6	1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6-triamine (1:1)	vP	measured half life = 913 d (soil)	vM	read-across min. Dow/Kow = 2.0 (neutral)	T	STOTRE_2			neg. emissions
260-375-3/ 56773-42-3	Tetraethylammonium heptadecafluorooctanesulphonate	vP	on SVHC list - vPvB substance	vM	exp min. Doc/Koc = 0.0 (anionic)	T	SVHC	DW&GW	A; E; I	unknown
268-957-9/ 68155-37-3	Amines, N-C12-18-alkyltrimethylenedi-	vP	measured half life = 227 d (soil)	vM	read-across min. Dow/Kow = -2.8 (ionizable)	T	STOTRE_1; DNEL			66
271-756-9/ 68607-24-9	Quaternary ammonium compounds, C20-22-alkyltrimethyl, chlorides	vP	measured half life = 255 d (soil)	vM	exp min. Doc/Koc = 2.1 (cationic)	T	STOTRE_2			unknown
276-014-8/ 71786-60-2	Ethanol, 2,2'-iminobis-, N-C12-18-alkyl derivs.	vP	measured half life = 227 d (soil)	vM	exp min. Dow/Kow = -0.8 (ionizable)	T	ecotox			neg. emissions
430-550-0/ 1671-49-4	4-mesyl-2-nitrotoluene	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 2.3 (neutral)	T	Rep_2			unknown
688-332-8/ 199119-58-9	sodium (4,6-dimethoxypyrimidin-2-yl)carbamoyl-[[3-(2,2,2-trifluoroethoxy)-2-pyridyl]sulfonyl]azanide	vP	measured half life = 170 d (soil)	vM	exp min. Doc/Koc = 1.5 (anionic)	T	ecotox			unknown

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
700-242-3/ 62037-80-3	ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = -5.1 (anionic)	T	STOTRE_2			neg. emissions
201-132-3/ 78-67-1	2,2'-dimethyl-2,2'-azodipropiononitrile	vP	measured half life = 1,093 d (fresh water)	vM	exp min. Doc/Koc = 2.0 (neutral)	Pot.T	Cramer; Class; III			22
202-095-6/ 91-76-9	6-phenyl-1,3,5-triazine-2,4-diyldiamine	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 1.4 (ionizable)	Pot.T	Cramer; Class; III			neg. emissions
202-425-9/ 95-50-1	1,2-dichlorobenzene	vP	measured half life = 191 d (soil)	vM	exp min. Doc/Koc = 2.7 (neutral)	Pot.T	Cramer; Class; III			neg. emissions
205-861-8/ 156-62-7	Calcium cyanamide	vP	measured half life = 242 d (soil)	vM	exp min. Doc/Koc = 1.3 (anionic)	Pot.T	Cramer; Class; III			unknown
206-841-1/ 382-28-5	2,2,3,3,5,5,6,6-octafluoro-4-(trifluoromethyl)morpholine	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)	vM	exp min. Doc/Koc = 0.2 (ionizable)	Pot.T	Cramer; Class; III			71
208-796-3/ 542-02-9	6-methyl-1,3,5-triazine-2,4-diyldiamine	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Dow/Kow = -0.7 (ionizable)	Pot.T	Cramer; Class; III			104
209-143-5/ 556-88-7	1-nitroguanidine	vP	measured half life = 102 d (fresh water)	vM	QSAR min. Dow/Kow = -1.1 (ionizable)	Pot.T	Cramer; Class; III			91
221-201-1/ 3030-47-5	Bis(2-dimethylaminoethyl)(methyl)amine	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Dow/Kow = 0.1 (ionizable)	Pot.T	Cramer; Class; III			62
221-220-5/ 3033-62-3	N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Dow/Kow = 0.5 (ionizable)	Pot.T	Cramer; Class; III			108
224-548-7/ 4404-43-7	4,4'-bis[4-[bis(2-hydroxyethyl)amino]-6-anilino-1,3,5-triazin-2-yl]amino]stilbene-2,2'-disulphonic acid	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 A (old version) (Ready Biodegradabiltiy: Modified AFNOR Test)	vM	exp min. Doc/Koc = 2.5 (zwitterion)	Pot.T	Cramer; Class; III			unknown
226-789-3/ 5468-75-7	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methylphenyl)-3-oxobutyramide]	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Dow/Kow = 0.5 (ionizable)	Pot.T	Cramer; Class; III			unknown
226-939-8/ 5567-15-7	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-chloro-2,5-dimethoxyphenyl)-3-oxobutyramide]	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Dow/Kow = 0.0 (ionizable)	Pot.T	Cramer; Class; III			unknown
227-877-4/ 6022-22-6	Disodium 4,4'-diamino-9,9',10,10'-tetrahydro-9,9',10,10'-tetraoxo[1,1'-bianthracene]-3,3'-disulphonate	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. Dow/Kow = -1.1 (anionic)	Pot.T	Cramer; Class; III			unknown

