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Abstract: A prioritization framework for PMT/vPvM Substances under REACH for registrants, regulators, researchers and the water sector

A framework was developed to facilitate the prioritization PMT/vPvM substances that require immediate action from REACH registrants, regulators, researchers and the water sector to safeguard our drinking water resources against contamination. The developed framework is the result of stakeholder surveys, monitoring campaigns, laboratory investigations, literature reviews and a stakeholder workshop. The prioritization framework for PMT/vPvM substances is based on the following five prioritization categories: i) the PMT/vPvM hazard; ii) the REACH emission likelihood; iii) the analytical and monitoring gaps; iv) the remediation gaps and v) the exposure level. To implement this prioritization framework, 176 substances were selected based on several considerations that would fully explore a range of outcomes. The selection criteria included whether or not they meet PMT/vPvM criteria, data gaps regarding the PMT/vPvM hazard assessment, whether they contain a perfluoroalkyl substructure or triazine substructure, suspicion of being present in German drinking water resources and current knowledge of detection methods.

The PMT/vPvM hazard assessment was conducted for all 176 substances, and it was found that 99 met the PMT/vPvM criteria. The REACH emission likelihood could be derived for 152 of the 176 substances, and it was found that 133 of them had either a "high" (84 substances) or "very high" (49 substances) REACH emission likelihood. The analytical and monitoring gaps and the remediation gaps were investigated for 150 of the substances by carrying out surveys of analytical labs and water treatment facilities throughout Germany, as well as through original experimental work. From this investigation, 26 substances were considered to have a minor or major analytical gap, and 58 substances to have a major monitoring gap. There were substantial remediation gaps for the investigated substances, as 78 could not be removed by activated carbon (AC) filtration nor ozonation, 22 could only be removed by ozonation and 31 could only by removed by AC filtration. The exposure levels were investigated by a monitoring study of 78 of the 176 substances within 13 drinking water source areas in German at two different time points. This was complimented by a literature review which found monitoring data for 12 substances not included in the monitoring campaign. From this, 10 substances were considered ubiquitous at high concentrations, 28 ubiquitous at low concentrations, and 36 that were monitored only in local regions at either high or low concentrations. From the investigation of these five prioritization categories, this prioritization framework identified 43 PMT/vPvM substances of the highest-priority, 23 substances of high-priority and 33 of moderate-priority for follow up. The prioritization framework presented here can serve as an early warning system to identify immediate threats and the need for action for PMT/vPvM substances. It can readily be applied to other substances than those considered in this study.

Kurzbeschreibung: Ein Priorisierungsrahmenwerk für PMT/vPvM-Stoffe im Rahmen von REACH für Registranten, Regulierungsbehörden, Forscher und den Wassersektor

Ein Priorisierungsrahmenwerk wurde entwickelt, um die Auswahl derjenigen PMT/vPvM-Stoffe zu unterstützen, die sofortige Maßnahmen durch REACH-Registranten, Regulierungsbehörden, Forschern und dem Wassersektor erfordern, um die Trinkwasserressourcen vor einer Kontamination zu schützen. Das entwickelte Rahmenwerk ist das Ergebnis von Stakeholder-Befragungen, Monitoringkampagnen, Laboruntersuchungen, Literaturrecherchen und einem Stakeholder-Workshop. Das Rahmenwerk für die Priorisierung von PMT/vPvM-Stoffen basiert auf den folgenden fünf Priorisierungskategorien: I) die PMT/vPvM-Gefahrenbewertung; II) die REACH-Emissionswahrscheinlichkeit; III) die Analytik- und Monitoringlücken; IV) die Wasseraufbereitungslücke und v) das Expositionsniveau. Zur Umsetzung dieses Priorisierungsrahmenwerks wurden 176 Stoffe auf der Grundlage mehrerer Überlegungen ausgewählt. Zu den Auswahlkriterien gehörten, ob sie die PMT/vPvM-Kriterien erfüllen oder nicht, Datenlücken in Bezug auf die PMT/vPvM-Bewertung, ob sie eine Perfluoralkyl-Substruktur oder Triazin-Substruktur enthalten, der Verdacht, in deutschen Trinkwasserressourcen vorhanden zu sein, und aktuelle Kenntnisse zu Analytikmethoden.

Die PMT/vPvM-Gefahrenbewertung wurde für alle 176 Stoffe durchgeführt, und es wurde festgestellt, dass 99 die PMT/vPvM-Kriterien erfüllten. Die REACH-Emissionswahrscheinlichkeit konnte für 152 der 176 Stoffe abgeleitet werden, und es wurde festgestellt, dass 133 von ihnen entweder eine „hohe“ (84 Stoffe) oder „sehr hohe“ (49 Stoffe) REACH-Emissionswahrscheinlichkeit aufwiesen. Die Analyse- und Monitoringlücken und die Wasseraufbereitungslücke wurden für 150 der Stoffe durch eine Umfrage bei Analyselaboren und Wasseraufbereitungsanlagen in ganz Deutschland sowie durch eigene experimentelle Arbeiten untersucht. Bei dieser Untersuchung wurde festgestellt, dass 26 Stoffe eine geringe bis erhebliche Analytiklücke und 58 Stoffe eine erhebliche Monitoringlücke aufweisen. Es gab erhebliche Wasseraufbereitungslücken für die untersuchten Substanzen, da 78 weder durch Aktivkohlefilter noch durch Ozonung entfernt werden können, 22 können nur durch Ozonung und 31 nur durch Aktivkohlefilter entfernt werden. Die Expositionswerte wurden durch eine Monitoringstudie von 78 der 176 Substanzen in 13 Trinkwassereinzugsgebieten zu zwei verschiedenen Zeitpunkten untersucht. Dies wurde durch eine Literaturrecherche ergänzt, in der Monitoringdaten für 12 Stoffe gefunden wurden, die nicht in die Monitoringkampagne aufgenommen wurden. Davon waren 10 der Substanzen allgegenwärtig in hohen Konzentrationen, 28 allgegenwärtig in niedrigen Konzentrationen und 36, die in lokalen Regionen entweder in hohen oder niedrigen Konzentrationen überwacht wurden. Aus der Bewertung dieser fünf Priorisierungskategorien ergeben sich durch das Priorisierungsrahmenwerk 43 PMT/vPvM-Stoffe mit höchster Priorität, 23 Stoffe mit hoher Priorität und 33 Stoffe mit mittlerer Priorität für Folgemaßnahmen. Das hier vorgestellte Priorisierungsrahmenwerk kann als Frühwarnsystem dienen, um eine unmittelbare Bedrohungen oder Besorgnis durch andere als in dieser Studie berücksichtigen PMT/vPvM- oder potenzielle PMT/vPvM-Stoffe zu identifizieren.

Table of contents

List of figures

List of tables

List of abbreviations

AC	Activated Carbon
AOF	Adsorbable organic fluorine
BVT	Bed Volumes Treated
CMR	Carcinogenic, mutagenic, toxic for reproduction
DIN ISO EN	Deutsches Institut fuer Normung (German Institute for Standardisation)
DNEL	Derived no effect level
DOC	Dissolved organic carbon
D_{OW}	Octanol-water distribution coefficient for all species
DT50	The half-life of a substance in soil
DWS	Drinking water supplier
E-score	Emission-score
EC10	Concentration of a chemical that shows effects for 10% of the test animals
EN	Europaische Norm (European standard)
FTS	Fluorotelomersulfonate
HILIC	Hydrophilic interaction liquid chromatography
HPLC	High-performance liquid chromatography
LC_{50}	Concentration of a chemical that results in a mortality of 50% of the test animals
log K_{oc}	Soil sorption coefficient normalized to the total organic carbon
LSER	Linear solvation energy relationship
M	Mobility criterion
MS	Mass spectrometry
MS/MS	Tandem mass spectrometry
P	Persistent criterion
PBT	Persistent, bioaccumulative and toxic
PNEC	Predicted no-effect concentration
NOEC	No observed effect concentration
PAC	Powdered activated carbon
PFAA	Perfluoroalkyl acids
PFAS	Per and polyfluoroalkyl acids
PFCA	Perfluorocarboxylic acids
PFPrA	Perfluorpropanoic acid

PFSA	Perfluorosulfonic acids
PM	Persistent and mobile in the aquatic environment
PMT	Persistent, mobile and toxic
RPLC	Reverse Phase Liquid Chromatography
RMM	Risk management measures
RMOA	Risk management option analysis
RO	Reverse Osmosis
RPLC	Reverse Phase Liquid Chromatography
SMARTS	SMiles ARbitrary Target Specification
SMILES	Simplified molecular-input line-entry system
STOT RE	Specific target organ toxicity - repeat exposure
T	Toxicity criterion
TFA	Trifluoroacetic acid
TFMSA	Trifluoromethyl sulfonic acid
TPA	Tonnes per annum
UVCB	Substances of "Unknown or Variable composition, Complex reaction products or Biological material"
vP	Very persistent criterion
vM	Very mobile criterion
vPvB	Very persistent, very bioaccumulative
vPvM	Very persistent, very mobile

Summary

PMT/vPvM substances have the intrinsic chemical properties to be widely distributed in the sources of our drinking water, and in particular groundwater and bank filtrate, when emitted at low-levels. For most PMT/vPvM substances there is no emission data, and many also have limited information on analytical methods or monitoring data. Many PMT/vPvM substances are also typically resistant to advanced water treatment, though there is often little information about this. Further, PMT/vPvM substances that are registered in REACH can vary exposure levels. To best manage and mitigate real or potential risks of PMT/vPvM substances, a prioritization framework for PMT/vPvM substances is needed. One key advantage of a prioritization framework is that it does not require the intense amount of data or assumptions that quantitative risk assessments or exposure models often require. Prioritization frameworks can be based on the availability of known data as well as the status of existing knowledge gaps to spot red flags.

This report presents such a prioritization framework. The prioritization framework was the outcome of a large-scale research project initiated in 2019. It takes in to consideration the views of diverse stakeholders, including industry, regulators, researchers and the water sector. The prioritization framework includes the categories presented in Summary Box 1.

Summary Box 1. Categories of the prioritization framework for PMT/vPvM substances

- **PMT/vPvM hazard**: This category indicates the PMT/vPvM conclusion, as defined in Neumann and Schliebner (2019), and as assessed in Arp and Hale (2023).
- **REACH Emission Likelihood**: This category indicates the likelihood that emissions could be occurring, based on REACH registered volumes, monitoring data and the emission-score (E-score) as presented in Arp and Hale (2019)
- **Analytical and monitoring gaps**: This category indicates the current state of analytical development and monitoring activities of the substance
- **Remediation gap**: This category indicates the technology and investment costs required to remove the substance from drinking water
- **Exposure level**: This category is related to the "analytical and monitoring gap" category, but is focussed on documented concentrations in the following drinking water source media: bank filtrate, groundwater, raw water and drinking water.
- **Overall prioritization level**. This category indicates the overall prioritization based on all individual categories.

To implement this prioritization framework, 176 substances were selected based on several considerations that would fully explore a range of outcomes. The selection criteria included whether they meet PMT/vPvM criteria, data gaps regarding the PMT/vPvM hazard assessment, whether they contain a perfluoroalkyl substructure or triazine substructure, suspicion of being present in German drinking water reources and current knowledge of detection methods.

The **PMT/vPvM hazard category** is based on Arp and Hale (2023), which presents an updated guidance for assessing the PMT/vPvM hazard. The 176 substances selected exhibited a wide range of PMT/vPvM assessment conclusions, ranging from PMT/vPvM substances (99 substances), substances that were persistent and mobile but with no high-quality consensus conclusions that the criteria for T is met (38 substances), substances requiring more data to assess if the PMT/vPvM criteria is met (20 substances), substances that are not PMT/vPvM substances (18 substances) and 1 substance where there was not sufficient data to make an assessment.

The **REACH emission likelihood category** is based on REACH registered volumes, monitoring data and the emission-score (E-score), as presented in Arp and Hale (2019). The E-score is based on REACH registered use categories and volumes. Most of the 176 substances selected had a high or very high REACH emission likelihood (133 substances), whereas 21 had a medium or low REACH emission likelihood and there were 22 substances where this could not be assessed as they were not REACH registered but were impurities or transformation products of REACH registered substances.

The **analytical and monitoring gaps** are considered as one category and not two because, in practice, there is a lot of overlap between these two gaps. Broadly speaking the analytical gap refers to substances that are not analysed because there is no method currently available to analyse the substance. The monitoring gap refers to substances that could be monitored using existing methods but currently are not. To investigate this gap, surveys were sent to water analysis labs throughout Germany. Results show that for 26 of the 176 substances there is either a major or minor analytical gap, for 87 substances there is a major or minor monitoring gap, and for 27 substances there was extensive monitoring information (26 of the selected substances were not included in the survey).

The **remediation gap** focussed on the two most commonly available advanced treatment methodologies: activated carbon (AC) filtration and ozonation. The gap was investigated through a screening approach based on structure (the *Hot-Target-approach*), experiments for substances commonly detected from the monitoring campaign, and interviews with 13 German water treatment companies. It was concluded that 78 of the 176 substances could not be treated with either ozonation or activated carbon filtration, 22 substances could be treated with ozonation only, 31 substances could be treated with activated carbon filtration only, and 19 substances could be treated with both methods (an evaluation was not made for 26 of the substances).

To assess the **exposure level**, an intensive monitoring campaign was conducted for 13 regions of drinking water abstraction throughout Germany, covering the Danube, Elbe, Ems, Havel, Main, Neckar, Rhine, Sieg, river basins as well as the lakes Constance and Tegel. The sampling included surface waters, bank filtrate, groundwater and raw water. The monitoring campaign included 78 of the 176 selected substances, including 16 PMT/vPvM substances that have not previously been monitored for in the literature. In addition, the literature review presented in (Arp et al., 2023a) was also used to assess the exposure level, as this report contained monitoring data from the literature for 58 of the 176 substances. From this monitoring study and literature review, data was available for 90 of the 176 selected substances. 10 substances were considered ubiquitous at high concentrations, 28 ubiquitous at low concentrations, 36 substances as present in local environments but not ubiquitous, and 16 substances as monitored commonly and not detected.

The **overall prioritization level** was developed for REACH registered substances. Two of the classes in this category were previously defined in (Arp et al., 2023b): the High-Priority class and the Moderate-Priority class. These are PMT/vPvM substances registered under REACH that were registered with volumes > 10 tpa or between 1-10 tpa, respectively. The Highest-Priority class is introduced in this report, and refers to substances met the High-Priority class but also have an additional prioritization concern at the highest level, such as major analytical gap, unavailability of remediations methods, or ubiquitous detection at high concentrations. The "Potential-Priority" class refers to substances that could meet the PMT/vPvM criteria if more data were available, such as persistent and mobile substances that did not meet the vPvM criteria and for which there are no high-quality consensus conclusions that the criteria for T is met. The "Lowest-Priority" class refers to substances that do not meet the PMT/vPvM criteria. From this analysis, 43 substances were considered Highest-Priority, 23 substances were considered High-Priority, 33 substances were considered Moderate-Priority, 65 substances were considered Potential-Priority and 11 substances were considered Lowest-Priority (with also 1 substance for which an overall prioritization could not be made). The 43 Highest-Priority PMT/vPvM substances are those that should be given the most attention by industry, regulators and the water sector for strategies to prevent pollution under REACH. Substances that were considered of Potential-priority should also be investigated in order to obtain more persistence, mobility or toxicity data, so that a final conclusion on the PMT/vPvM hazard assessment can be made. Such a final conclusion would affect the overall prioritization level.

In addition to the prioritization framework, various communication and dissemination activities were conducted as part of this project, as shown in the appendices. This work includes hosting a large online workshop (attended by over 500 participants), developing an updated website for PMT/vPvM substances hosted by the UBA, publishing 12 popular and scientific articles, in addition to presenting this work at many different forums, including a keynote at SETAC Copenhagen (Arp, 2022). The appendix also contains 10 fact sheets which were developed within the project for selected substances that met the PMT/vPvM criteria or are precursors of them.