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
244-751-4/ 22042-96-2	[[(phosphonomethyl)imino]bis[(ethylenenitrilo)bis(methylene)]]tetrakisphosphonic acid, sodium salt	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	QSAR min. Dow/Kow = -14.3 (anionic)	Pot.T	Cramer; Class; III			60
244-776-0/ 22094-93-5	2,2'-[(2,2',5,5'-tetrachloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Dow/Kow = 0.5 (ionizable)	Pot.T	Cramer; Class; III			neg. emissions
252-575-4/ 35453-19-1	5-amino-2,4,6-triiodoisophthalic acid	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	QSAR min. Dow/Kow = 0.6 (ionizable)	Pot.T	Cramer; Class; III			102
255-449-7/ 41583-09-9	1,3,5-triazine-2,4,6-triamine phosphate	vP	measured half life = 913 d (soil)	vM	exp min. Dow/Kow = -2.3 (ionizable)	Pot.T	Cramer; Class; III			89
263-212-4/ 61792-09-4	Pentasodium pentahydrogen [[(phosphonatomethyl)imino]bis[ethane-2,1-diylnitrilobis(methylene)]]tetrakisphosphonate	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	QSAR min. Dow/Kow = -14.3 (anionic)	Pot.T	Cramer; Class; III			75
271-878-2/ 68610-86-6	Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(o-anisyl and 2,4-xylyl) derivs.	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Dow/Kow = 0.8 (ionizable)	Pot.T	Cramer; Class; III			81
277-242-0/ 73037-34-0	Disodium oxybis[methylbenzenesulphonate]	vP	expert conclusion (Berger et al. 2018)	vM	QSAR min. Dow/Kow = -1.7 (anionic)	Pot.T	Cramer; Class; III			unknown
406-080-7/ 83016-70-0	2-[(2-[2-(dimethylamino)ethoxy]ethyl)methylamino]ethanol	vP	expert conclusion (Berger et al. 2018)	vM	QSAR min. Dow/Kow = -2.9 (ionizable)	Pot.T	Cramer; Class; III			unknown
476-160-4/ -	sodium 4,4-dimethyl-2,5-dioxoimidazolidin-1-ide	vP	measured half life = 590 d (water/sediment)	vM	QSAR min. Dow/Kow = -0.9 (anionic)	Pot.T	Cramer; Class; III			unknown
601-093-6/ 111453-32-8	rac-5-Amino-N-(2,3-dihydroxypropyl)-2,4,6-triiodoisophthalamic acid	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	QSAR min. Dow/Kow = 0.1 (ionizable)	Pot.T	Cramer; Class; III			unknown

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
601-601-6/ 119345-04-9	Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated, sodium salts	vP	measured half life = 980 d (sediment)	vM	exp min. Dow/Kow = -2.7 (anionic)	Pot.T	Cramer; Class; III			neg. emissions
700-183-3/ 52299-25-9	bis(nonafluorobutyl)phosphinic acid	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Dow/Kow = -1.1 (ionizable)	Pot.T	Cramer; Class; III			unknown
700-570-7/ 1217271-49-2	1,6-Bis[2,2-dimethyl-3-(N-morpholino)-propylideneamino]-hexane	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test) July 17, 1992	vM	QSAR min. Dow/Kow = 0.1 (ionizable)	Pot.T	Cramer; Class; III			unknown
700-616-6/ 849608-59-9	Tetra potassium 5,5'-[ethane-1,2-diylbis[thio-1,3,4-thiadiazole-5,2-diyldiazene-2,1-diyl(5-amino-3-tert-buyl-1H-pyrazole-4,1-diyl)]}diisophthalate	vP	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	QSAR min. Dow/Kow = -3.4 (anionic)	Pot.T	Cramer; Class; III			36
209-813-7/ 593-85-1	Diguanidinium carbonate	vP	measured half life = 174 d (fresh water)	vM	QSAR min. Dow/Kow = -4.2 (anionic)	Not T	-			unknown
253-256-2/ 36888-99-0	5,5'-(1H-isoindole-1,3(2H)-diylidene)dibarbituric acid	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Dow/Kow = 0.3 (ionizable)	Not T	-			neg. emissions
603-373-3/ 129909-90-6	4-amino-N-(1,1-dimethylethyl)-4,5-dihydro-3-(1-methylethyl)-5-oxo-1H-1,2,4-triazole-1-carboxamide	vP	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 1.4 (ionizable)	Not T	-			neg. emissions
202-479-3/ 96-12-8	1,2-dibromo-3-chloropropane	vP	measured half life = 529 d (soil)	M	QSAR min. Dow/Kow = 2.5 (neutral)	T	Carc_1b; muta_1b; muta_2; Rep_1a; STOTRE_2; Susp_ED			neg. emissions
219-006-1/ 2312-35-8	Propargite	vP	measured half life = 169 d (soil)	M	exp min. Doc/Koc = 3.6 (neutral)	T	ecotox; Carc_2			neg. emissions
235-166-5/ 12108-13-3	Tricarbonyl(methylcyclopentadienyl) manganese	vP	expert conclusion (Berger et al. 2018)	M	exp min. Doc/Koc = 3.4 (anionic)	T	Carc_2; STOTRE_1			unknown
246-807-3/ 25307-17-9	2,2'-(octadec-9-enylimino)bisethanol	vP	measured half life = 227 d (soil)	M	exp min. Dow/Kow = 1.9 (ionizable)	T	ecotox			45

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
269-927-8/ 68391-08-2	Alcohols, C8-14, γ-ω-perfluoro	vP	measured half life = 202,521 d (soil)	M	QSAR min. Dow/Kow = 2.9 (neutral)	T	Rep_2; STOTRE_2			unknown
691-719-4/ 1072957-71-1	N-[9-(dichloromethylidene)-1,2,3,4-tetrahydro-1,4-methanonaphthalen-5-yl]-3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxamide	vP	measured half life = 881 d (soil)	M	exp min. Doc/Koc = 3.7 (ionizable)	T	ecotox			neg. emissions
201-167-4/ 79-01-6	Trichloroethylene	P	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 2.2 (neutral)	T	SVHC	DW	G	96
201-758-7/ 87-62-7	2,6-xylidine	P	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 1.3 (ionizable)	T	Carc_2			3
201-808-8/ 88-19-7	Toluene-2-sulphonamide	P	expert conclusion (Berger et al. 2018)	vM	QSAR min. Dow/Kow = 0.9 (neutral)	T	Carc_1a; Carc_2			93
203-458-1/ 107-06-2	1,2-dichloroethane	P	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 1.1 (neutral)	T	SVHC			68
204-616-2/ 123-30-8	4-aminophenol	P	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 0.6 (ionizable)	T	muta_2; STOTRE_2			9
204-661-8/ 123-91-1	1,4-dioxane	P	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = -0.5 (neutral)	T	Carc_2; STOTRE_1; STOTRE_2	DW	E	30
204-809-1/ 126-86-3	2,4,7,9-tetramethyldec-5-yne-4,7-diol	P	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 1.6 (neutral)	T	STOTRE_2			30
205-411-0/ 140-31-8	2-piperazin-1-ylethylamine	P	expert conclusion (Berger et al. 2018)	vM	QSAR min. Dow/Kow = -3.6 (ionizable)	T	Rep_2; STOTRE_1			unknown
206-022-9/ 288-88-0	1,2,4-triazole	P	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 1.6 (ionizable)	T	Rep_2	DW	E	neg. emissions
210-734-5/ 622-40-2	2-morpholinoethanol	P	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = -1.9 (ionizable)	T	Carc_1b			neg. emissions
212-201-2/ 768-94-5	Amantadine	P	expert conclusion (Berger et al. 2018)	vM	QSAR min. Dow/Kow = 0.5 (ionizable)	T	Rep_2			19
212-634-7/ 834-12-8	Ametryn	P	measured half life = 143 d (soil)	vM	exp min. Doc/Koc = 1.8 (ionizable)	T	ecotox	DW&GW	H	neg. emissions
214-302-7/ 1120-24-7	Decyldimethylamine	P	measured half life = 180 d (soil)	vM	exp min. Dow/Kow = -1.5 (ionizable)	T	ecotox; Susp_ED			3

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
218-760-9/ 2226-96-2	4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	P	expert conclusion (Berger et al. 2018)	vM	QSAR min. Dow/Kow = 0.1 (ionizable)	T	STOTRE_2			neg. emissions
220-666-8/ 2855-13-2	3-aminomethyl-3,5,5-trimethylcyclohexylamine	P	expert conclusion (Berger et al. 2018)	vM	exp min. Dow/Kow = -1.3 (ionizable)	T	Susp_ED			neg. emissions
223-772-2/ 4065-45-6	Sulisobenzone	P	expert conclusion (Berger et al. 2018)	vM	exp min. Doc/Koc = 2.0 (ionizable)	T	Rep_2; Susp_ED			22
226-109-5/ 5281-04-9	Calcium 3-hydroxy-4-[(4-methyl-2-sulphonatophenyl)azo]-2-naphthoate	P	expert conclusion (Berger et al. 2018)	vM	exp min. Dow/Kow = 0.7 (anionic)	T	STOTRE_2			62
253-733-5/ 37971-36-1	2-phosphonobutane-1,2,4-tricarboxylic acid	P	measured half life = 139 d (soil)	vM	QSAR min. Dow/Kow = -7.7 (ionizable)	T	STOTRE_2			39
269-915-2/ 68390-97-6	Amines, C16-18-alkyldimethyl	P	measured half life = 180 d (soil)	vM	read-across min. Dow/Kow = -0.5 (ionizable)	T	ecotox			unknown
269-923-6/ 68391-04-8	Amines, C12-18-alkyldimethyl	P	measured half life = 180 d (soil)	vM	read-across min. Dow/Kow = 0.8 (ionizable)	T	ecotox			unknown
283-464-9/ 84649-84-3	Amines, C12-14-alkyldimethyl	P	measured half life = 180 d (soil)	vM	read-across min. Dow/Kow = 0.8 (ionizable)	T	ecotox			unknown
445-550-6/ 155661-07-7	rac-[(2R,4R)-2-(2,4-DICHLOROPHENYL)-2-(1H-1,2,4-TRIAZOL-1-YLMETHYL)-1,3-DIOXOLAN-4-YL]METHYL METHANESULFONATE MONOHYDROCHLORIDE	P	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Doc/Koc = 2.5 (neutral)	T	STOTRE_2			unknown
203-997-2/ 112-69-6	Hexadecyldimethylamine	P	measured half life = 180 d (soil)	M	read-across min. Dow/Kow = 1.2 (ionizable)	T	ecotox; Susp_ED			unknown
204-002-4/ 112-75-4	Dimethyl(tetradecyl)amine	P	measured half life = 180 d (soil)	M	read-across min. Dow/Kow = 1.2 (ionizable)	T	ecotox; Susp_ED			neg. emissions
204-371-1/ 120-12-7	Anthracene	P	On SVHC list - PBT substance	M	exp min. Doc/Koc = 3.6 (neutral)	T	SVHC	GW	H	7

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
204-694-8/ 124-28-7	Dimantine	P	measured half life = 180 d (soil)	M	read-across min. Dow/Kow = 1.2 (ionizable)	T	ecotox; Susp_ED			50
236-740-8/ 13472-08-7	2,2'-azobis[2-methylbutyronitrile]	P	expert conclusion (Berger et al. 2018)	M	exp min. Dow/Kow = 2.1 (neutral)	T	STOTRE_2			unknown
268-220-1/ 68037-96-7	Amines, (C16-18 and C18-unsatd. alkyl)dimethyl	P	measured half life = 180 d (soil)	M	read-across min. Dow/Kow = 1.2 (ionizable)	T	ecotox			unknown
270-414-6/ 68439-70-3	Amines, C12-16-alkyldimethyl	P	measured half life = 180 d (soil)	M	read-across min. Dow/Kow = 1.2 (ionizable)	T	ecotox			75
200-300-3/ 56-93-9	Benzyltrimethylammonium chloride	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	QSAR min. Dow/Kow = -1.0 (cationic)	T	muta_2	DW	F	71
200-663-8/ 67-66-3	Chloroform	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 2.0 (neutral)	T	Carc_2; muta_2; Rep_2; STOTRE_1; STOTRE_2	DW&GW	H	11
200-664-3/ 67-68-5	Dimethyl sulfoxide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 0.6 (neutral)	T	Carc_2; muta_2; STOTRE_2			unknown
200-819-5/ 74-88-4	Iodomethane	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 0.9 (neutral)	T	Carc_2			15
200-864-0/ 75-35-4	1,1-dichloroethylene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 1.4 (neutral)	T	Carc_1b; Carc_2; STOTRE_1; STOTRE_2			neg. emissions
200-900-5/ 75-77-4	Chlorotrimethylsilane	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)	vM	read-across min. Dow/Kow = 1.2 (neutral)	T	Carc_2			15
200-915-7/ 75-91-2	tert-butyl hydroperoxide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. Dow/Kow = 0.8 (neutral)	T	muta_2			22