Zusammenfassung

PMT/vPvM-Stoffe besitzen die intrinsischen Stoffeigenschaften, die dazu führen können, dass sie sich in den Ressourcen unserer Trinkwässer weit verbreiten, insbesondere im Grundwasser und im Uferfiltrat, selbst dann, wenn sie nur in niedrigen Konzentrationen freigesetzt werden. Für die meisten PMT/vPvM-Stoffe liegen keine Emissionsdaten vor, und für viele fehlen Analytikmethoden oder Monitoringdaten. PMT/vPvM-Stoffe unterscheiden sich hinsichtlich ihrer Resistenz gegen fortgeschrittene technische Wasseraufbereitung. Auch sind viele PMT/vPvM-Stoffe typischerweise resistent gegen Wasseraufbereitung, aber es liegt in vielen Fällen dazu keine Bewertung vor. Weiterhin weisen REACH-registrierte PMT/vPvM-Stoffe sehr unterschiedliche Expositionsniveaus auf. Um die tatsächlichen oder potenziellen Risiken von PMT/vPvM-Stoffen bestmöglich zu beherrschen und zu mindern, ist ein Priorisierungsrahmenwerk für PMT/vPvM-Stoffe erforderlich. Ein wesentlicher Vorteil eines Priorisierungsrahmenwerks besteht darin, dass er nicht die intensive Menge an Daten oder Annahmen erfordert, die bei der quantitativen Risikobewertungen oder Expositionsmodellen häufig erforderlich sind. Priorisierungsrahmen können auf der Verfügbarkeit bekannter Daten sowie mit bestehenden Wissenslücken basieren, um Warnsignale zu erkennen.

Dieser Bericht stellt einen solchen Priorisierungsrahmen vor. Der Priorisierungsrahmen ist das Ergebnis eines langjährigen Forschungsprojekts, initiiert 2019. Es berücksichtigt die Ansichten verschiedener Interessenträger, darunter Industrie, Regulierungsbehörden, Forscher und dem Wasserversorgungssektor. Der Priorisierungsrahmen umfasst die in Kasten 1 dargestellten Kategorien.

Kasten 1. Kategorien des Priorisierungsrahmens für PMT/vPvM-Stoffe

- **PMT/vPvM-Gefährlichkeit:** Diese Kategorie gibt die PMT/vPvM-Schlussfolgerung an, wie sie in Neumann und Schliebner (2019) definierte und in Arp und Hale (2023) bewertet wurde.
- **REACH-Emissionswahrscheinlichkeit:** Diese Kategorie gibt die Wahrscheinlichkeit an, dass Emissionen auftreten können, basierend auf REACH registrierten Verwendungsmengen und des in Arp und Hale (2019) dargestellten Emissions-Scores (E-score).
- **Analytik- und Monitoringlücken:** Diese Kategorie gibt an, wie für den Stoff der aktuelle Stand bei der Entwicklung neuer Analytikmethoden und beim Umweltmonitoring ist.
- **Wasseraufbereitungslücke:** Diese Kategorie gibt die Technologie- und Investitionskosten an, die erforderlich sind, um den Stoff aus dem Trinkwasser zu entfernen.
- **Expositionshöhe:** Diese Kategorie bezieht sich auf die Kategorie „Analytik- und Monitoringlücken“, aber is fokusiert auf bereits bekannt Konzentrationen in den Trinkwasserresourcen: Uferfiltrat, Grundwasser, Rohwasser und Trinkwasser.
- **Gesamtprioritätsebene:** Diese Kategorie gibt die Gesamtpriorität auf der Grundlage aller einzelnen Kategorien an.

Zur Umsetzung dieses Priorisierungsrahmens wurden 176 Stoffe auf der Grundlage mehrerer Erwägungen ausgewählt, um eine Reihe von Ergebnissen vollständig zu untersuchen. Zu den Auswahlkriterien gehörten, ob sie die PMT/vPvM-Kriterien erfüllen, Datenlücken hinsichtlich der PMT/vPvM-Gefahrenbewertung, ob sie eine perfluorierte Alkylunterstruktur oder Triazin-

Unterstruktur enthalten, der Verdacht, ob sie in Trinkwasserressourcen in Deutschland vorkommen und der aktuelle Wissenstand zur Analytikmethode.

Die Kategorie **PMT/vPvM-Gefährlichkeit** basiert auf Arp und Hale (2023) die aktualisierten Leitlinien für die Bewertung der PMT/vPvM-Eigenschaften präsentieren. Die 176 ausgewählten Stoffe wiesen ein breites Spektrum von PMT/vPvM-Schlussfolgerungen auf. Diese reichten von PMT/vPvM-Stoffen (99 Stoffe) über Stoffe, die persistent und mobil sind, ohne einen Konsens von hoher Qualität darüber, dass das T-Kriterium erfüllt ist (38 Stoffe), bis hin zu Stoffen, für die mehr Daten erforderlich sind, um zu beurteilen zu können, ob die PMT/vPvM-Kriterien erfüllt sind (20 Stoffe), und Stoffe, die keine PMT/vPvM-Stoffe sind (18 Stoffe), sowie ein Stoff, für den keine ausreichenden Daten für eine PMT/vPvM-Bewertung vorlagen.

Die Kategorie **REACH-Emissionswahrscheinlichkeits** basiert auf unter REACH-registrierten Mengen, Monitoringdaten und dem Emissions-Score (E-Score), wie in Arp und Hale (2019) definiert. Der E-Score basiert auf den unter REACH-registrierten Verwendungskategorien und -mengen. Die meisten der 176 ausgewählten Stoffe wiesen eine hohe oder sehr hohe REACH-Emissionswahrscheinlichkeit auf (133 Stoffe), während 21 Stoffe eine mittlere oder niedrige REACH-Emissionswahrscheinlichkeit aufwiesen und es 22 Stoffe gab, bei denen dies nicht bewertet werden konnte, da sie nicht REACH-registriert waren, sondern Verunreinigungen oder Transformationsprodukte von REACH-registrierten Stoffen.

Die Kategorie **Analytik- und Monitoringlücken** werden als eine und nicht als zwei getrennte Kategorien betrachtet, da es in der Praxis viele Überschneidungen zwischen diesen beiden Lücken gibt. Grob gesagt bezieht sich die Analytiklücke auf Stoffe, die nicht analysiert werden, da es derzeit gar keine Analytikmethoden des Stoffes gibt. Die Monitoringlücke bezieht sich auf Stoffe, die mit den bestehenden Analytikmethoden überwacht werden könnten, dies aber derzeit nicht passiert. Um diese Lücke zu untersuchen, wurden Umfragebögen an Wasseranalytiklabore in ganz Deutschland verschickt. Die Ergebnisse zeigen, dass für 26 der 176 Stoffe eine erhebliche oder geringfügige Analytiklücke, für 87 der 176 Stoffe eine erhebliche oder geringfügige Monitoringlücke und für 27 der 176 Stoffe umfangreiche Monitoringdaten vorlagen. 26 der 176 Stoffe wurden nicht in die Umfrage einbezogen.

Die Kategorie **Wasseraufbereitungslücke** betrachtet die beiden am häufigsten verfügbaren fortgeschrittenen Behandlungsmethoden: Aktivkohlefilter und Ozonung. Die Lücke wurde mit Hilfe des strukturbasierten Screening-Ansatzes (Hot-Target-Ansatz), Experimenten für häufig im Monitoring detektieren Stoffe sowie Interviews mit 13 deutschen Wasserversorgern bewertet. Es wurde festgestellt, dass 78 der 176 Stoffe weder mit Aktivkohlefilter noch mit Ozonung Aktivkohlefiltration behandelt werden können, 22 der 176 Stoffe nur mit Ozonung behandelt werden können, 31 der 176 Stoffe nur mit Aktivkohlefilter behandelt werden können und nur 19 der 176 Stoffe können mit beiden Methoden behandelt werden. 26 der 176 der Stoffe wurden nicht in die Bewertung einbezogen.

Zur Bewertung der Kategorie **Expositionshöhe** wurde eine intensive Monitoringkampagne für 13 Trinkwassereinzugsgebiete in ganz Deutschland durchgeführt, die die Flussgebiete von Donau, Elbe, Ems, Havel, Main, Neckar, Rhein, Sieg sowie die Seen Konstanz und Tegel umfasste. Die Probenahme umfasste Oberflächenwasser, Uferfiltrat, Grundwasser und Rohwasser. Die Monitoringkampagne umfasste 78 der 176 ausgewählten Stoffe, darunter 16 PMT/vPvM-Stoffe, die zuvor in der Literatur niemals detektiert wurden. Darüber hinaus wurde die in (Arp et al., 2023a) vorgestellte Literaturrecherche zur Bewertung der Kategorie Expositionshöhe herangezogen, da dieser Bericht Monitoringdaten aus der Literatur für 58 der 176 Stoffe enthielt. Aus der Monitoringkampagne und der Literaturrecherche lagen Daten für 90 der 176 Stoffe vor. 10 der 176 Stoffe sind ubiquitär in hohen Konzentrationen, 28 der 176

Stoffe sind ubiquitär in niedrigen Konzentrationen, 36 der 176 Stoffe sind in lokal detektiert und 16 der 176 Stoffe sind häufig überwacht aber nicht nachgewiesen.

Die **Gesamtprioritätsebene** wurde für REACH-registrierte Stoffe definiert. Zwei der Unterkategorien in dieser Kategorie wurden zuvor in (Arp et al., 2023b) definiert: die hohe Prioritätskategorie und die mittlere Prioritätskategorie. Dabei handelt es sich um unter REACH registrierte PMT/vPvM-Stoffe, die mit Mengen > 10 tpa bzw. zwischen 1 und <10 tpa registriert wurden. Die höchste Prioritätskategorie wird in diesem Bericht eingeführt und bezieht sich auf Stoffe, die die hohe Prioritätskategorie erfüllen und darüber hinaus ein zusätzliches Prioritätskriterium der höchsten Stufe aufweisen, wie z.B. eine erhebliche Analytiklücke, die Nichtverfügbarkeit von Wasseraufbereitungsmethoden oder der ubiquitäre Nachweis mit hohen Konzentrationen. Die Unterkategorie "Potenzielle Priorität" bezieht sich auf Stoffe, die die PMT/vPvM-Kriterien vermutlich erfüllen, falls mehr Daten zur Verfügung stünden, wie z.B. persistente und mobile Stoffe, die zwar die vPvM-Kriterien nicht erfüllen, für die es aber keine abschließende Bewertung gibt, ob das T-Kriterium erfüllt ist. Die Klasse "Niedrigste Priorität" bezieht sich auf Stoffe, die die PMT/vPvM-Kriterien nicht erfüllen.

Bei dieser Analyse wurden 43 der 176 Stoffe als höchst prioritär, 23 der 176 Stoffe als hoch prioritär, 33 der 176 Stoffe als mäßig prioritär, 65 Stoffe als potenziell prioritär und 11 Stoffe als am wenigsten prioritär eingestuft. Für ein Stoff konnte keine Gesamtpriorisierung vorgenommen werden. Die 43 PMT/vPvM-Stoffe mit der höchsten Priorität sind diejenigen, denen die Industrie, die Aufsichtsbehörden und der Wassersektor die größte Aufmerksamkeit widmen sollten um gemeinsam Strategien zur Minimierung der Emissionen aus REACH-registrierten Verwendungen zu erreichen. Stoffe, die als potenziell prioritär eingestuft wurden, sollten ebenfalls untersucht werden, um mehr Daten zur Persistenz, Mobilität oder Toxizität zu erhalten, damit eine abschließende PMT/vPvM-Bewertung erfolgen kann. Eine solche abschließende PMT/vPvM-Bewertung würde sich auf die Gesamtpriorisierungsstufe auswirken.

Zusätzlich zum Priorisierungsrahmenwerk wurden im Rahmen dieses Projekts viele Aktivitäten zur Kommunikation und Verbreitung durchgeführt, die in den Anhängen aufgelistet sind. Dazu gehören die Organisation des dritten PMT-Workshops (online, mit über 500 Teilnehmenden), die Entwicklung einer aktualisierten Website für PMT/vPvM-Stoffe, die vom UBA gehostet wird, die Veröffentlichung von 12 populären und wissenschaftlichen Artikeln sowie die Präsentation dieser Arbeit auf vielen verschiedenen Konferenzen, einschließlich einer Hauptvortrag (*keynote*) auf der SETAC Europe 2022 in Kopenhagen (Arp, 2022). Der Anhang enthält außerdem 10 Datenblätter (*fact sheets*) die im Rahmen dieses Projekts für ausgewählte PMT/vPvM-Stoffe oder deren Vorläufer zusammengetragen wurden.

This report is part of research project (FKZ 3719 65 408 0) that started in 2019 to address several aims related to the implementation and utilization of the PMT/vPvM criteria to assist REACH registrants, regulators, researchers and the water sector to help develop strategies for managing these hazardous substances. The key results of this project are presented in four reports:

Arp, H.P.H., Hale, S.E. (2023):
REACH: Guidance and Methods for the Identification and Assessment of PMT/vPvM Substances.
UBA TEXTE 19/2023. Neumann, M., Schliebner, I. [ed.], ISSN 1862-4804. German Environment Agency (UBA), Dessau-Roßlau, Germany, 66 pages
https://www.umweltbundesamt.de/publikationen/reach-guidance-methods-for-the-identification

Arp, H.P.H., Hale, S.E., Neumann, M. (2023):
PMT/vPvM assessment of REACH registered Substances Detected in Wastewater Treatment Plant Effluent, Freshwater Resources and Drinking Water.
UBA TEXTE 20/2023. Neumann, M., Schliebner, I. [ed.], ISSN 1862-4804 German Environment Agency (UBA), Dessau-Roßlau, Germany, 259 pages
https://www.umweltbundesamt.de/publikationen/pmtvpvm-assessment-of-reach-registered-substances

Arp, H.P.H., Hale, S.E., Schliebner, I., Neumann, M. (2023):
Prioritised PMT/vPvM substances in the REACH registration database.
UBA TEXTE 21/2023. Neumann, M., Schliebner, I. [ed.], ISSN 1862-4804. German Environment Agency (UBA), Dessau-Roßlau, Germany, 177 pages
https://www.umweltbundesamt.de/publikationen/prioritised-pmtvpvm-substances-in-the-reach

Arp, H.P.H., Hale, S.E., Borchers, U., Valkov V., Wiegand, L., Zahn, D., Neuwald, I., Nödler, K. Scheurer, M. (2023):
A prioritization framework for PMT/vPvM Substances under REACH for registrants, regulators, researchers and the water sector.
UBA TEXTE 22/2023. Neumann, M., Schliebner, I. [ed.], ISSN 1862-4804. German Environment Agency (UBA), Dessau-Roßlau, Germany, 238 pages
https://www.umweltbundesamt.de/publikationen/a-prioritization-framework-for-pmtvpvm-substances

This report (UBA TEXTE 22/2023) is the fourth in the series, which presents a prioritization framework for PMT/vPvM substances under REACH. The other three reports present: updated guidance and methods for the identification and assessment of PMT/vPvM substances registered under REACH (UBA TEXTE 19/2023); an investigation of the number of substances detected in six water media that are in the REACH registration database and meet the PMT/vPvM criteria (UBA TEXTE 20/2023); and, the UBA list of prioritized PMT/vPvM substances in the REACH registration database (UBA TEXTE 21/2023).