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
201-114-5/ 78-40-0	Triethyl phosphate	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. Doc/Koc = -0.3 (neutral)	T	Carc_1b; muta_2			19
201-152-2/ 78-87-5	1,2-dichloropropane	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. Doc/Koc = 1.3 (neutral)	T	Carc_1b			neg. emissions
201-209-1/ 79-46-9	2-nitropropane	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = -1.7 (ionizable)	T	Carc_1b; muta_2			unknown
201-245-8/ 80-05-7	4,4'-isopropylidenediphenol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 A (Inherent Biodegradability: Modified SCAS Test)	vM	exp min. Doc/Koc = 2.3 (ionizable)	T	SVHC	DW&GW	A; D; J; K	42
201-250-5/ 80-09-1	4,4'-sulphonyldiphenol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = -0.3 (ionizable)	T	Susp_ED	DW	F	85
201-286-1/ 80-51-3	4,4'-oxydi(benzenesulphonohydrazide)	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	QSAR min. Dow/Kow = 0.2 (ionizable)	T	muta_2; STOTRE_2			neg. emissions
201-304-8/ 80-73-9	1,3-dimethylimidazolidin-2-one	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	QSAR min. Dow/Kow = -0.4 (neutral)	T	Rep_2; STOTRE_2			85
201-325-2/ 81-11-8	4,4'-diaminostilbene-2,2'-disulphonic acid	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	QSAR min. Dow/Kow = -2.7 (ionizable)	T	Susp_ED			22
201-604-9/ 85-42-7	Cyclohexane-1,2-dicarboxylic anhydride	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. Doc/Koc = 2.3 (neutral)	T	SVHC			14
201-831-3/ 88-44-8	4-aminotoluene-3-sulphonic acid	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	QSAR min. Dow/Kow = -1.7 (ionizable)	T	Susp_ED			96
201-853-3/ 88-72-2	2-nitrotoluene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 1.9 (neutral)	T	Carc_1b; Carc_2; muta_1b; Rep_2			17
201-854-9/ 88-73-3	1-chloro-2-nitrobenzene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 2.5 (neutral)	T	Carc_1b; Carc_2; muta_2; Rep_2;			101

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
							STOTRE_1; STOTRE_2			
201-857-5/ 88-75-5	2-nitrophenol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = -1.3 (ionizable)	T	STOTRE_2			66
202-049-5/ 91-20-3	Naphthalene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	vM	exp min. Doc/Koc = 2.5 (neutral)	T	Carc_2; STOTRE_1			neg. emissions
202-394-1/ 95-14-7	Benzotriazole	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 1.5 (ionizable)	T	muta_2	DW	A; E	54
202-430-6/ 95-54-5	o-phenylenediamine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Dow/Kow = -0.6 (ionizable)	T	Carc_2; muta_2			neg. emissions
202-486-1/ 96-18-4	1,2,3-trichloropropane	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. Doc/Koc = 1.9 (neutral)	T	SVHC			36
202-577-6/ 97-39-2	1,3-di-o-tolylguanidine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Dow/Kow = -3.0 (ionizable)	T	Carc_1b; Rep_2	DW	F	neg. emissions
202-605-7/ 97-74-5	Tetramethylthiuram monosulphide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Dow/Kow = 1.2 (neutral)	T	STOTRE_2			75
202-679-0/ 98-54-4	4-tert-butylphenol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Doc/Koc = 1.9 (neutral)	T	Rep_2; STOTRE_1; Susp_ED			70
202-705-0/ 98-83-9	2-phenylpropene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 2.8 (neutral)	T	Rep_2			100
202-716-0/ 98-95-3	Nitrobenzene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Doc/Koc = 1.7 (neutral)	T	SVHC			unknown
202-797-2/ 99-88-7	4-isopropylaniline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 1.2 (ionizable)	T	ecotox			89

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
202-808-0/ 99-99-0	4-nitrotoluene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 2.0 (neutral)	T	STOTRE_2; Susp_ED			neg. emissions
202-809-6/ 100-00-5	1-chloro-4-nitrobenzene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 2.1 (neutral)	T	Carc_2; muta_2; STOTRE_2			102
202-852-0/ 100-43-6	4-vinylpyridine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Dow/Kow = 0.2 (ionizable)	T	muta_2			3
202-870-9/ 100-61-8	N-methylaniline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. Doc/Koc = 0.3 (ionizable)	T	STOTRE_1; STOTRE_2			neg. emissions
202-905-8/ 100-97-0	Methenamine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Dow/Kow = -7.5 (ionizable)	T	Rep_2; STOTRE_1			neg. emissions
202-977-0/ 101-80-4	4,4'-oxydianiline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 1.2 (ionizable)	T	SVHC			39
203-135-5/ 103-69-5	N-ethylaniline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Dow/Kow = 1.1 (ionizable)	T	STOTRE_2			neg. emissions
203-400-5/ 106-46-7	1,4-dichlorobenzene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 2.4 (neutral)	T	Carc_2			neg. emissions
203-401-0/ 106-47-8	4-chloroaniline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. Doc/Koc = 1.2 (ionizable)	T	Carc_1b; Carc_2; muta_2; STOTRE_1; STOTRE_2			neg. emissions
203-402-6/ 106-48-9	4-chlorophenol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 0.9 (ionizable)	T	Susp_ED			17
203-509-8/ 107-66-4	Dibutyl hydrogen phosphate	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. Doc/Koc = -8.3 (anionic)	T	Carc_2			45
203-560-6/ 108-20-3	Diisopropyl ether	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 0.6 (neutral)	T	Rep_2			9

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
203-581-0/ 108-42-9	3-chloroaniline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 1.5 (ionizable)	T	ecotox; Carc_1b; STOTRE_1; STOTRE_2			neg. emissions
203-604-4/ 108-67-8	Mesitylene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 2.9 (neutral)	T	STOTRE_1			neg. emissions
203-639-5/ 109-01-3	1-methylpiperazine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. Doc/Koc = 2.9 (ionizable)	T	Rep_2			51
203-646-3/ 109-09-1	2-chloropyridine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 0.8 (neutral)	T	STOTRE_2			81
203-924-4/ 111-96-6	Bis(2-methoxyethyl) ether	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. Dow/Kow = -0.4 (neutral)	T	SVHC			22
204-065-8/ 115-10-6	Dimethyl ether	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test) Slightly Modified.	vM	exp min. Doc/Koc = -0.4 (neutral)	T	Carc_1a; muta_1b			1
204-340-2/ 119-64-2	1,2,3,4-tetrahydronaphthalene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 2.7 (neutral)	T	Carc_2; Susp_ED			neg. emissions
204-341-8/ 119-65-3	Isoquinoline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 1.8 (ionizable)	T	Carc_1b			105
204-429-6/ 120-83-2	2,4-dichlorophenol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 0.0 (ionizable)	T	Susp_ED			21
204-783-1/ 126-33-0	Tetrahydrothiophene 1,1-dioxide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	QSAR min. Dow/Kow = -0.4 (neutral)	T	Rep_1b			unknown
207-529-8/ 479-27-6	1,8-naphthylenediamine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	QSAR min. Dow/Kow = 1.3 (ionizable)	T	Carc_2; muta_2			unknown
207-586-9/ 482-89-3	2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. Doc/Koc = 2.9 (ionizable)	T	STOTRE_2			unknown

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
208-792-1/ 541-73-1	1,3-dichlorobenzene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 2.6 (neutral)	T	STOTRE_2; Susp_ED			62
209-967-5/ 599-61-1	3,3'-sulphonyldianiline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 1.8 (ionizable)	T	STOTRE_2; Susp_ED			neg. emissions
209-968-0/ 599-64-4	4-(α,α-dimethylbenzyl)phenol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 3.0 (ionizable)	T	STOTRE_2; Susp_ED			neg. emissions
210-036-0/ 603-35-0	Triphenylphosphine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Dow/Kow = 2.6 (neutral)	T	Carc_1a; STOTRE_2			unknown
210-248-3/ 611-06-3	1,3-dichloro-4-nitrobenzene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Doc/Koc = 2.5 (neutral)	T	Carc_1b; Carc_2; muta_2; Rep_2			neg. emissions
210-438-6/ 615-60-1	4-chloro-o-xylene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 1.2 (neutral)	T	STOTRE_2			unknown
213-059-4/ 920-66-1	1,1,1,3,3,3-hexafluoropropan-2-ol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = -0.5 (ionizable)	T	Rep_2			neg. emissions
214-189-4/ 1112-39-6	Dimethoxydimethylsilane	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)	vM	exp min. Doc/Koc = 0.7 (neutral)	T	Rep_1b; Rep_2; STOTRE_1			30
215-311-9/ 1321-12-6	Nitrotoluene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 1.9 (neutral)	T	Carc_1b; muta_1b; Rep_2; STOTRE_2			93
217-157-8/ 1758-73-2	Aminoiminomethanesulphinic acid	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 A (new version) (Ready Biodegradability: DOC Die Away Test)	vM	QSAR min. Dow/Kow = -4.3 (zwitterion)	T	STOTRE_2			39
217-168-8/ 1761-71-3	4,4'-methylenebis(cyclohexylamine)	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = -3.6 (ionizable)	T	STOTRE_2; Susp_ED			22

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
218-747-8/ 2224-33-1	Butan-2-one O,O',O''-(vinylsilylidyne)trioxime	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	vM	exp min. Dow/Kow = 0.0 (ionizable)	T	Carc_2; STOTRE_2			54
219-754-9/ 2524-03-0	O,O-dimethyl phosphorochloridothioate	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	QSAR min. Dow/Kow = 1.4 (neutral)	T	muta_2			neg. emissions
220-237-5/ 284-95-7	N,N-dimethylacrylamide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 1.3 (neutral)	T	muta_2			30
221-111-2/ 3006-86-8	Cyclohexylidenebis[tert-butyl] peroxide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test) 17th July 1992	vM	exp min. Doc/Koc = 2.7 (neutral)	T	Carc_2; muta_2			unknown
221-374-3/ 3081-01-4	N-(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 2.5 (ionizable)	T	ecotox			38
221-375-9/ 3081-14-9	N,N'-bis(1,4-dimethylpentyl)-p-phenylenediamine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 1.5 (ionizable)	T	ecotox			62
222-182-2/ 3380-34-5	Triclosan	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. Doc/Koc = 0.9 (ionizable)	T	ecotox; Susp_ED	GW	A; D; K	neg. emissions
222-733-7/ 3590-84-9	Tetraoctyltin	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Dow/Kow = -4.0 (neutral)	T	STOTRE_2			neg. emissions
223-055-4/ 3710-84-7	N,N-diethylhydroxylamine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Dow/Kow = -0.2 (ionizable)	T	muta_2			unknown
225-716-2/ 5026-74-4	p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test) July 17, 1992	vM	exp min. Doc/Koc = 1.9 (ionizable)	T	Carc_2; muta_2; Rep_2; STOTRE_2			71
226-736-4/ 5460-09-3	Sodium hydrogen 4-amino-5-hydroxynaphthalene-2,7-disulphonate	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	QSAR min. Dow/Kow = -4.2 (anionic)	T	Susp_ED			unknown