1. Introduction

Persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM) substances have the intrinsic substance properties to contaminate drinking water sources, even if they are far away from the emission source or the contamination occurred long ago. (Neumann and Schliebner, 2019). Though all PMT/vPvM substances share the same serious intrinsic hazard of harming the water cycle, including drinking water, they do not all share the same chance of exposure, nor risk, nor necessitate the same prioritization for investigation or further risk mitigation measures. For instance, PMT/vPvM substances that only exist in the patent literature or are manufactured in small quantities would not need to be prioritized over a PMT/vPvM substance that has been produced in large quantities for several years and is ubiquitously detected in drinking water.

To best manage and mitigate real or potential risks, a prioritization framework for PMT/vPvM substances is needed. One key advantage of a prioritization framework is that it does not require the intense amount of data or assumptions that risk assessments often require, as prioritization frameworks can be based on the availability of known data. Prioritization frameworks can be based on the availability of known data as well as the status of existing knowledge gaps to spot red flags.

This report presents such a prioritization framework. The development of this prioritization framework was the result of a large research project initiated in 2019. The prioritization framework took into consideration the views of diverse stakeholders, including industry, regulators, researchers and the water sector. The prioritization framework was developed based on the results of surveys with analytical labs (Chapter 6), surveys with water treatment facilities (Chapter 7), an intensive monitoring campaign of PMT/vPvM substances in German Drinking water sources (Chapter 8) and replies to a live poll at an online workshop to assess the key data gaps regarding PMT/vPvM substances (Annex C).

This prioritization framework can be used to identify which PMT/vPvM substances registered under REACH require immediate risk management measures (RMM) by industry, the development of risk management option analysis (RMOA) by regulators, the closure of data gaps by researchers, and the implementation of remediation strategies from the water sector.

2. The Prioritization Framework for PMT/vPvM substances

The prioritization framework for PMT/vPvM substances presented in this report consists of six categories as presented in Box 1.

Box 1. Categories of the prioritization framework for PMT/vPvM substances

- **PMT/vPvM hazard**: This category indicates the PMT/vPvM conclusion, as defined in Neumann and Schliebner (2019), and as assessed in Arp and Hale (2023).
- **REACH Emission Likelihood**: This category indicates the likelihood that emissions could be occurring, based on REACH registered volumes, monitoring data and the emission-score (E-score) as presented in Arp and Hale (2019)
- **Analytical and Monitoring gaps**: This category indicates the current state of analytical development and monitoring activities
- **Remediation gap**: This category indicates the technology and investment costs required to remove the substance from drinking water
- **Exposure level**: This category is related to the "analytical and monitoring gap" category but is focussed on documented concentrations in the following drinking water source media: bank filtrate, groundwater, raw water and drinking water.
- **Overall prioritization level**. This category indicates the overall prioritization based on all individual categories.

For each of the six categories in the prioritization framework, a different classification scheme exists, to indicate a high or low level of concern related to the prioritization category. Each classification uses a similar traffic-light type colour scheme, as presented in Table 1, from green (Lowest-Priority), to light yellow (Potential-Priority), to dark yellow (Moderate-Priority), to light red (High-Priority) to dark red (Highest-Priority). Importantly, there is also a category for unknown categorizations, coloured white, which indicates that the data gaps are too substantial to make assignment, either because the data does not exist, or the assessment was not yet performed.

The first two categories, PMT/vPvM hazard and REACH Emission Likelihood are the same as applied to REACH registered substances in Arp and Hale (2023) and (Arp et al., 2023b), using the same colour scheme as in Table 1. Further information about these two hazard categories is presented in Chapters 4 and 5, respectively. The remaining prioritization categories are unique to this report. They are presented in further detail in Chapter 6 (Analytical and Monitoring gap), Chapter 7 (Remediation Gap) and Chapter 10 (Overall Prioritization Level).

Table 1: The prioritization framework for PMT/vPvM substances registered under REACH

PMT/vPvM hazard	REACH Emission Likelihood	Analytical & Monitoring Gaps	Remediation Gap	Exposure Level	Overall Prioritization Level
Unknown/ insufficient data	Unknown/ confidential/Not REACH registered	Unknown/ Not assessed	Remediation potential with AC and ozone unknown or difficult to estimate	No monitoring data currently available	Unknown/insufficient data
vPvM & PMT or vPvM	**Very high or High:** high E-score, detection in environment required for "very high", otherwise "high"	**Major analytical gap:** Not monitored because the substance can only be analysed by advanced / specialized methods	**No O3&AC:** Compounds that cannot be eliminated using AC or ozonation	**Ubiquitously detected and occasionally at high concentrations** in drinking water sources (greater than 0.1 µg/L or the PNEC if known)	**Highest-Priority** PMT/vPvM substance with registration volumes > 10 tpa, very high or high emission likelihood, and at least one other
PMT		**Minor analytical gap:** Not monitored, but method development feasible	**O3 only:** Compounds that can be removed using ozonation only	**Ubiquitous but generally at low concentrations** in drinking water sources (less than 0.1 µg/L or the PNEC if known)	**High-Priority** PMT/vPvM substance with registration volume > 10 tpa
PM	**Medium:** low E-score or intermediate under REACH that is detected in drinking water sources	**Major monitoring gap:** Not monitored, but could be monitored using current methods	**AC only:** Compounds that can be removed using AC only	**Local contamination and occasionally at high concentrations** in drinking water sources	**Moderate-Priority** PMT/vPvM substances with registration volume < 10 tpa or are suspected impurity/transformation products.
Potential PMT/vPvM		**Minor monitoring gap:** Monitored regularly, but by less than 20% of water quality labs	**Both O3&AC**: Compounds that can be removed by using both AC or ozonation	**Local contamination but generally at low concentrations** in drinking water sources	**Potential-Priority** All other cases, except if "Not PMT/vPvM"
Not PMT/vPvM	**Low:** low E-score or intermediate substance, not detected in drinking water sources	**No Monitoring gap:** Monitored regularly, but more than 20% of water quality labs	**Conventional:** Compounds that can be removed with conventional techniques	**Monitored commonly, not found:** Extensive monitoring showed no presence in sources of drinking water	**Lowest-Priority** Substance is "Not PMT/vPvM"

3. The 176 Substances considered

For the development and implementation of the PMT/vPvM prioritization framework a total of 176 substances were selected, as presented in Table 2. The selection of these substances was based on several considerations that would fully explore a range of outcomes within the framework. The selection criteria included whether or not they meet PMT/vPvM criteria, data gaps regarding the PMT/vPvM hazard assessment, whether they contain a perfluoroalkyl substructure or triazine substructure, suspicion of being present in German drinking water resources and current knowledge of detection methods.

The starting point for this was the list of 122 PMT/vPvM substances, registered under REACH, that were prioritized in Arp and Hale (2019). A research question related to this list was to see the number of these substances that would no longer be considered PMT/vPvM substances due to stricter requirements for the toxicity data in the updated guideline (Arp and Hale, 2023), as well as more recent data related to persistency and mobility. It should be noted that there were 3 substances that were removed from the list in Arp and Hale (2019), due to unit errors in the P/vP dossier data used to make the assessment. These three were cyanamide (420-04-2), calcium cyanamide (156-62-7) and chlorotrimethylsilane (CAS 75-77-4). Therefore, a total of 119 of the priority PMT/vPvM substances in Arp and Hale (2019) were considered. These substances are listed in Table 2.

A second research question that was considered in the selection of substances was related to grouping PMT/vPvM substances based on a common moiety that appears to be associated with PMT/vPvM substances, or their transform products. Two such substances groups were selected, those with triazine rings and those with a short perfluorinated alkyl group (i.e. short-chain PFAS). Known triazine containing substances that meet the PMT/vPvM criteria include melamine, atrazine, and cyanuric acid (Arp and Hale, 2019). It is hypothesized that many substances containing a triazine ring can transform themselves to melamine or cyanuric acid, and further, many of the transformation products of melamine and cyanuric acid are themselves persistent and mobile (Zheng et al., 2021). Five additional triazines were added as follows: ammeline (CAS 645-92-1) and ammelide (CAS 645-93-2), which are known transformation products of melamine that contain an s-triazine ring (Zheng et al., 2021), as well as the REACH registered substances 2,4,6-trichloro-1,3,5-triazine (CAS 108-77-0), sodium p-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]benzenesulphonate (CAS 4156-21-2) and 1,3,5-triazine-2,4,6(1H,3H,5H)-trithione, trisodium salt (17766-26-6). It is also hypothesized that substances containing a short-chain PFAS can transform in the environment to smaller substances where the short-chain PFAS sub-moiety remains. Known short-chain PFAS that are considered PMT/vPvM substances, include PFBS (CAS 29420-49-3) and GenX (CAS 62037-80-3). These substances have recently been added to the list of Substances of Very High Concern (SVHC) because their PMT/vPvM properties were considered to be an equivalent level of concern to PBT/vPvB substances (Hale et al. 2020). From the list of REACH registered substances as of September 2019, 28 additional short-chain PFAS were identified that were not already prioritized (see Table 2), and these were referred to as "short-chain PFAS – REACH". For clarity, these "short-chain PFAS – REACH" are ether themselves short-chain PFAS or suspected precursors of them.

A third research question that was the basis for substance selection was related to PFAS substances that are not REACH registered, due to the general concern about PFAS, and also

because several PFAS substances can be transformation daughter products of REACH registered substances (Zhang et al., 2021). For this purpose, an additional 24 PFAS were also selected for inclusion. Though all additional 24 substances are persistent, they very in mobility as well as toxicity. These additional PFAS were all included in the monitoring study in this report (Chapter 8) and are therefore called the "monitoring PFAS" in Table 2.

The "Reason for inclusion" of each of the 176 substances is presented in Table 2, along with the number of substances that could be assessed using each prioritization category, as described in the subsequent chapters.

Table 2: The 176 substances considered for the PMT/vPvM Prioritization Framework, and the Prioritization Categories for which they could be assessed

CAS	EC	Substance	Reason for inclusion	PMT/vPvM hazard (Chapter 4) (175 of 176)	REACH Emission Likelihood (Chapter 5) (154 of 176)	Analytical & Monitoring Gaps (Chapter 6) (150 of 176)	Remediation Gap (Chapter 7) (150 of 176)	Exposure Level: Literature study (Arp et al., 2023a) (58 of 176)	Exposure Level: Monitoring (Chapter 8) (76 out of 176)
288-88-0	206-022-9	1,2,4-triazole	Arp and Hale (2019)	x	x	X	x	x	x
13674-87-8	237-159-2	Tris(2-chloro-1-methylethyl) phosphate	Arp and Hale (2019)	x	x	X	x	x	
3622-84-2	222-823-6	N-butylbenzenesulphonamide	Arp and Hale (2019)	x	x	X	x	x	
56-23-5	200-262-8	Carbon tetrachloride	Arp and Hale (2019)	x	x	X	x	x	x
67-66-3	200-663-8	Chloroform	Arp and Hale (2019)	x	x	X	x	x	x
71-55-6	200-756-3	1,1,1-trichloroethane	Arp and Hale (2019)	x	x	x	x	x	x
115-27-5	204-077-3	Chlorendic anhydride	Arp and Hale (2019)	x	x	x	x		
13472-08-7	236-740-8	2,2'-azobis[2-methylbutyronitrile]	Arp and Hale (2019)	x	x	x	x		
22042-96-2	244-751-4	Diethylenetriaminepenta(methylenephosphonic acid), sodium salt	Arp and Hale (2019)	x	x	x	x		
61792-09-4	263-212-4	Pentasodium diethylenetriaminepentamethylenephosphonate	Arp and Hale (2019)	x	x	x	x		
78-67-1	201-132-3	2,2'-dimethyl-2,2'-azodipropiononitrile	Arp and Hale (2019)	x	x	x	x		
123-91-1	204-661-8	1,4-dioxane	Arp and Hale (2019)	x	x	x	x	x	x
102-06-7	203-002-1	1,3-diphenylguanidine	Arp and Hale (2019)	x	x	x	x	x	x
97-39-2	202-577-6	1,3-di-o-tolylguanidine	Arp and Hale (2019)	x	x	x	x	x	
2855-13-2	220-666-8	3-aminomethyl-3,5,5-trimethylcyclohexylamine	Arp and Hale (2019)	x	x	x	x	x	x
3030-47-5	221-201-1	Bis(2-dimethylaminoethyl)(methyl)amine	Arp and Hale (2019)	x	x	x	x		x
75-35-4	200-864-0	1,1-dichloroethylene	Arp and Hale (2019)	x	x	x	x	x	x
78-51-3	201-122-9	Tris(2-butoxyethyl) phosphate	Arp and Hale (2019)	x	x	x	x	x	
162881-26-7	423-340-5	Phenyl bis(2,4,6-trimethylbenzoyl)-phosphine oxide	Arp and Hale (2019)	x	x	x	x		

CAS	EC	Substance	Reason for inclusion	PMT/vPvM hazard (Chapter 4) (175 of 176)	REACH Emission Likelihood (Chapter 5) (154 of 176)	Analytical & Monitoring Gaps (Chapter 6) (150 of 176)	Remediation Gap (Chapter 7) (150 of 176)	Exposure Level: Literature study (Arp et al., 2023a) (58 of 176)	Exposure Level: Monitoring (Chapter 8) (76 out of 176)
94239-04-0	428-100-3	2-fluoro-6-trifluoromethylpyridine	Arp and Hale (2019)	x	x	x	x		
95-14-7	202-394-1	Benzotriazole	Arp and Hale (2019)	x	x	x	x	x	x
108-78-1	203-615-4	Melamine	Arp and Hale (2019)	x	x	x	x	x	x
834-12-8	212-634-7	Ametryn	Arp and Hale (2019)	x	x	x	x	x	
91-76-9	202-095-6	6-phenyl-1,3,5-triazine-2,4-diyldiamine	Arp and Hale (2019)	x	x	x	x		x
108-80-5	203-618-0	cyanuric acid	Arp and Hale (2019)	x	x	x	x	x	x
382-28-5	206-841-1	2,2,3,3,5,5,6,6-octafluoro-4-(trifluoromethyl)morpholine	Arp and Hale (2019)	x	x	x	x		x
29420-49-3	249-616-3	PFBS	Arp and Hale (2019)	x	x	x	x	x	x
76-05-1	200-929-3	Trifluoroacetic acid	Arp and Hale (2019)	x	x	x	x	x	x
1493-13-6	216-087-5	Trifluoromethanesulphonic acid	Arp and Hale (2019)	x	x	x	x	x	x
541-73-1	208-792-1	1,3-dichlorobenzene	Arp and Hale (2019)	x	x	x	x	x	x
56-93-9	200-300-3	Benzyltrimethylammonium chloride	Arp and Hale (2019)	x	x	x	x	x	x
51-28-5	200-087-7	2,4-dinitrophenol	Arp and Hale (2019)	x	x	x	x	x	
106-93-4	203-444-5	1,2-dibromoethane	Arp and Hale (2019)	x	x	x	x	x	x
108-90-7	203-628-5	Chlorobenzene	Arp and Hale (2019)	x	x	x	x	x	x
156-60-5	205-860-2	trans-dichloroethylene	Arp and Hale (2019)	x	x	x	x	x	x
280-57-9	205-999-9	1,4-diazabicyclooctane	Arp and Hale (2019)	x	x	x	x		x
3033-62-3	221-220-5	N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	Arp and Hale (2019)	x	x	x	x		x
38083-17-9	253-775-4	Climbazole	Arp and Hale (2019)	x	x	x	x	x	x
52556-42-0	258-004-5	Sodium 3-(allyloxy)-2-hydroxypropanesulphonate	Arp and Hale (2019)	x	x	x	x		x
622-40-2	210-734-5	2-morpholinoethanol	Arp and Hale (2019)	x	x	x	x		x
75-01-4	200-831-0	Chloroethylene	Arp and Hale (2019)	x	x	x	x	x	x
75-71-8	200-893-9	Dichlorodifluoromethane	Arp and Hale (2019)	x	x	x	x	x	x
78-87-5	201-152-2	1,2-dichloropropane	Arp and Hale (2019)	x	x	x	x	x	x
81-07-2	201-321-0	1,2-benzisothiazol-3(2H)-one 1,1-dioxide	Arp and Hale (2019)	x	x	x	x	x	x