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
229-563-2/ 6610-29-3	4-methylthiosemicarbazide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. Dow/Kow = -1.0 (ionizable)	T	DNEL			unknown
229-654-7/ 6640-24-0	1-(m-chlorophenyl)piperazine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	QSAR min. Dow/Kow = 0.3 (ionizable)	T	Rep_2			88
229-713-7/ 6674-22-2	1,8-diazabicyclo[5.4.0]undec-7-ene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. Doc/Koc = -6.0 (ionizable)	T	Carc_1b; muta_2			6
229-962-1/ 6864-37-5	2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	exp min. Doc/Koc = -2.2 (ionizable)	T	STOTRE_2; Susp_ED			unknown
230-625-6/ 7226-23-5	Tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 E (Ready biodegradability: Modified OECD Screening Test)	vM	exp min. Doc/Koc = 0.9 (neutral)	T	Rep_2			neg. emissions
230-847-3/ 7336-20-1	Disodium 4,4'-diaminostilbene-2,2'-disulphonate	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	QSAR min. Dow/Kow = -3.1 (anionic)	T	Susp_ED			neg. emissions
231-274-1/ 7474-78-4	3,4-diaminobenzenesulphonic acid	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	QSAR min. Dow/Kow = -2.7 (ionizable)	T	Susp_ED			54
237-163-4/ 13676-54-5	1,1'-(methylenedi-p-phenylene)bismaleimide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Doc/Koc = 3.0 (neutral)	T	muta_2			unknown
242-424-0/ 18559-94-9	Salbutamol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. Dow/Kow = -0.6 (ionizable)	T	Susp_ED			unknown
245-366-4/ 22984-54-9	Butan-2-one O,O',O''-(methylsilylidyne)trioxime	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	vM	exp min. Dow/Kow = 0.0 (ionizable)	T	STOTRE_2			neg. emissions
246-836-1/ 25321-14-6	Dinitrotoluene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 1.0 (neutral)	T	Carc_1b; muta_2; Rep_2; STOTRE_2			22

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
248-394-5/ 27310-25-4	7-aminonaphthalene-1,3,5-trisulphonic acid	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	QSAR min. Dow/Kow = -5.0 (ionizable)	T	Susp_ED			45
255-255-2/ 41198-08-7	O-(4-bromo-2-chlorophenyl) O-ethyl S-propyl phosphorothioate	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Doc/Koc = 3.0 (neutral)	T	ecotox			neg. emissions
256-435-3/ 49701-24-8	4-amino-2,5-dimethoxy-N-methylbenzenesulphonamide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Dow/Kow = 0.3 (ionizable)	T	Susp_ED			neg. emissions
258-004-5/ 52556-42-0	Sodium 3-(allyloxy)-2-hydroxypropanesulphonate	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	QSAR min. Dow/Kow = -2.9 (anionic)	T	Rep_2			neg. emissions
258-904-8/ 53988-10-6	1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 1.9 (ionizable)	T	Rep_2; STOTRE_2			neg. emissions
267-122-6/ 67801-01-8	Barium bis[5-chloro-4-ethyl-2-[(2-hydroxy-1-naphthyl)azo]benzenesulphonate]	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Dow/Kow = 0.1 (anionic)	T	Susp_ED			neg. emissions
269-929-9/ 68391-11-7	Pyridine, alkyl derivs.	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	read-across min. Dow/Kow = -0.1 (ionizable)	T	Carc_1a; Carc_1b; muta_1a; muta_1b; STOTRE_2			unknown
275-662-9/ 71604-74-5	m-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. Doc/Koc = 1.9 (ionizable)	T	muta_2; STOTRE_2			75
283-482-7/ 84650-02-2	Distillates (coal tar), benzole fraction	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	vM	exp min. Doc/Koc = 1.4 (neutral)	T	Carc_1a; Carc_1b; muta_1b; Rep_2; STOTRE_1			unknown
298-842-9/ 93839-71-5	4-[[(2-aminophenyl)methyl]amino]cyclohexyl acetate	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	QSAR min. Dow/Kow = 0.3 (ionizable)	T	Susp_ED			98
400-600-6/ 71868-10-5	2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. Doc/Koc = 1.9 (ionizable)	T	Rep_1b			unknown

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
402-860-6/ 110553-27-0	4,6-bis(octylthiomethyl)-o-cresol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. Doc/Koc = 2.0 (neutral)	T	ecotox			unknown
405-800-7/ 27955-94-8	4,4',4"-(ethan-1,1,1-triyl)triphenol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. Doc/Koc = 1.7 (ionizable)	T	Susp_ED			unknown
411-280-2/ 74091-64-8	2,5-bis-isocyanatomethyl-bicyclo[2.2.1]heptane	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = 0.2 (ionizable)	T	STOTRE_1			91
423-800-5/ 7305-71-7	2-amino-5-methylthiazole	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	QSAR min. Dow/Kow = 0.3 (ionizable)	T	STOTRE_2			unknown
428-100-3/ 94239-04-0	2-fluoro-6-trifluoromethylpyridine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	vM	exp min. Doc/Koc = 1.7 (neutral)	T	STOTRE_2			unknown
480-070-0/ 85-27-8	4-(1-Phenylethyl)-benzene-1,3-diol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	vM	exp min. Doc/Koc = 1.5 (ionizable)	T	Susp_ED			unknown
483-270-6/ -	Tin, dioctylbis(2,4-pentanedionato-κO2,κO4)-	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Doc/Koc = 0.9 (neutral)	T	Rep_2; STOTRE_2			unknown
500-033-5/ 25068-38-6	4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	vM	exp min. Doc/Koc = 2.1 (neutral)	T	Susp_ED			unknown
601-329-8/ 114798-26-4	[2-butyl-4-chloro-1-({4-[2-(2H-1,2,3,4-tetrazol-5-yl)phenyl]phenyl}methyl)-1H-imidazol-5-yl]methanol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	read-across min. Dow/Kow = 1.0 (ionizable)	T	Lact; Rep_1b; Rep_2			neg. emissions
609-335-2/ 3717-40-6	N,N-dimethyl-1-adamantanamine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 B (Inherent biodegradability: Zahn-Wellens/EMPA Test)	vM	QSAR min. Dow/Kow = 0.9 (ionizable)	T	Rep_2			45
611-210-2/ 54914-95-3	sodium 2-amino-5-methylbenzenesulfonate	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	QSAR min. Dow/Kow = -1.7 (anionic)	T	Susp_ED			unknown
614-637-2/ 68603-75-8	No IUPAC name	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 310 (Ready	vM	exp min. Doc/Koc = 1.6 (ionizable)	T	ecotox			unknown