CAS	EC	Substance	Reason for inclusion	PMT/vPvM hazard (Chapter 4) (175 of 176)	REACH Emission Likelihood (Chapter 5) (154 of 176)	Analytical & Monitoring Gaps (Chapter 6) (150 of 176)	Remediation Gap (Chapter 7) (150 of 176)	Exposure Level: Literature study (Arp et al., 2023a) (58 of 176)	Exposure Level: Monitoring (Chapter 8) (76 out of 176)
83016-70-0	406-080-7	2-[(2-[2-(dimethylamino)ethoxy]ethyl)methylamino]ethanol	Arp and Hale (2019)	x	x	x	x		x
88-72-2	201-853-3	2-nitrotoluene	Arp and Hale (2019)	x	x	x	x		x
88-73-3	201-854-9	1-chloro-2-nitrobenzene	Arp and Hale (2019)	x	x	x	x		x
95-50-1	202-425-9	1,2-dichlorobenzene	Arp and Hale (2019)	x	x	x	x	x	x
99-99-0	202-808-0	4-nitrotoluene	Arp and Hale (2019)	x	x	x	x		x
108-42-9	203-581-0	3-chloroaniline	Arp and Hale (2019)	x	x	x	x		
123-30-8	204-616-2	4-aminophenol	Arp and Hale (2019)	x	x	x	x		
67-68-5	200-664-3	Dimethyl sulfoxide	Arp and Hale (2019)	x	x	x	x		
78-40-0	201-114-5	Triethyl phosphate	Arp and Hale (2019)	x	x	x	x	x	
87-62-7	201-758-7	2,6-xylidine	Arp and Hale (2019)	x	x	x	x	x	
102-08-9	203-004-2	1,3-diphenyl-2-thiourea	Arp and Hale (2019)	x	x	x	x		
109-01-3	203-639-5	1-methylpiperazine	Arp and Hale (2019)	x	x	x	x		
100-43-6	202-852-0	4-vinylpyridine	Arp and Hale (2019)	x	x	x	x		
100-61-8	202-870-9	N-methylaniline	Arp and Hale (2019)	x	x	x	x		
121-47-1	204-473-6	3-aminobenzenesulphonic acid	Arp and Hale (2019)	x	x	x	x		
129909-90-6	603-373-3	4-amino-N-(1,1-dimethylethyl)-4,5-dihydro-3-(1-methylethyl)-5-oxo-1H-1,2,4-triazole-1-carboxamide	Arp and Hale (2019)	x	x	x	x		
1758-73-2	217-157-8	Aminoiminomethanesulphinic acid	Arp and Hale (2019)	x	x	x	x		
1761-71-3	217-168-8	4,4'-methylenebis(cyclohexylamine)	Arp and Hale (2019)	x	x	x	x		
2226-96-2	218-760-9	4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	Arp and Hale (2019)	x	x	x	x		
2440-22-4	219-470-5	2-(2H-benzotriazol-2-yl)-p-cresol	Arp and Hale (2019)	x	x	x	x		
25321-09-9	246-835-6	Diisopropylbenzene	Arp and Hale (2019)	x	x	x	x		
27955-94-8	405-800-7	4,4',4''-(ethan-1,1,1-triyl)triphenol	Arp and Hale (2019)	x	x	x	x		
2680-03-7	220-237-5	N,N-dimethylacrylamide	Arp and Hale (2019)	x	x	x	x		
3710-84-7	223-055-4	N,N-diethylhydroxylamine	Arp and Hale (2019)	x	x	x	x		

CAS	EC	Substance	Reason for inclusion	PMT/vPvM hazard (Chapter 4) (175 of 176)	REACH Emission Likelihood (Chapter 5) (154 of 176)	Analytical & Monitoring Gaps (Chapter 6) (150 of 176)	Remediation Gap (Chapter 7) (150 of 176)	Exposure Level: Literature study (Arp et al., 2023a) (58 of 176)	Exposure Level: Monitoring (Chapter 8) (76 out of 176)
37971-36-1	253-733-5	2-phosphonobutane-1,2,4-tricarboxylic acid	Arp and Hale (2019)	x	x	x	x		
4065-45-6	223-772-2	Sulisobenzone	Arp and Hale (2019)	x	x	x	x		
556-88-7	209-143-5	1-nitroguanidine	Arp and Hale (2019)	x	x	x	x		
593-85-1	209-813-7	Diguanidinium carbonate	Arp and Hale (2019)	x	x		x		
6331-96-0	700-413-2	2-amino-4,5-dichlorobenzenesulfonic acid	Arp and Hale (2019)	x	x	x	x		
6674-22-2	229-713-7	1,8-diazabicyclo[5.4.0]undec-7-ene	Arp and Hale (2019)	x	x	x	x		
73037-34-0	277-242-0	Disodium oxybis[methylbenzenesulphonate]	Arp and Hale (2019)	x	x	x	x		
76-03-9	200-927-2	Trichloroacetic acid	Arp and Hale (2019)	x	x	x	x		
80-51-3	201-286-1	4,4'-oxydi(benzenesulphonohydrazide)	Arp and Hale (2019)	x	x	x	x		
97-74-5	202-605-7	Tetramethylthiuram monosulphide	Arp and Hale (2019)	x	x	x	x		
121-82-4	204-500-1	Perhydro-1,3,5-trinitro-1,3,5-triazine	Arp and Hale (2019)	x	x	x	x	x	
126-86-3	204-809-1	2,4,7,9-tetramethyldec-5-yne-4,7-diol	Arp and Hale (2019)	x	x	x	x	x	
2312-35-8	219-006-1	Propargite	Arp and Hale (2019)	x	x	x	x		
345-92-6	206-466-3	Bis(4-fluorophenyl) ketone	Arp and Hale (2019)	x	x	x	x		
100-97-0	202-905-8	Methenamine	Arp and Hale (2019)	x	x	x	x	x	
107-46-0	203-492-7	Hexamethyldisiloxane	Arp and Hale (2019)	x	x	x	x		
107-66-4	203-509-8	Dibutyl hydrogen phosphate	Arp and Hale (2019)	x	x	x	x		
108-20-3	203-560-6	Diisopropyl ether	Arp and Hale (2019)	x	x	x	x	x	
110553-27-0	402-860-6	4,6-bis(octylthiomethyl)-o-cresol	Arp and Hale (2019)	x	x	x	x		
1112-39-6	214-189-4	Dimethoxydimethylsilane	Arp and Hale (2019)	x	x	x	x		
119-61-9	204-337-6	Benzophenone	Arp and Hale (2019)	x	x	x	x	x	
119-64-2	204-340-2	1,2,3,4-tetrahydronaphthalene	Arp and Hale (2019)	x	x	x	x		

CAS	EC	Substance	Reason for inclusion	PMT/vPvM hazard (Chapter 4) (175 of 176)	REACH Emission Likelihood (Chapter 5) (154 of 176)	Analytical & Monitoring Gaps (Chapter 6) (150 of 176)	Remediation Gap (Chapter 7) (150 of 176)	Exposure Level: Literature study (Arp et al., 2023a) (58 of 176)	Exposure Level: Monitoring (Chapter 8) (76 out of 176)
12108-13-3	235-166-5	Tricarbonyl(methylcyclopentadienyl)manganese	Arp and Hale (2019)	x	x	x			
1671-49-4	430-550-0	4-mesyl-2-nitrotoluene	Arp and Hale (2019)	x	x	x	x		
25068-38-6	500-033-5	4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane	Arp and Hale (2019)	x	x	x	x		
2554-06-5	219-863-1	2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane	Arp and Hale (2019)	x	x	x	x		
26471-62-5	247-722-4	m-tolylidene diisocyanate	Arp and Hale (2019)	x	x	x	x		
3006-86-8	221-111-2	Cyclohexylidenebis[tert-butyl] peroxide	Arp and Hale (2019)	x	x	x	x		
3468-63-1	222-429-4	1-[(2,4-dinitrophenyl)azo]-2-naphthol	Arp and Hale (2019)	x	x	x	x		
34690-00-1	252-156-6	[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methylene)]]tetrakisphosphonic acid	Arp and Hale (2019)	x	x	x	x		
482-89-3	207-586-9	2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	Arp and Hale (2019)	x	x	x	x		
5026-74-4	225-716-2	p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	Arp and Hale (2019)	x	x	x	x		
5281-04-9	226-109-5	Calcium 3-hydroxy-4-[(4-methyl-2-sulphonatophenyl)azo]-2-naphthoate	Arp and Hale (2019)	x	x	x	x		
53988-10-6	258-904-8	1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione	Arp and Hale (2019)	x	x	x	x		
584-84-9	209-544-5	4-methyl-m-phenylene diisocyanate	Arp and Hale (2019)	x	x	x	x		
599-61-1	209-967-5	3,3'-sulphonyldianiline	Arp and Hale (2019)	x	x	x	x		
6864-37-5	229-962-1	2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)	Arp and Hale (2019)	x	x	x	x		
68937-41-7	273-066-3	Phenol, isopropylated, phosphate (3:1)	Arp and Hale (2019)	x	x	x	x		

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68987-63-3	273-501-7	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, chlorinated	Arp and Hale (2019)	x	x	x			
71604-74-5	275-662-9	m-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	Arp and Hale (2019)	x	x	x	x		
71868-10-5	400-600-6	2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one	Arp and Hale (2019)	x	x	x	x		
7226-23-5	230-625-6	Tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one	Arp and Hale (2019)	x	x	x	x		
74091-64-8	411-280-2	2,5-bis-isocyanatomethyl-bicyclo[2.2.1]heptane	Arp and Hale (2019)	x	x	x	x		
75-91-2	200-915-7	tert-butyl hydroperoxide	Arp and Hale (2019)	x	x	x	x		
77-73-6	201-052-9	3a,4,7,7a-tetrahydro-4,7-methanoindene	Arp and Hale (2019)	x	x	x	x		
80-08-0	201-248-4	Dapsone	Arp and Hale (2019)	x	x	x	x	x	
80-15-9	201-254-7	α,α-dimethylbenzyl hydroperoxide	Arp and Hale (2019)	x	x	x	x		
80-43-3	201-279-3	Bis(α,α-dimethylbenzyl) peroxide	Arp and Hale (2019)	x	x	x	x		
90268-24-9	290-824-9	Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(4-chloro-2,5-dimethoxyphenyl and 2,4-xylyl) derivs.	Arp and Hale (2019)	x	x	x	x		
121-03-9	204-445-3	4-nitrotoluene-2-sulphonic acid	Arp and Hale (2019)	x	x	x	x		x
5165-97-9	225-948-4	Sodium 2-methyl-2-[(1-oxoallyl)amino]propanesulphonate	Arp and Hale (2019)	x	x	x	x	x	x
90076-65-6	415-300-0	Lithium bis(trifluoromethylsulfonyl)imide	short-chain PFAS-REACH	x	x	x	x		x

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27619-97-2	248-580-6	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonic acid	short-chain PFAS-REACH	x	x	x	x	x	x
431-47-0	207-074-5	Methyl trifluoroacetate	short-chain PFAS-REACH	x	x	x	x		
62037-80-3	700-242-3	Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate	short-chain PFAS-REACH	x	x	x	x	x	x
17527-29-6	241-527-8	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate	short-chain PFAS-REACH	x	x	x	x		x
2144-53-8	218-407-9	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl methacrylate	short-chain PFAS-REACH	x	x	x	x		x
428-59-1	207-050-4	Trifluoro(trifluoromethyl)oxirane	short-chain PFAS-REACH	x	x	x	x		
1187-93-5	214-703-7	Trifluoro(trifluoromethoxy)ethylene	short-chain PFAS-REACH	x	x	x	x		
700874-87-9	615-064-0	{difluoro[(1,2,2-trifluoroethenyl)oxy]methoxy}trifluoromethane	short-chain PFAS-REACH	x	x	x	x		
1623-05-8	216-600-2	1,1,1,2,2,3,3-heptafluoro-3-[(trifluorovinyl)oxy]propane	short-chain PFAS-REACH	x	x	x	x		
756-13-8	436-710-6	1,1,1,2,2,4,5,5,5-nonafluoro-4-(trifluoromethyl)-3-pentanone	short-chain PFAS-REACH	x	x	x	x		
355-93-1	206-596-0	2,2,3,3,4,4,5,5-octafluoropentyl methacrylate	short-chain PFAS-REACH	x	x	x	x		x
85857-16-5	288-657-1	Trimethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	short-chain PFAS-REACH	x	x	x	x		x
78560-45-9	278-947-6	Trichloro(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	short-chain PFAS-REACH	x	x	x	x		x
51851-37-7	257-473-3	Triethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	short-chain PFAS-REACH	x	x	x	x		x
1190931-27-1	682-238-0	Ammonium difluoro{[2,2,4,5-tetrafluoro-5-	short-chain PFAS-REACH	x	x	x	x		

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		(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate							
908020-52-0	700-323-3	Ammonium difluoro[1,1,2,2-tetrafluoro-2-(pentafluoroethoxy)ethoxy]acetate	short-chain PFAS-REACH	x	x	x	x		
34454-97-2	252-043-1	1,1,2,2,3,3,4,4,4-nonafluoro-N-(2-hydroxyethyl)-N-methylbutane-1-sulphonamide	short-chain PFAS-REACH	x	x	x	x		x
34455-00-0	252-044-7	1,1,2,2,3,3,4,4,4-nonafluoro-N,N-bis(2-hydroxyethyl)butane-1-sulphonamide	short-chain PFAS-REACH	x	x	x	x		
67584-55-8	266-733-5	2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl acrylate	short-chain PFAS-REACH	x	x	x	x		
67584-59-2	266-737-7	2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl methacrylate	short-chain PFAS-REACH	x	x	x	x		
80475-32-7	279-481-6	N-[3-(dimethylamino)propyl]-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonamide N-oxide	short-chain PFAS-REACH	x	x	x	x		x
88992-45-4	811-523-6	2-hydroxy-N,N,N-trimethyl-3-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)thio]propan-1-aminium chloride	short-chain PFAS-REACH	x	x	x	x		
34455-29-3	252-046-8	Carboxymethyldimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulphonyl]amino]propylammonium hydroxide	short-chain PFAS-REACH	x	x	x	x		
62880-93-7	811-522-0	sodium 2-methyl-2-({3-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)thio]propanoyl}amino)propane-1-sulfonate	short-chain PFAS-REACH	x	x	x	x		