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
			Biodegradability - CO2 in Sealed Vessels (Headspace Test)							
618-706-8/ 91161-71-6	(2E)-N,6,6-trimethyl-N-(1-naphthylmethyl)hept-2-en-4-yn-1-amine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	vM	exp min. Dow/Kow = 0.3 (ionizable)	T	ecotox			unknown
679-514-8/ 154279-60-4	4,4'-methylenebis(N-sec-butylcyclohexamine)	Pot. P/vP++	weight-of-evidence (this study): QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	vM	exp min. Doc/Koc = -1.0 (ionizable)	T	ecotox			107
200-681-6/ 68-22-4	Norethisterone	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. Dow/Kow = 2.7 (neutral)	T	Carc_1b; Carc_2; Lact; Rep_1a; Rep_1b; Rep_2; STOTRE_2; Susp_ED			108
201-052-9/ 77-73-6	3a,4,7,7a-tetrahydro-4,7-methanoindene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	M	exp min. Dow/Kow = 2.8 (neutral)	T	Rep_1a; Rep_2; STOTRE_1; STOTRE_2			neg. emissions
201-254-7/ 80-15-9	α,α-dimethylbenzyl hydroperoxide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test) (1981)	M	exp min. Doc/Koc = 3.1 (neutral)	T	muta_2; STOTRE_1; STOTRE_2			neg. emissions
201-279-3/ 80-43-3	Bis(α,α-dimethylbenzyl) peroxide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	M	exp min. Doc/Koc = 4.0 (neutral)	T	Rep_2			51
201-696-0/ 86-74-8	Carbazole	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 E (Ready biodegradability: Modified OECD Screening Test) adopted 1981	M	exp min. Doc/Koc = 3.5 (neutral)	T	Carc_2; muta_2			neg. emissions
201-806-7/ 88-17-5	α,α,α-trifluoro-o-toluidine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. Dow/Kow = 2.3 (neutral)	T	STOTRE_2			71
202-396-2/ 95-16-9	Benzothiazole	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test) (1992)	M	exp min. Dow/Kow = 2.0 (ionizable)	T	STOTRE_2			neg. emissions
202-551-4/ 97-00-7	1-chloro-2,4-dinitrobenzene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. Dow/Kow = 2.2 (neutral)	T	muta_2; STOTRE_1; STOTRE_2			unknown

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
202-588-6/ 97-52-9	4-nitro-o-anisidine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	M	exp min. Dow/Kow = 1.2 (ionizable)	T	Carc_2; muta_2			42
203-002-1/ 102-06-7	1,3-diphenylguanidine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	M	exp min. Dow/Kow = 1.4 (ionizable)	T	Rep_2	DW	F	75
203-004-2/ 102-08-9	1,3-diphenyl-2-thiourea	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	M	exp min. Dow/Kow = 2.0 (ionizable)	T	Rep_2; STOTRE_2			11
203-697-1/ 109-70-6	1-bromo-3-chloropropane	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	QSAR min. Dow/Kow = 2.0 (neutral)	T	Carc_1b; Carc_2; muta_2; Rep_2; STOTRE_2			105
203-865-4/ 111-40-0	2,2'-iminodi(ethylamine)	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	M	exp min. Doc/Koc = 4.0 (ionizable)	T	Rep_1b			neg. emissions
204-337-6/ 119-61-9	Benzophenone	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	M	exp min. Doc/Koc = 3.1 (neutral)	T	Carc_2; STOTRE_2; Susp_ED			45
204-419-1/ 120-71-8	6-methoxy-m-toluidine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	M	exp min. Dow/Kow = 1.1 (ionizable)	T	SVHC			7
204-501-7/ 121-86-8	2-chloro-4-nitrotoluene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	M	QSAR min. Dow/Kow = 2.9 (neutral)	T	STOTRE_2			unknown
207-096-5/ 434-03-7	Ethisterone	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	M	exp min. Dow/Kow = 2.7 (neutral)	T	ecotox; Carc_2; Lact; Rep_1a; Rep_2; Susp_ED			neg. emissions
218-817-8/ 2243-62-1	1,5-naphthylenediamine	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	M	QSAR min. Dow/Kow = 1.1 (ionizable)	T	Carc_2			neg. emissions

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
219-372-2/ 2425-85-6	1-(4-methyl-2-nitrophenylazo)-2-naphthol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 C (Ready Biodegradability: Modified MITI Test (I))	M	exp min. Dow/Kow = 3.7 (ionizable)	T	ecotox			neg. emissions
219-470-5/ 2440-22-4	2-(2H-benzotriazol-2-yl)-p-cresol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. Doc/Koc = 3.0 (ionizable)	T	STOTRE_2; Susp_ED			75
219-863-1/ 2554-06-5	2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)	M	exp min. Doc/Koc = 3.8 (neutral)	T	ecotox			68
220-481-2/ 2781-10-4	Dibutyltin bis(2-ethylhexanoate)	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	M	exp min. Dow/Kow = 2.6 (neutral)	T	muta_2; Rep_1b; Rep_2; STOTRE_1; STOTRE_2; DNEL			93
224-638-6/ 4433-79-8	4'-chloro-2',5'-dimethoxyacetoacetanilide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	M	exp min. Dow/Kow = 1.7 (ionizable)	T	STOTRE_2			42
228-782-0/ 6358-64-1	4-chloro-2,5-dimethoxyaniline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	M	exp min. Dow/Kow = 1.8 (ionizable)	T	STOTRE_2; Susp_ED			unknown
237-159-2/ 13674-87-8	Tris[2-chloro-1-(chloromethyl)ethyl] phosphate	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	M	exp min. Doc/Koc = 3.7 (neutral)	T	Carc_2; STOTRE_2	DW	J	81
246-835-6/ 25321-09-9	Diisopropylbenzene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	M	exp min. Doc/Koc = 3.8 (neutral)	T	STOTRE_2			neg. emissions
246-910-3/ 25376-45-8	Diaminotoluene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	M	exp min. Doc/Koc = 3.4 (ionizable)	T	Carc_1b; muta_2; Rep_2; STOTRE_2			neg. emissions
247-094-1/ 25550-51-0	Hexahydromethylphthalic anhydride	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	M	read-across min. Dow/Kow = 2.1 (neutral)	T	SVHC			30