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2926-29-6	911-467-3	trifluoromethanesulfinate (triflinate)	short-chain PFAS-REACH	x	x		x		x
40573-09-9	442-390-9	1,1,2,2,3,3-hexafluoro-1-trifluoromethoxy-3-trifluorovinyloxypropane	short-chain PFAS-REACH	x	x	x	x		x
21615-47-4	244-479-6	Ammonium undecafluorohexanoate (PFHxA)	short-chain PFAS-REACH	x	x	x	x	x	x
211-455-1	211-455-1	ammeline	triazine	x		x	x		x
645-93-2	645-93-2	ammelide	triazine	x		x	x		
108-77-0	203-614-9	2,4,6-trichloro-1,3,5-triazine	triazine	x	x	x	x		
4156-21-2	223-989-2	Sodium p-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]benzenesulphonate	triazine	x	x	x	x		
17766-26-6	241-749-5	1,3,5-triazine-2,4,6(1H,3H,5H)-trithione, trisodium salt	triazine		x	x	x		
2058-94-8	218-165-4	Perfluoroundecanoic acid (PFUnDA)	monitoring PFAS	x				x	x
307-55-1	206-203-2	Perfluorododecanoic acid (PFDoDA)	monitoring PFAS	x				x	x
68259-12-1	-	Perfluorononane sulfonic acid (PFNS)	monitoring PFAS	x				x	x
67906-42-7, 335-77-3	206-401-9	Perfluorodecane sulfonic acid (PFDS)	monitoring PFAS	x				x	x
920-66-1	213-059-4	1,1,1,3,3,3-hexafluoropropan-2-ol	monitoring PFAS	x	x				x
422-05-9	207-012-7	2,2,3,3,3-pentafluoropropanol	monitoring PFAS	x	x				x
15290-77-4	430-710-1	1,1,2,2,3,3,4-heptafluorocyclopentane	monitoring PFAS	x	x				x
375-22-4	206-786-3	Perfluorobutanoic acid (PFBA)	monitoring PFAS	x				x	x
2706-90-3	220-300-7	Perfluoropentanoic acid (PFPA)	monitoring PFAS	x				x	x
375-85-9	206-798-9	Perfluoroheptanoic acid (PFHpA)	monitoring PFAS	x				x	x
335-67-1	206-402-4	Perfluorooctanoic acid (PFOA)	monitoring PFAS	x				x	x

CAS	EC	Substance	Reason for inclusion	PMT/vPvM hazard (Chapter 4) (175 of 176)	REACH Emission Likelihood (Chapter 5) (154 of 176)	Analytical & Monitoring Gaps (Chapter 6) (150 of 176)	Remediation Gap (Chapter 7) (150 of 176)	Exposure Level: Literature study (Arp et al., 2023a) (58 of 176)	Exposure Level: Monitoring (Chapter 8) (76 out of 176)
72629-94-8	276-745-2	Perfluorotridecanoic acid (PFTrDA)	monitoring PFAS	x					x
375-95-1	206-801-3	Perfluorononanoic acid (PFNA)	monitoring PFAS	x				x	x
335-76-2	206-400-3	Perfluorodecanoic acid (PFDA)	monitoring PFAS	x				x	x
2706-91-4	220-301-2	Perfluoropentanesulfonic acid (PFPS)	monitoring PFAS	x				x	x
3871-99-6, 355-46-4	206-587-1	Perfluorohexanesulfonic acid (PFHxS)	monitoring PFAS	x				x	x
375-92-8	206-800-8	Perfluoroheptane sulfonic acid (PFHpS)	monitoring PFAS	x				x	x
1763-23-1, 56773-42-3	217-179-8; 260-375-3	Perfluorooctane sulfonic acid (PFOS)	monitoring PFAS	x	x			x	x
79780-39-5	279-259-9	Perfluorododecane sulfonic acid (PFDoDS)	monitoring PFAS	x				x	x
422-64-0	207-021-6	Perfluoropropanoic acid (PFPrA)	monitoring PFAS	x					x
376-06-7	206-803-4	Perfluorotetradecanoic acid (PFTetrA)	monitoring PFAS	x					x
354-88-1	-	Perfluoroethanesulfonic acid (PFEtS)	monitoring PFAS	x					
423-41-6	-	Perfluoropropanesulfonic acid (PFPrS)	monitoring PFAS	x					x
-	477-710-6	tris(pentafluoroethyl)trifluorophosphate (FAP)	monitoring PFAS	x					x

4. Category: PMT/vPvM Hazard

The PMT/vPvM hazard categories are summarized in Table 3, which is adapted from Arp and Hale (2023). The PMT/vPvM assessment distribution for the 176 selected substances are presented in

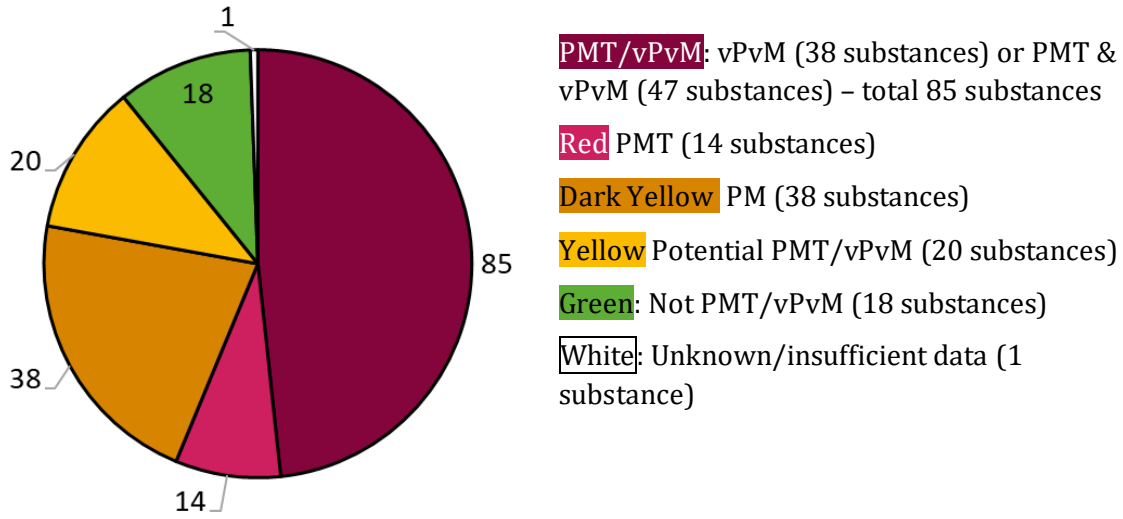
Figure 1, and the detailed PMT/vPvM assessment for selected substances is presente in Annex A.

Table 3: Traffic light colour scheme representing the PMT/vPvM conclusion including the corresponding level of data availability

Criteria or PMT/vPvM conclusion	Explanation
Insufficient data	Data missing or data quality too poor or inconsistent to make a screening level assessment
vPvM	High quality data or sufficient weight-of-evidence that the criteria for vP (very Persistent) and vM (very Mobile) is met
vPvM & PMT	High quality data or sufficient weight-of-evidence that the criteria for vP, vM and T (toxic) criteria are met
PMT	High quality data or sufficient weight-of-evidence that the criteria for P (persistent), M (mobile) and T (toxic), or vP, M and T or P, vM and T are met
PM	High quality data or sufficient weight-of-evidence that the criteria for P and M, or vP and M, or P and vM are met, but there are currently no high-quality consensus conclusions that the criteria for T is met
Potential PMT/vPvM	Screening data or low-quality data indicates that the criteria for P/vP and M/vM could potentially be met
Not PMT/vPvM	High quality data or sufficient weight-of-evidence that either the criteria for P and/or M are not met

Source: (Arp and Hale, 2023)

Figure 1: Distribution of the PMT/vPvM Hazard classes amongst the 176 substances



Source: Original Figure

The majority of the 176 substances selected met the PMT/vPvM criteria, including 14 PMT substances, 38 vPvM substances and 47 PMT & vPvM substances, giving a total of 99 substances. Of the remainder, there were 38 PM substances, 20 Potential PMT/vPvM substances, 18 Not PMT/vPvM substances, and 1 substance for which there was insufficient data to perform an assessment. It was expected that the majority of substances would meet the PMT/vPvM criteria, as those selected were either considered as such in Arp and Hale (2019), or for the short-chain PFAS and triazines they were selected because they were either suspected of being PMT/vPvM substance or capable of transforming into one.

23 of the prioritized PMT/vPvM substances in Arp and Hale (2019) were re-assessed as PM substances due to higher harmonization requirements for how the toxicity data was considered in Arp and Hale (2023), this reduced the number of the 176 substances that met the PMT/vPvM criteria. There were also 17 PMT/vPvM substances in Arp and Hale (2019) re-evaluated as "Potential PMT/vPvM" due to the greater data quality requirements of Arp and Hale (2023) compared to Arp and Hale (2019), and 10 substances that were now considered "Not PMT/vPvM substances" due to newer data that indicated the P/vP criteria was no longer met. A comparison of the PMT/vPvM evaluations in Arp and Hale (2023) with Arp and Hale (2019) can be found in Annex A.

Regarding the 28 substances with a short-chain PFAS moiety, 8 of them met the PMT/vPvM criteria, 12 met the PM criteria and are hypothesised to be parent substances that can transform to PMT/vPvM substances, and 9 are considered either "Not PMT/vPvM" or "Potential PMT/vPvM", but suspected parents of PMT/vPvM transformation substances (Annex A).

Regarding the 24 "monitoring PFAS substances", 19 of these met the PMT/vPvM criteria, 2 were considered PM substances due to lack of read-across data to imply toxicity, and the 3 longer chain PFAS (PFTrDA CASRN72629-94-8, PFDoDS CASRN 79780-39-5 and PFTetrDA CAS 376-06-7) were considered "Not PMT/vPvM" as they did not meet the mobility criteria.

Regarding the 5 added triazines, their assessment went from "unknown/insufficient data" (the triazine 1,3,5-triazine-2,4,6(1H,3H,5H)-trithione, trisodium salt, CASRN 17766-26-6), three were considered "Potential PMT/vPvM" due to the presence of screening data that the PMT/vPvM

criteria could be med, and in one was a PM substance as there was no current evidence indicating toxicity. Overall there was a lack of data for these triazines to make a definitive assessment.

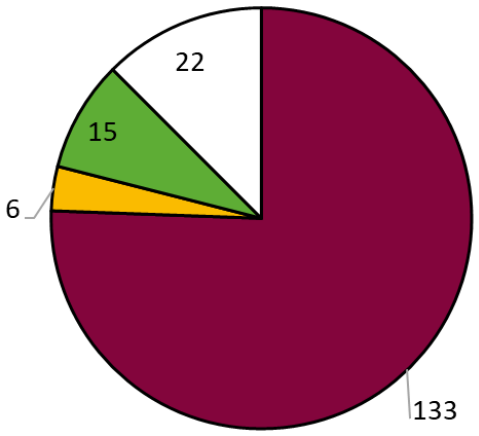
5. Category: REACH Emission Likelihood

The REACH Emission Likelihood Category in the prioritization framework is defined in more detail in Table 4. This category indicates the likelihood that emissions could be occurring, based on the by utilizing indirect indicators REACH registered volumes, the emission-score (E-score) as presented in Arp and Hale (2019). The E-score is based REACH tonnages and registered use categories (Schulze et al., 2018). If a substance is registered under REACH as a non-intermediate and has an E-score above the median value, its REACH Emission Likelihood category was considered "high"; if additionally, the substances had already been detected in drinking water, raw water, bank filtrate or groundwater, its REACH Emission Likelihood category was considered "very high". The literature review of monitoring data for the 176 substances was presented as part of Arp et al., (2023a). For the remaining REACH substances, the "REACH Emission Likelihood category" was considered "medium" if monitoring data in these drinking water relevant media were available. For all remaining substances the REACH Emission Likelihood category was considered "low" (Table 4). The distribution of this category for the 176 substances is presented in Figure 2.

Table 4: REACH Emission Likelihood category assignment

REACH emission likelihood category	Detected in drinking water, raw water, bank filtrate or ground water	Registration type in REACH	E-Score
Very High	Yes	Full	Top 50'th percentile
	-	-	-
High	No	Full	Top 50'th percentile
	-	-	-
Medium	Yes	Full	Lower 50'th percentile
	Yes	Intermediate	-
Low	No	Full	Lower 50'th percentile
	No	Intermediate	-

Figure 2: Distribution of the REACH Emission Likelihood classes amongst the 176 substances



Source: Original Figure

Dark red: high E-score, detection in environment required for "very high" (49 substances), otherwise "high" (84 substances) (total 133 substances)

Yellow: low E-score or intermediate under REACH that is detected in drinking water sources required for "medium" (6 substances)

Green: low E-score or intermediate substance, not detected in drinking water sources required for "low" (15 substances)

White: Not registered under REACH (22 substances)

The majority of the 176 substances had a REACH Emission Likelihood score that was very high (49 substance) or high (84 substances), totalling 133 substances. These were mostly comprised of the substances in Arp and Hale (2019), which were prioritized in part because of their very high or high REACH Emission Likelihood score, here 105 of the 119 substances from Arp and Hale (2019) were either "high" or "very high", whereas 3 were "medium" and 11 were "low".

Of the short-chain PFAS substances registered under REACH, 25 of 28 of them had a "very high" (3 substances) or "high" (22 substances) REACH Emission Likelihood scores, with the remaining being either "medium" (2 substances) or "low" (1 substances) REACH Emission Likelihood scores. Of the 24 monitoring PFAS, 20 were not registered under REACH and the remaining substances were either "medium" (2 substances) or "low" (2 substances). Some of these monitoring PFAS were selected because of legacy emissions, in some cases with restrictions put in place by the Stockholm Convention around the time REACH was implemented in 2007.

Of the triazines, three of them had a "high" REACH Emission Likelihood score, and the transformation products of melamine (ammeline and ammelide) were considered "Not REACH".

There were 22 substances where the REACH Emission Likelihood score could not be assessed, because they were not REACH registered but were impurities or transformations substances of REACH registered substances (e.g. PFAS that can be potential degradation products or unknown impurities of REACH registered PFAS).

6. Category: Analytical and Monitoring Gap

Analytical and monitoring gaps are considered as one category and not two because, in practice, there is a lot of overlap between these two gaps. Broadly speaking the analytical gap refers to chemicals that are not analysed because there is currently no available method. The monitoring gap can refer both to substances that can be measured but are not, due to lack of interest/client requests, but also because of analytical gap issues. To assess and assign the category analytical and monitoring gap for each of the 176 substances survey data from water analysis labs were used, along with literature queries, as presented in Table 5.

Table 5: Classes of the Analytical and Monitoring Gap Prioritization Category

Criteria or PMT/vPvM conclusion	Explanation
Not included/not assessable	Substances that were not included in the survey, and therefore the analytical and monitoring gap is unknown.
Major Analytical Gap	There is an extreme analytical gap. The substances is not monitored because it can only be analysed by advanced / specialized methods that are unknown to the surveyed labs.
Minor Analytical Gap	This class is both an analytical and monitoring gap. It refers to substances that are not monitored due to both lack of methods and client requests, but for cases where method development is potentially feasible.
Major Monitoring Gap	This class is also both an analytical and monitoring gap. It refers to substances that are not monitored due to both lack of methods and client requests, but in cases where existing methods could be applied with little need for development (e.g. using commonly available instrumentation).
Minor Monitoring Gap	This class refers to substances that are monitored regularly, but by less than 20% of labs in the survey. The threshold was chosen to reflect the percentage of water analysis labs in Germany that are research labs, and therefore more likely to be monitoring for emerging substances than non-research labs.
No Monitoring Gap	Monitored regularly, but more than 20% of water quality labs

Two surveys containing a list of 150 of the 176 substances presented in Chapter 3 were sent to 27 analytical labs throughout Germany. The first survey was sent with a submission deadline of early November 2020; the follow-up survey was sent in out based on the results of the first survey, with a deadline of April 2021. Many of the surveyed labs are dedicated specifically to examining drinking water quality. In total, 27 labs of different sizes answered the survey within the deadline. Twelve of these were commercial labs (including the labs of the three project partners: IWW, TZW and HSF), eleven were federal labs (of the 16 federal states), and four were labs of water suppliers. The surveys were answered anonymously to facilitate maximum participation. Due to the number and locations of the labs included in this work, the survey is considered representative of the overall picture of water monitoring in Germany.

The questions in first survey were relevant for addressing both analytical gaps and monitoring gaps individually. Participating labs were asked to supply the following information about each of the 150 substances related to the Analytical and Monitoring gap:

- is the substance regularly analysed by your lab?

- could it be analysed if necessary using equipment and methods currently available in your lab?

In early 2021, a second survey was set out to obtain more information about the substances that the labs said they did not analyse for further clarification. The specific questions in this second survey were:

- Is this due to analytical problems (e.g. missing reference substances, limitations of instrumentation)
- Is this due to a lack of request from their clients?

When the labs answered that they were able to analyse a particular substance, they were also asked which method they used.

6.1 Analytical and Monitoring Gap

The results of the analytical gap for the 150 substances were as follows:

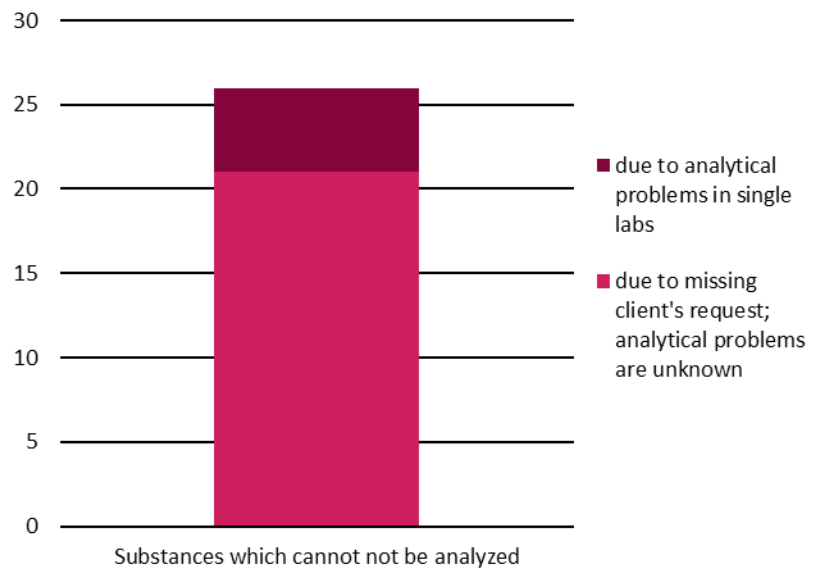
i) There were 66 substances analysed regulatory by at least one lab,

ii) There were 58 substances which could be analysed if specifically requested

iii) There were 26 substances which could not be analysed if specifically requested .

In order to better understand the reasons why 26 of the substances could not be analysed, the results of the second survey were considered (Figure 3). Single labs reported analytical problems for five of the 26 substances, and these substances were therefore categorized as analytical gap substances. These substances are: p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline, m-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline, Cyclohexylidenebis[tert-butyl] peroxide, α,α-dimethylbenzyl hydroperoxide, and Bis(α,α-dimethylbenzyl) peroxide. However, for the remaining 21 substances, the labs stated that they could not be analysed because they are not specifically requested by clients, but methods could potentially be developed. It must however be borne in mind that analytical problems are still possible for these substances, but that they have not been encountered due to lack of client request.

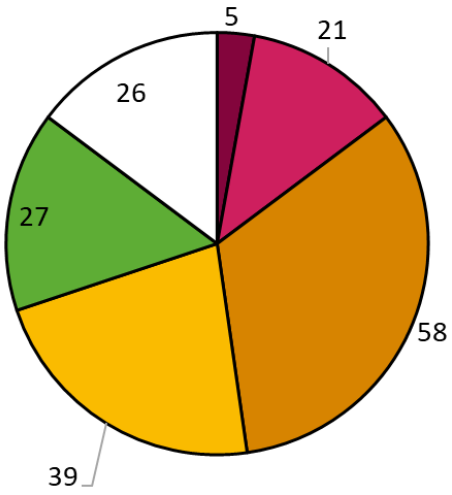
Figure 3: Number of substances which cannot be analysed by any of the surveyed labs



Source: Original Figure

Based on the survey results, the selected 176 substances were grouped according to the Analytical and Monitoring gap category presented in Figure 4.

Figure 4: Distribution of the analytical and monitoring gap prioritization categories for the 176 selected substances



Source: Original Figure

Major Analytical Gap: Not monitored because the substance can only be analysed by advanced / specialized methods (5 substances)

Minor Analytical Gap Not monitored, but method development feasible (21 substances)

Major Monitoring Gap The analytical gap is not substantial, the substance is not monitored but could be using current methods (58 substances)

Minor Monitoring Gap if the substance is monitored regularly, but by less than 20% of water surveyed labs. (39 substances)

No Monitoring Gap: Monitored regularly, but more than 20% of water quality labs (27 substances)

White: Substance not included/assessed (26 substances)

As shown Figure 4, of the 176 substances considered, there are 27 substances where there was no monitoring gap (green category, analysed regularly by at least 20% of the labs surveyed) and 39 for which there was a minor monitoring gap (yellow category, by at least one surveyed lab). For 58 substances there was a major monitoring gap (dark yellow category, methods exist but have not been implement due to lack of requests). Regarding the 26 substances that had an analytical gap, there were 21 with a minor analytical gap (red category, not monitored but

method development feasible) and 5 substances for which analytical methods do not yet exist and thus had a major analytical gap (dark red category).

6.2 Analytical Methods

For the PMT/vPvM substances that the labs analysed regularly or could analyse if requested, the labs were additionally asked which method they used. By evaluating the answers to this question based on the expertise of the labs participating in this project, methods can be recommended for 82 of the 150 substances based on the most common responses and thus method suitability. These methods are shown in Table 6 in bold letters. For the remaining 68 substances, suitable methods were identified based on the expertise of the authors of this study.

Table 6: Recommended analytical methods for the 150 PMT/vPvM substances considered in this study

Method and standard abbreviations include DIN = Deutsches Institut fur Normung (German Institute for Standardisation), ISO = International Standardization Organization (also means "equal" in Greek), EN = Europaische Norm (European standard), GC = gas chromatography, LC = liquid chromatography, RPLC = reverse phase liquid chromatography, HILIC = Hydrophilic interaction liquid chromatography, MS = mass spectrometry, MS/MS = tandem mass spectrometry

Substance name	Recommended method	Substance name	Recommended method	Substance name	Recommended method
[[(phosphonomethyl)imino]bis[(ethylenenitrilo)bis(methylene)]]tetrakisphosphonic acid, sodium salt	**LC-MS/MS**	2-nitrotoluene	**GC-MS**	Diisopropyl ether	**DIN EN ISO 10301:1997-08**
[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methylene)]]tetrakisphosphonic acid	**LC-MS/MS**	2-phosphonobutane-1,2,4-tricarboxylic acid	**LC-MS/MS**	Diisopropylbenzene	**DIN EN ISO 10301:1997-08**
{difluoro[(1,2,2-trifluoroethenyl)oxy]methoxy}trifluoromethane	GC-MS	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonic acid	**LC-MS/MS**	Dimethoxydimethylsilane	GC-MS
1,1,1,2,2,3,3-heptafluoro-3-[(trifluorovinyl)oxy]propane	GC-MS	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate	**GC-MS**	Dimethyl sulfoxide	LC-MS/MS
1,1,1,2,2,4,5,5,5-nonafluoro-4-(trifluoromethyl)-3-pentanone	GC-MS	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl methacrylate	**GC-MS**	Disodium oxybis[methylbenzenesulphonate]	LC-MS/MS
1,1,1-trichloroethane	**DIN EN ISO 10301:1997-08**	3,3'-sulphonyldianiline	**LC-MS/MS**	Hexamethyldisiloxane	GC-MS
1,1,2,2,3,3,4,4,4-nonafluoro-N-(2-hydroxyethyl)-N-methylbutane-1-sulphonamide	**GC-MS**	3a,4,7,7a-tetrahydro-4,7-methanoindene	GC-MS	Lithium bis(trifluoromethylsulfonyl)imide	**HILIC-MS/MS**

Substance name	Recommended method	Substance name	Recommended method	Substance name	Recommended method
1,1,2,2,3,3,4,4,4-nonafluoro-N,N-bis(2-hydroxyethyl)butane-1-sulphonamide	GC-MS	3-aminobenzenesulphonic acid	**HILIC-MS/MS**	m-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	**LC-MS/MS**
1,1,2,2,3,3-hexafluoro-1-trifluoromethoxy-3-trifluorovinyloxypropane	**GC-MS**	3-aminomethyl-3,5,5-trimethylcyclohexylamine	**HILIC-MS/MS**	Melamine	**LC-MS/MS**
1,1-dichloroethylene	**DIN EN ISO 10301:1997-08**	3-chloroaniline	**GC-MS**	Methenamine	**LC-MS/MS**
1,2,3,4-tetrahydronaphthalene	**GC-MS**	4,4',4''-(ethan-1,1,1-triyl)triphenol	GC-MS	Methyl trifluoroacetate	GC-MS
1,2,4-triazole	**LC-MS/MS**	4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane	GC-MS	m-tolylidene diisocyanate	LC-MS/MS
1,2-benzisothiazol-3(2H)-one 1,1-dioxide	LC-MS/MS	4,4'-methylenebis(cyclohexylamine)	**LC-MS/MS**	N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	**HILIC-MS/MS**
1,2-dibromoethane	**DIN EN ISO 10301:1997-08**	4,4'-oxydi(benzenesulphonohydrazide)	LC-MS/MS	N,N-diethylhydroxylamine	GC-MS
1,2-dichlorobenzene	**DIN EN ISO 10301:1997-08**	4,6-bis(octylthiomethyl)-o-cresol	LC-MS/MS	N,N-dimethylacrylamide	GC-MS
1,2-dichloropropane	**DIN EN ISO 10301:1997-08**	4-amino-N-(1,1-dimethylethyl)-4,5-dihydro-3-(1-methylethyl)-5-oxo-1H-1,2,4-triazole-1-carboxamide	LC-MS/MS	N-[3-(dimethylamino)propyl]-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonamide N-oxide	**RPLC-MS/MS**

Substance name	Recommended method	Substance name	Recommended method	Substance name	Recommended method
1,3-dichlorobenzene	**DIN EN ISO 10301:1997-08**	4-aminophenol	**LC-MS/MS**	N-butylbenzenesulphonamide	**LC-MS/MS**
1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione	GC-MS	4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	GC-MS	N-methylaniline	**GC-MS**
1,3-di-o-tolylguanidine	**HILIC-MS/MS**	4-mesyl-2-nitrotoluene	LC-MS/MS	p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	**LC-MS/MS**
1,3-diphenyl-2-thiourea	**HILIC-MS/MS**	4-methyl-m-phenylene diisocyanate	LC-MS/MS	Pentasodium pentahydrogen [[(phosphonatomethyl)imino]bis[ethane-2,1-diylnitrilobis(methylene)]]tetrakis phosphonate	LC-MS/MS
1,3-diphenylguanidine	**LC-MS/MS**	4-nitrotoluene	**GC-MS**	Perhydro-1,3,5-trinitro-1,3,5-triazine	GC-MS
1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	LC-MS/MS	4-nitrotoluene-2-sulphonic acid	**RPLC-MS/MS**	Phenol, isopropylated, phosphate (3:1)	LC-MS/MS
1,4-diazabicyclooctane	**HILIC-MS/MS**	4-vinylpyridine	GC-MS	Phenyl bis(2,4,6-trimethylbenzoyl)-phosphine oxide	**HILIC-MS/MS**
1,4-dioxane	**DIN EN ISO 17943:2016-10**	6-phenyl-1,3,5-triazine-2,4-diyldiamine	**HILIC-MS/MS**	Pigment Yellow 176	LC-MS/MS
1,8-diazabicyclo[5.4.0]undec-7-ene	GC-MS	Ametryn	**HILIC-MS/MS**	Potassium 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulphonate	**LC-MS/MS**

Substance name	Recommended method	Substance name	Recommended method	Substance name	Recommended method
1-[(2,4-dinitrophenyl)azo]-2-naphthol	LC-MS/MS	Aminoiminomethanesulphinic acid	LC-MS/MS	Propargite	GC-MS
1-chloro-2-nitrobenzene	**GC-MS**	Ammelide	**HILIC-MS/MS**	sodium 2-methyl-2-({3-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)thio]propanoyl}amino)propane-1-sulfonate	LC-MS/MS
1-methylpiperazine	**HILIC-MS/MS**	Ammeline	**HILIC-MS/MS**	Sodium 2-methyl-2-[(1-oxoallyl)amino]propanesulphonate	**HILIC-MS/MS**
1-nitroguanidine	LC-MS/MS	Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate	**RPLC-MS/MS**	Sodium 3-(allyloxy)-2-hydroxypropanesulphonate	**HILIC-MS/MS**
2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	LC-MS/MS	Ammonium difluoro[1,1,2,2-tetrafluoro-2-(pentafluoroethoxy)ethoxy]acetate	GC-MS	Sodium p-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]benzenesulphonate	LC-MS/MS
2-(2H-benzotriazol-2-yl)-p-cresol	GC-MS	Ammonium difluoro{[2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	GC-MS	Sulisobenzone	LC-MS/MS
2,2,3,3,4,4,5,5-octafluoropentyl methacrylate	**GC-MS**	Ammonium undecafluorohexanoate	**RPLC-MS/MS**	tert-butyl hydroperoxide	**GC-MS**
2,2,3,3,5,5,6,6-octafluoro-4-(trifluoromethyl)morpholine	**GC-MS**	Benzophenone	**GC-MS**	Tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one	GC-MS
2,2'-azobis[2-methylbutyronitrile]	GC-MS	Benzotriazole	**LC-MS/MS**	Tetramethylthiuram monosulphide	GC-MS
2,2'-dimethyl-2,2'-azodipropiononitrile	GC-MS	Benzyltrimethylammonium chloride	**HILIC-MS/MS**	trans-dichloroethylene	**DIN EN ISO**

Substance name	Recommended method	Substance name	Recommended method	Substance name	Recommended method
					10301:1997-08
2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)	LC-MS/MS	Bis(2-dimethylaminoethyl)(methyl)amine	**HILIC-MS/MS**	Tricarbonyl(methylcyclopentadienyl)manganese	LC-MS/MS
2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane	GC-MS	Bis(4-fluorophenyl) ketone	GC-MS	Trichloro(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	GC-MS
2,4,6-trichloro-1,3,5-triazine	**not possible, hydrolysis in water**	Bis(α,α-dimethylbenzyl) peroxide	GC-MS	Trichloroacetic acid	**GC-MS**
2,4,7,9-tetramethyldec-5-yne-4,7-diol	GC-MS	Calcium 3-hydroxy-4-[(4-methyl-2-sulphonatophenyl)azo]-2-naphthoate	LC-MS/MS	Triethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	**GC-MS**
2,4-dinitrophenol	**GC-MS**	Carbon tetrachloride	**DIN EN ISO 10301:1997-08**	Triethyl phosphate	**GC-MS**
2,5-bis-isocyanatomethyl-bicyclo[2.2.1]heptane	LC-MS/MS	Carboxymethyldimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulphonyl]amino]propylammonium hydroxide	LC-MS/MS	Trifluoro(trifluoromethoxy)ethylene	GC-MS
2,6-xylidine	**GC-MS**	Chlorobenzene	DIN EN ISO 10301:1997-08	Trifluoro(trifluoromethyl)oxirane	GC-MS

Substance name	Recommended method	Substance name	Recommended method	Substance name	Recommended method
2-[(2-[2-(dimethylamino)ethoxy]ethyl)methylamino]ethanol	**LC-MS/MS**	Chloroform	**DIN EN ISO 10301:1997-08**	Trifluoroacetic acid	**LC-MS/MS**
2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl acrylate	GC-MS	Climbazole	**LC-MS/MS**	Trifluoromethanesulphonic acid	**HILIC-MS/MS**
2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl methacrylate	GC-MS	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, chlorinated	LC-MS/MS	Trimethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	GC-MS
2-amino-4,5-dichlorobenzenesulfonic acid	**HILIC-MS/MS**	Cyanuric acid	**HILIC-MS/MS**	Tris(2-butoxyethyl) phosphate	**GC-MS**
2-fluoro-6-trifluoromethylpyridine	GC-MS	Cyclohexylidenebis[tert-butyl] peroxide	LC-MS/MS	Tris(2-chloro-1-methylethyl) phosphate	**GC-MS**
2-hydroxy-N,N,N-trimethyl-3-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)thio]propan-1-aminium chloride	LC-MS/MS	Dapsone	**LC-MS/MS**	Vinylchlorid	**DIN EN ISO 10301:1997-08**
2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one	GC-MS	Dibutyl hydrogen phosphate	**HILIC-MS/MS**	α,α-dimethylbenzyl hydroperoxide	GC-MS
2-morpholinoethanol	**HILIC-MS/MS**	Dichlorodifluoromethane	GC-MS		

7. Category: Remediation Gap

The Remediation Gap category is an important consideration regarding the management of PMT/vPvM substances, as, according to the EU Water Framework Directive (2000/60/EC (European Commission, 2000a)), "*Member States shall ensure the necessary protection for the bodies of water identified [...] in order to reduce the level of purification treatment required in the production of drinking water*." Therefore, technical water treatment methods can be considered as methods of risk management of PMT/vPvM substances registered under REACH.