EC/ CAS	Name	P conc.	P rationale	M conc.	M rationale	T conc.	T rationale	Known in DW or GW[a]	DW or GW Study[b]	Relative emission rank[c]
248-097-0/ 26898-17-9	Dibenzyltoluene	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. Doc/Koc = 3.6 (neutral)	T	ecotox			99
253-292-9/ 36968-27-1	4-[[4-(aminocarbonyl)phenyl]azo]-3-hydroxy-N-(2-methoxyphenyl)naphthalene-2-carboxamide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 302 C (Inherent Biodegradability: Modified MITI Test (II))	M	QSAR min. Dow/Kow = 3.6 (ionizable)	T	muta_2			85
253-775-4/ 38083-17-9	Climbazole	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	M	exp min. Doc/Koc = 3.5 (ionizable)	T	ecotox			81
270-986-7/ 68512-65-2	Resin acids and Rosin acids, esters with ethylene glycol	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	read-across min. Dow/Kow = 2.4 (neutral)	T	Rep_2			unknown
273-066-3/ 68937-41-7	Phenol, isopropylated, phosphate (3:1)	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 D (Ready Biodegradability: Closed Bottle Test)	M	exp min. Doc/Koc = 3.7 (neutral)	T	Rep_2; STOTRE_2			unknown
273-227-8/ 68953-84-4	1,4-Benzenediamine, N,N'-mixed Ph and tolyl derivs.	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 F (Ready Biodegradability: Manometric Respirometry Test)	M	exp min. Dow/Kow = 3.8 (neutral)	T	ecotox			unknown
276-017-4/ 71786-67-9	Benzyl(3-hydroxyphenacyl)methylammonium chloride	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	QSAR min. Dow/Kow = 0.5 (cationic)	T	Susp_ED			unknown
277-553-1/ 73612-34-7	Barium bis[6-chloro-4-[(2-hydroxy-1-naphthyl)azo]toluene-3-sulphonate]	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. Dow/Kow = 2.0 (anionic)	T	Susp_ED			unknown
423-340-5/ 162881-26-7	Phenyl bis(2,4,6-trimethylbenzoyl)-phosphine oxide	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. Doc/Koc = 3.9 (neutral)	T	ecotox			unknown
425-280-5/ 114772-54-2	4'-Bromomethylbiphenyl-2-carbonitrile	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. Doc/Koc = 3.4 (neutral)	T	muta_2			unknown
604-045-2/ 137862-53-4	(2S)-3-methyl-2-(N-{[2'-(1H-1,2,3,4-tetrazol-5-yl)-[1,1-biphenyl]-4-yl]methyl}pentanamido)butanoic acid	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	exp min. Dow/Kow = 1.2 (ionizable)	T	Rep_1a; Rep_2	DW	E	neg. emissions
688-269-6/ 641571-11-1	3-(4-Methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)aniline	Pot. P/vP++	weight-of-evidence (this study) based on all QSARs and screen tests, e.g. 301 B (Ready Biodegradability: CO2 Evolution Test)	M	QSAR min. Dow/Kow = 1.9 (ionizable)	T	Susp_ED			unknown

Footnotes to Table 1.

a) DW = reported above detection limits in treated or distributed drinking water; GW = reported above detection limits in ground water areas isolated from emission sources.
b) A = Loos et al. (2010); D = Lapworth et al. (2012); E = Schmidt (2017); F = Berger et al. (2017); G = European Drinking Water Directive, Regulation 98/83/EC.; H = Kuhlmann et al. (2010) and Skark et al. (2011); I = Kaboré et al. (2018); J = Stackelberg et al. (2007); K = Benotti et al. (2008).
c) The relative emission rank system is presented in Schulze et al. (2018); essentially this system gives a rank based on produced tonnages of the substance and a list of Environmental Release Categories (ERCs) registered in REACH. The actual score is not presented due to potential sensitivity (as confidential tonnage data could be back-calculated); instead the rank of the actual score is presented relative to other substances on the list, with the lower the score implying a higher likelihood of emissions relative to other substances on this list. "unknown" = not enough registration data was available to make a score; "neg. emissions" = the substance is registered to be used in a way that only negligible emissions are anticipated.

7 From PMT/vPvM Hazard to Risk Mitigation Measures

The proposed PMT/vPvM assessment can be used to identify if a substance has intrinsic properties that indicate a potential hazard to contaminate sources of drinking water. However, a substance meeting the hazard criteria does not necessarily imply that it will be a threat to water sources. This will depend to a very large extent on how the substance is ultimately used and how much is emitted. The overriding purpose of this initiative is that substances that meet or could meet the PMT/vPvM criteria be used in a way that mitigates their risk of appearing or accumulating in potential drinking water sources.

The recent position paper by UBA (Neumann and Schliebner, 2017) underscores that there are several similarities between PMT/vPvM and PBT/vPvB substances in terms of hazards; therefore, the paper suggests that similar to PBT/vPvB substances, PMT/vPvM substances should be assessed with the steps outlined in Annex I (4.0.2) of the REACH regulation:

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

For PMT/vPvM substances, "Step 1: Comparison with the Criteria" is essentially the exercise conducted in this report. However, all conclusions in this report are subject to change, upon the emergence of higher quality data than used in this present assessment.

The next step "Step 2: Emission Characterization" would 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 (European Chemical Agency, 2017). These can be largely applied to PMT/vPvM assessments, with the exception that water cycle enrichment and potential accumulation in local drinking water resources should be additionally considered.

Following such assessments, manufacturers, importers and downstream users would be able to develop risk mitigation measures to protect drinking water quality from undue contamination. Local authorities, water suppliers and regulators would also be encouraged to work with manufacturers, importers and downstream to ensure the mitigation measures adequately protect the sources of our drinking water (Neumann and Schliebner, 2017).

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