The classes of the remediation gap category (Table 7) were based on advanced and conventional methods used in water treatment common in Europe. For the advanced methods, both ozonation and activated carbon (AC) filtration were considered, and conventional methods refer to simpler water treatment techniques like aeration (which can remove volatile substances) or sand filtration. State-of-the-art water treatment methods, such as reverse osmosis and nanofiltration, as well as alternative destruction methods like ultraviolet radiation and chlorine disinfection, were not considered here, in part due to lack of widespread adaptation in Europe.

Table 7: Classes of the Remediation Gap Prioritization Category

Criteria or PMT/vPvM conclusion	Explanation
Not included/not assessable	Substances that were not included or assessed
No O3&AC	Substances that cannot be eliminated using AC or ozonation
O3 Only	Substances that can be removed using ozonation only
AC Only	Substances that can be removed using AC only
Both O3&AC	Substances that can be removed by using both ozonation or AC
Standard methods	Substances that can be removed with conventional techniques

The reason why "ozonation only" was given a higher prioritization category (red) than AC only (dark yellow), is due to the comparative rarity and extra expense for ozonation, as well as ozonation potentially leading to hazardous by-products.

To begin, and as explained in the first section of this chapter, 150 of the 176 selected substances were screened for their potential removability using AC or ozonation using the *Hot-Target-approach*. For some substances that are most frequently detected in the monitoring campaign of Chapter 8, a refined assessment was conducted (i.e. literature review and experimental work).

In the second section of this chapter, further details about the challenges German drinking water producers face to analyse, monitor or remediated these substances are given. Interviews were designed to learn about current technologies at German waterworks and the awareness of the water suppliers concerning PMT/vPvM substances.

7.1 Remediation of prioritized PMT/vPvM substances by AC filtration and ozonation

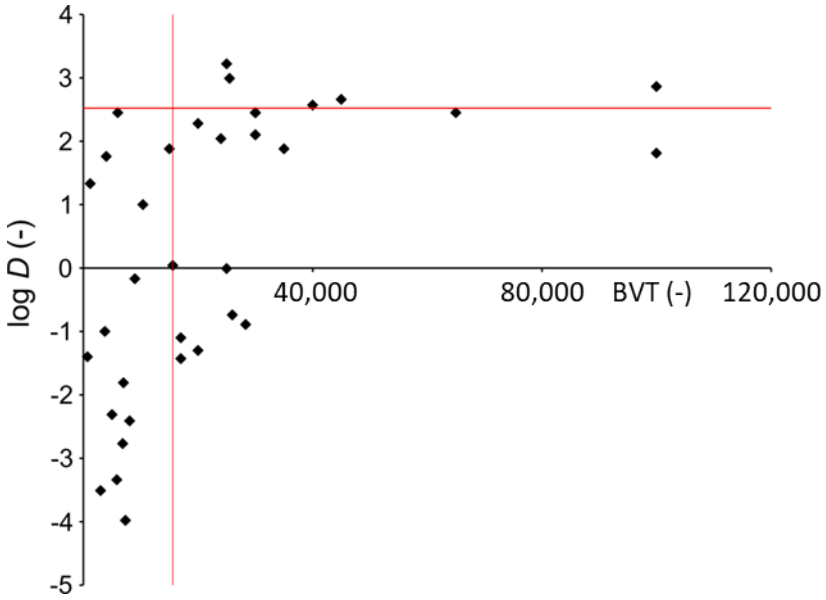
The screening for removal potential of prioritized PMT/vPvM substances by AC filtration and ozonation was performed using the *Hot-Target-approach*.

7.1.1. AC filtration within the *Hot-Target-approach*

AC filtration is an established method for removing lipophilic substances from the water phase. Therefore, measures of the lipophilicity of a substance (e.g. log K_{OW}, log K_{OC}, log D_{OW}) are significant prediction factors for the removal efficiency by this technique. In contrast to natural aquifer material, AC consists mostly (i.e. ≥ 85% (Sontheimer et al., 1988)) of organic carbon (OC). Therefore, it can be used to remove medium-polar substances that may overcome the underground passage during bank filtration. A standardized test was developed to assess the removal potential of organic substances by AC treatment at the project partner lab at TZW (Happel et al., 2009). An economically viable removal of a substance is achieved if the concentration of the tested substance in the effluent is lower than 10% of the concentration in the inflow (i.e. $c/c_0 \leq 10\%$) after 15,000 bed volumes treated (BVT). To derive the criteria used in the *Hot-Target-approach*, meta-analysis of TZW internal experimental data of the mentioned test was conducted to derive a log-*D*-cut-off value. Results showed that all investigated PMT/vPvM substances with a log D_{OW} of 2.5 or higher can be removed economically by AC treatment (Figure 5). Therefore, this value was selected as the cut-off for the assessment.

Figure 5: Number of bed volumes treated (BVT) at c/c_0 = 10% *vs.* log D_{OW} of different compounds (log D_{OW} calculated by Percepta/ACD-Labs).

The threshold values 15,000 BVT and log D_{OW} 2.5 highlighted by the red lines).

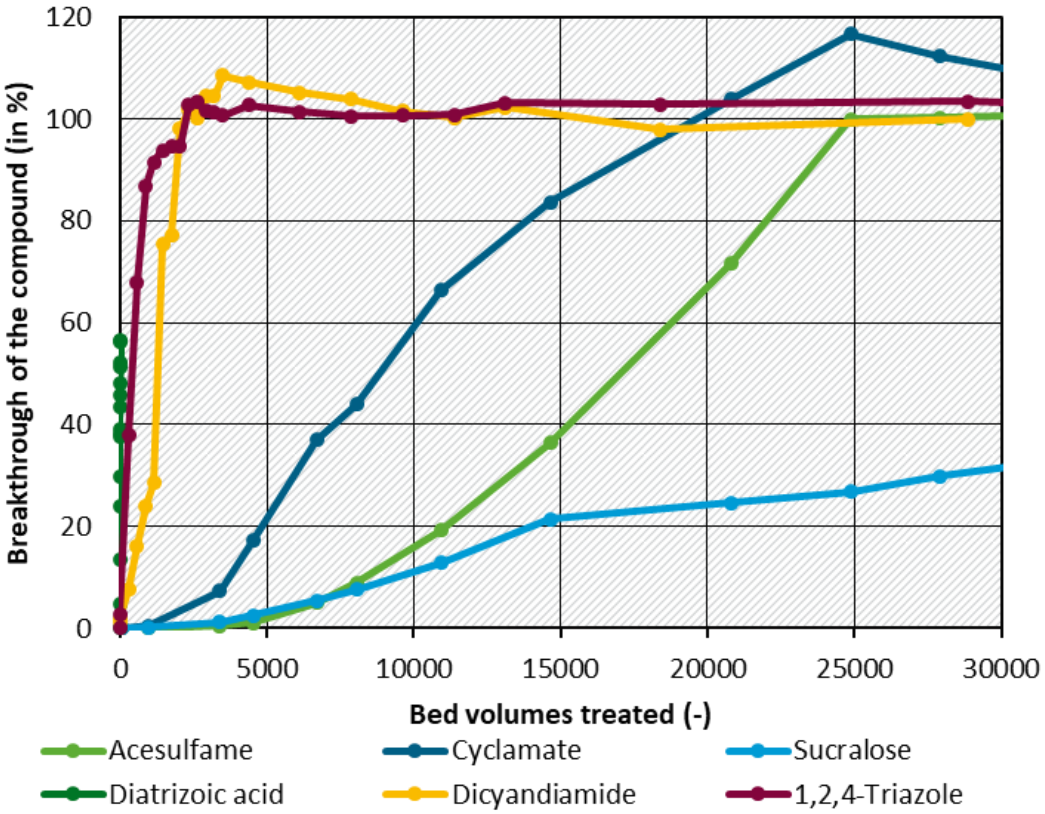


Source: Original Figure, slightly adapted from Nödler K. et al., 2018.

However, some PMT/vPvM substances can be removed economically with AC treatment despite showing lower log-*D*-values (e.g. the tested aromatic nitro compounds). It is well known that these compounds effectively adsorb to clay minerals (Haderlein et al., 1996). It is possible that the mineral fraction of the AC is also important for this group of substances and/or that there are additional interactions with the AC-material, which cannot be predicted by the log D_{OW} alone

(i.e. π-π-interactions). Therefore, using the derived cut-off is aligned with the use of the precautionary principle and is considered suitable for screening purposes which can then be followed by higher-tier compound-by-compound refinement. Selected experimental results of the tests are shown in Figure 6.

Figure 6: Early breakthrough of six vM substances registered under REACH in the small-scale filter test with activated carbon



Source: Original Figure

7.1.2. Ozonation within the *Hot-Target-screening*

Structural information for substances can be represented as SMILES strings (Simplified Molecular Input Line Entry Specification). For the *Hot-Target-approach*, a software tool was developed that scans the SMILES for defined substructures susceptible to fast reaction kinetics with ozone. The implementation of the software tool is based on the definition of chemical substructures using SMARTS (SMiles ARbitrary Target Specification), an extension of SMILES. Generally, (almost) every valid SMILES string is also a valid SMARTS string. The reverse is not true, because the extension allows the use of wildcards and logical operators, which enables an even more flexible and efficient search for substructures in chemical databases. For example, the wildcard symbol for any atom is an asterisk '*'. An arbitrary bond type is indicated with a tilde '~'. Further symbols or letters can be used to specify, for example, the charge, valence, connectivity or number of bonded hydrogen atoms for each atom. A detailed description of SMARTS with examples can be found on the website of the company Daylight[1].

[1] [Online]. Available: http://www.daylight.com/dayhtml/doc/theory/theory.smarts.html.

The C=C and C≡C bonds as well as aniline nitrogen were selected as substructures that show fast reaction kinetics with ozone (Duncan, 2005; Von Gunten, 2003). The integration of further substructures such as phenolic groups and other amines was omitted, since their reaction kinetics with ozone depend on their degree of ionisation and their respective relevant dissociation constants are often within the pH-range of raw water (7 to 9) (Schaffer and Licha, 2014; Von Gunten, 2003). In the case of the C=C bond, it is also taken into account that halogen substituents significantly decrease the reaction kinetics with ozone (Von Gunten, 2003). Therefore, C=C bonds with more than one halogen substituent are not covered by the SMART query.

A substance containing at least one of the listed structural elements reacts very quickly with ozone. Predictions about transformation products and associated risks cannot be made by using this approach.

7.1.3. Refinement of the *Hot-Target*-approach

The most abundant substances and substance groups from the monitoring study (see chapter 5) were individually checked for their removal potential (AC and ozonation), either by consulting the literature (preferably studies including full-scale waterworks) or by carrying out laboratory testing. The results of the *Hot-Target*-screening and the refined procedure are compared in section 7.1.3.7.

7.1.3.1. Per- and polyfluoroalkyl substances (PFAS)

For perfluoroalkyl acids (PFAAs), short-chain and long-chain representatives are assessed using a grouping approach. Previous studies have shown that there is no substantial removal of short-chain perfluorosulfonic acids (PFSA) (i.e. 5 or less perfluorinated carbons) and short-chain perfluorocarbonic acids (PFCA) (i.e. 6 or less perfluorinated carbons) by AC (Glover et al., 2018; Scheurer et al., 2017). Furthermore, the C-F moiety is highly resistant to oxidative treatments such as ozonation (Scheurer et al., 2017). This holds true for long-chain PFSA (6 or more perfluorinated carbons) and long-chain PFCA (7 or more perfluorinated carbons). Elimination of long-chain PFAAs by AC is possible (Glover et al., 2018), however, removal is limited in the presence of dissolved organic matter (Appleman et al., 2013). As a general rule for PFAS and AC, the longer the alkyl-chain, the better the removal.

7.1.3.2. The cyclic ether 1,4-dioxane

As learnt from studies at full-scale waterworks in Germany, the compound 1,4-dioxane cannot be sufficiently removed by ozonation and/or AC filtration (ARW, 2016).

7.1.3.3. The corrosion inhibitor 1*H*-benzotriazole

According to the study about organic micropollutants as process indicators reported by (Jekel et al., 2015), 1*H*-benzotriazole can be sufficiently eliminated by both ozonation and AC filtration.

7.1.3.4. The industrial chemical melamine

According to results from a full-scale waterworks in Germany, melamine cannot be removed by ozonation and there is very limited elimination by AC (only with fresh AC) (https://www.lw-online.de/fileadmin/lwonline/redaktion/pdf-dateien/publikationen/schriftenreihe/Beitrag_6_Winzenbacher_2015.pdf)

7.1.3.5. The sweetener saccharin

According to results from a German full-scale waterworks, there is no indication of the removal of saccharin by ozonation. However, effective removal by AC filtration, attributed to biological

degradation at aged AC sorption sites, has been reported (i.e., the AC acts as a bioreactor) (Scheurer et al., 2010).

7.1.3.6. The compounds 2-acrylamido-2-methylpropane sulfonic acid (AMPS), cyanuric acid, and diphenyl guanidine (DPG)

To the best of our knowledge, there is no published data on the removal of AMPS, cyanuric acid, and DPG by ozonation or AC treatment. Therefore, individual laboratory experiments were conducted.

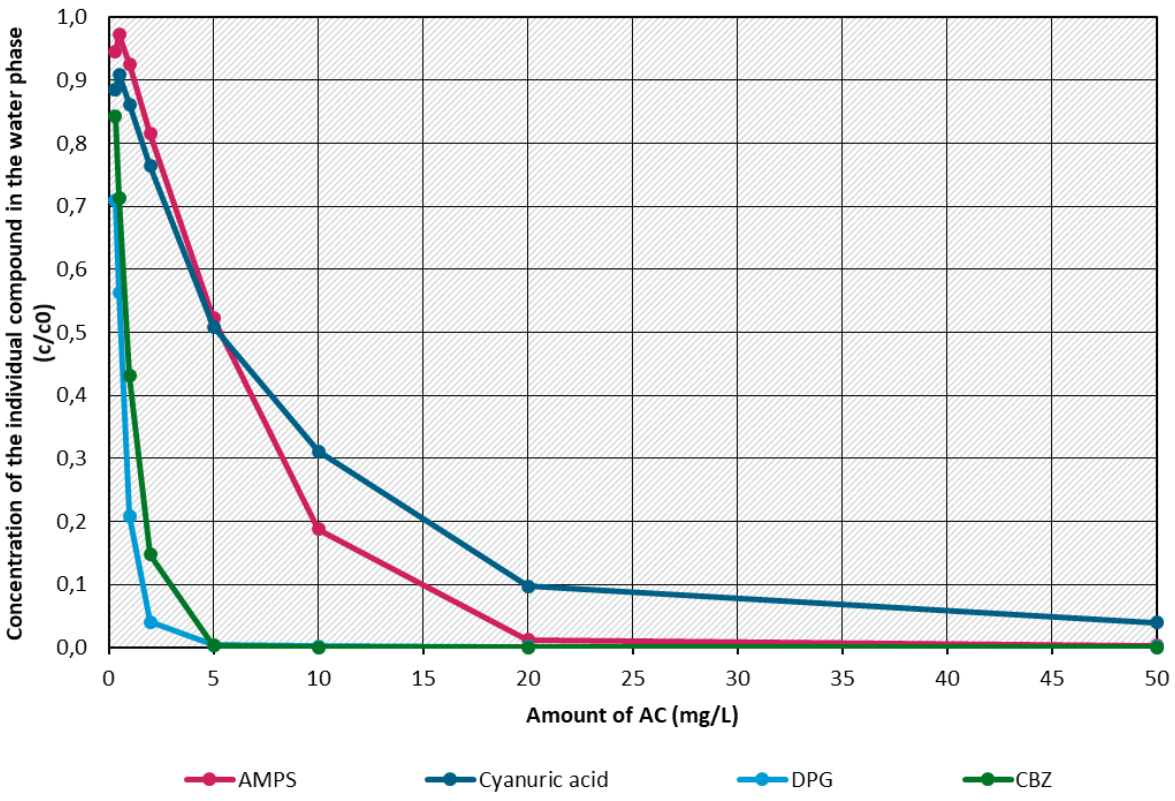
Ozonation experiments were carried out as batch experiments in 100-mL bottles (clear glass) using tap water (city of Karlsruhe, Germany; pH value of 7.3 and a dissolved organic carbon (DOC) concentration of 0.9 mg/L). The initial concentration of each substance was 1 µg/L. Ozone concentrations of 0.2, 0.5, and 1 mg/L were tested. The test batches were gently stirred using a magnetic stirrer. After defined ozone contact times of 1 minute to 60 minutes, samples were taken and the residual ozone was reduced using sodium thiosulfate. AMPS and DPG were efficiently removed (i.e. not detected after 5 min) even at the lowest ozone concentration. However, no elimination (i.e. < 20% elimination) was observed for cyanuric acid even at the highest ozone concentration and 60 min reaction time.

To evaluate the removability of the target substances by AC, adsorption isotherms were set up with eight different doses of powdered activated carbon (PAC) (0.3, 0.5, 1, 2, 5, 10, 20, and 50 mg/L). The AC used was PAC *Filtrasorb 300* (F 300; Chemviron Carbon, Feluy, Belgium) which is widely used in waterworks. The test mixtures were shaken horizontally for a period of 48 h and after the test, the samples were filtered to remove the PAC. Similar to the ozonation experiments, the initial concentration of each individually tested substance in the batch was 1 µg/L. To derive the elimination potential of the individual substances, the results were compared with the ones obtained for carbamazepine (CBZ). AC is well known to efficiently eliminate CBZ (Sperlich et al., 2017). Therefore, similar or stronger adsorption of the tested substances to AC than CBZ indicates efficient removal by this technique; lower adsorption is defined as insufficient removal of a substance by AC. The results are shown in

Figure 7. While DPG can be efficiently removed by AC, no removal is observed for AMPS and cyanuric acid.

Figure 7: Results of the experiments on removal of AMPS, cyanuric acid, and DPG by AC

CBZ was used as reference compound for efficient removal by means of AC



Source: Original Figure

7.1.3.7. Comparison of the *Hot-Target* assessment and refinement

A comparison of the *Hot-Target* assessment and the further refinement of conclusions based on experimental data is shown in Table 8. The comparison demonstrates that the *Hot-Target-approach* is a suitable tool for precautionary screening of data sets, i.e. there was no compound misleadingly labelled as removable. However, the results in Table 8 also show that experimental refinement is recommended.

Regarding the most abundant PMT/vPvM substances detected in the monitoring campaign (see chapter 6), there is a significant remediation gap for short-chain PFAAs (i.e. TFA, PFPrA, PFBA, PFBS), 1,4-dioxane, melamine, and cyanuric acid. For ozonation, the transformation products of 1*H*-benzotriazole, AMPS, and DPG with ozone and the potentially associated risks are unknown.

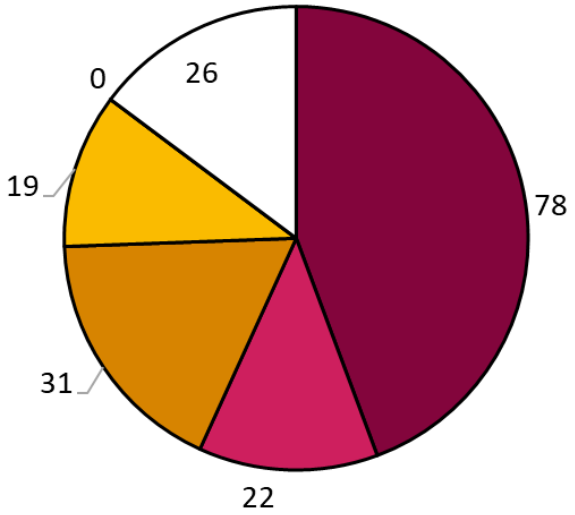
Table 8: Comparison of the *Hot-Target* approach and the evaluation based on experimental data

Compound/group	*Hot-Target*-screening	*Hot-Target*-screening	Experimental data	Experimental data
	Ozonation	AC filtration	Ozonation	AC filtration
Short-chain PFAA	No removal	No removal	No removal	No removal
Long-chain PFAA	No removal	Removal	No removal	Removal
1,4-Dioxane	No removal	No removal	No removal	No removal
1*H*-Benzotriazole	No removal	No removal	Removal	Removal
Melamine	No removal	No removal	No removal	No removal
Saccharin	No removal	No removal	No removal	Removal (biodegradation)
AMPS	Removal	No removal	Removal	No removal
Cyanuric acid	No removal	No removal	No removal	No removal
DPG	Removal	No removal	Removal	Removal

7.1.4. Remediation Gap Categorization

The final conclusions of the remediation gap categorization of the selected 176 substances after the *Hot-Target* screening approach and final refinement is presented in Figure 8. As is evident, the majority of substances included in the screening cannot be removed by AC (only 50 of the substances were considered to be removable by AC, of which 31 cannot be removed by ozonation), and only a similar minority can be removed by ozonation (41 substances). There were only 19 substances that are known to be removable by both methods. 76 substances were identified that need remediation methods that require next generation and rarely available remediation techniques (e.g. reverse osmosis or nanofiltration may be sufficient in some cases).

Figure 8: Results the Remediation Gap categories for the 152 PMT/vPvM substances considered



No O3 and AC: Compounds that cannot be eliminated using AC or ozonation (78 substances)

O3 only: Compounds that can be removed using ozonation only (22 substances)

AC only : Compounds that can be removed using AC only (31 substances)

Both O3&AC: Compounds that can be removed by using both AC or ozonation (19 substances)

Conventional: Compounds that can be removed with conventional techniques (0 substances)

White: Not assessable (26 substances)

Source: Original Figure

7.2 PMT/vPvM substances and technical treatment: current status for the German and European water sector

The 13 water companies which provided the water samples for the monitoring of German drinking water sources (see chapter 8), were asked to answer a survey about their awareness regarding the most frequently detected substances, the technical water treatment options present or planned at their waterworks, and their general concerns in terms of trace contaminants. Twelve of the 13 water companies responded. The questions asked and their answers given are summarized and discussed below.

Q1: Which substances currently pose the greatest challenges for your company in the production and supply of drinking water? *(Welche Stoffe stellen für Ihr Unternehmen derzeit die größten Herausforderungen bei der Trinkwassergewinnung und -versorgung dar?)*

Compound groups mentioned by more than one water company were PFAS (4 water companies), plant protection products (PPP) and PPP-metabolites (4 water companies) as well as pharmaceuticals and related transformation products (TPs) (3 water companies). Individual micropollutants mentioned by more than one water company are listed in Table 9. Dikegulac is used as a PPP and chlorothalonil M4 as well as *N*,*N*-dimethylsulfamide (DMS) are PPP-metabolites. Sulfamic acid is an inorganic REACH registered chemical. All other mentioned substances are PMT/vPvM substances covered by the REACH regulation.[2]

[2] Sulfamic acid is registered under REACH but, as an inorganic compound, not evaluated regarding its persistence. Therefore, this compound is by definition not included in PMT/vPvM-assessment as it falls outside the applicability domain.

Table 9: **Individually mentioned micropollutants representing the greatest challenges for the water companies who responded to the survey**

Substance	No. of water companies mentioning the substance
TFA	7
1,4-dioxane	3
Sulfamic acid	3
EDTA	3
Melamine	3
1*H*-benzotriazole	2
Chlorothalonil M4	2
Dikegulac	2
N,*N*-dimethylsulfamide (DMS)	2

Q2: Does your company have technical measures for the removal of organic trace substances in drinking water treatment or are you planning such treatment stages? Regarding your planning for the implementation of new techniques, please think about a period of 5 years. If your answer is "No, and not planned", please tell us the reasons for your statement. *(Verfügt Ihr Unternehmen in der Trinkwasseraufbereitung über technische Maßnahmen für die Entfernung organischer Spurenstoffe oder planen sie solche Aufbereitungsstufen? Hinsichtlich Ihrer Planung zur Implementierung neuer Techniken denken Sie bitte an einen Zeitraum von 5 Jahren. Falls Sie in einem Fall „Nein und nicht geplant" markiert haben sollten: Teilen Sie uns bitte die Gründe für Ihre Aussage mit.))*

The results in Table 10 show that – in terms of PMT/vPvM substances – AC filtration, which can be considered as most likely the least effective advanced treatment method, is the one which is currently the most applied. The fact that four water companies plan to implement RO is remarkable, as its implementation is considered the very last resort in water treatment. The large energy consumption and the disposal of RO-concentrates were given as the main reasons against the implementation of this technique. The formation of potentially harmful by-products was mentioned as the key drivers against the implementation of ozonation. Ozonation was mentioned by the water companies being more appropriate in advanced wastewater treatment. No objection was given regarding the implementation of AC filtration.

Table 10: **Summarized answers (i.e. total numbers) of the responding water suppliers about current and planned implementation of advanced treatment techniques**

Treatment technique	Yes	No, but planned	No, and not planned
Ozonation	3	0	9
Activated carbon filtration	6	3	3
Reverse osmosis (RO)	0	4	8
Misc. _____	-*	-*	-*

*other treatment methods were not mentioned by any of the participating water companies

In advanced water treatment, ozonation is typically followed by AC filtration (degradation of excess ozone and readily biodegradable ozonation products). Therefore, the survey demonstrated that 50% of the participating waterworks do not apply any advanced treatment step (i.e. no ozonation, activated carbon filtration, reverse osmosis). This observation is very well in line with results from a European survey. In 2014, Van Der Hoek (Van Der Hoek et al., 2014) published the results of the EurEau survey focusing on drinking water resources and drinking water treatment technologies applied in Europe. The study reported that 59% of European drinking water is produced without advanced treatment, following the request of the European Water Framework Directive (European Commission, 2000b) of limiting water treatment to natural processes.

The fact that no current standards are exceeded (i.e. limit values, health-related indication values, hygienic standards, etc.) in the produced drinking water was given as a general and comprehensive statement by the participating German water companies for *not* using any advanced treatment method at all (i.e. 50% of the water companies).[3] This simply means that there is no regulatory trigger to implement additional techniques and it highlights the general dilemma: Without exceeding standards, the ongoing or even increasing emissions of a particular compound to the water resources is not perceived as a problem. However, when new limit values for drinking water are introduced, or existing ones are decreased, pressure is put on the water supply sector as they struggle to meet the limit values and not on the polluters. This is especially true in the case of persistent compounds, as the contamination level will not rapidly decrease after phase-out of the substances (Cousins et al., 2020). This underlines the need for a paradigm shift from retrospective measures to proactive regulation taking into account the precautionary principle with regards to the emission of persistent and mobile substances. These policies should be coordinated over entire product life cycles as part of a transition to a circular economy. Prevention and restriction approaches are the only way to stop the accumulation of persistent compounds in the environment sustainably, and are therefore essential to effective protection of drinking water resources.

Q3: Before our investigation (i.e. before 2020), were you aware that the following substances occur in drinking water resources? *(Hatten Sie vor unserer Untersuchung (also vor 2020) Kenntnis darüber, dass nachfolgende Stoffe in Trinkwasserressourcen vorkommen?)*

The survey was sent to the water companies together with the analytical results of their raw water samples. The reason for asking this particular question was to identify potential

[3] Many PMT/vPvM-substances (microcontaminants in general) in drinking water are not regulated.

monitoring/awareness gaps for the most abundant PMT/vPvM substances detected in this project's monitoring. The results are summarized in Table 11. There was one water company who misinterpreted the question, and their answer was excluded from the analysis.

Table 11: **Total numbers (evaluable answers (n = 11) of the responding water suppliers (n = 12)) on the awareness of the occurrence of the most detected compounds/groups (this study) in drinking water resources**

*1 Number of total statements ≠ 11 which means that for these substances, not all water companies answered the question *2 regulated *3 not regulated

Subtance/substance group	Yes	No	*Total statements*[*1]
Trifluoroacetate (TFA) [*2]	11	0	*11*
Trifluoromethane sulfonate (TFMS)[*3]	2	9	*11*
Perfluoropropionate (PFPrA)[*3]	1	10	*11*
Per- and polyfluoroalkyl substances (PFAS) (in general) [*2]	9	2	*11*
1,4-dioxane[*2]	7	3	*10*
1*H*-benzotriazole[*2]	9	2	*11*
2-Acrylamido-2-methylpropane sulfonic acid (AMPS)[*3]	1	9	*10*
Melamine[*2]	7	4	*11*
Cyanuric acid[*3]	1	8	*9*
N,N'-diphenylguanidine (DPG)[*3]	1	8	*9*
Saccharin[*3]	8	2	*10*

The presence of TFA in German water resources is well known to the German water suppliers. This was expected, as in 2016 high concentrations of TFA reported in a German tap water sample resulted in public interest and many monitoring programs (Scheurer et al., 2017). The same is true for 1,4-dioxane (Rüdel et al., 2020). As is detailed in Chapter 6 related to the results from the survey about analytical methods, there is most likely a monitoring gap for 1,4-dioxane (i.e. there is no need to prove that regulatory standards are fulfilled which means there is no demand for analysis and hence a lack of driver for method development). As can be expected, knowledge on the presence of regulated compounds is larger than for non-regulated substances. The presence of AMPS, cyanuric acid, and DPG in water resources is currently not widely unknown.

PFAS in general are an important topic for the water suppliers, especially given the revised European Drinking Water Directive (DWD) (European Commission, 1998) and the recent assessment by the European Food and Safety Authority (EFSA) related to tolerable weekly intake values (Schrenk et al., 2020). However, apart from TFA, the presence of ultrashort-chain perfluoroalkyl acids (PFAA) such as TFMS and PFPrA was mostly unknown. The DWD does not consider perfluorinated chain lengths of less than three C atoms, which can easily explain the observed knowledge/awareness gap.

Q4: Which of the substances listed in question 3 do you consider problematic for your water supply and why? *(Welche der in Frage 3 aufgelisteten Stoffe halten Sie für problematisch für Ihre Wasserversorgung und warum?)*

The answers from the German water companies are summarized in Table 12. Frequent comments were related to toxicological relevance of the PMT/vPvM substances and difficulties related to remediation. Additional general comments were aimed at the lack of data related to the presence of PMT/vPvM substances in drinking water in general and the fact that toxicological data is insufficient.

Table 12: **PMT/vPvM substances considered problematic for the water suppliers and the reasons (summarized results)**

Compound / group	Reasons
TFA	• difficult to eliminate • image problem (regulation of 60 µg/L vs. 10 µg/L vs. precautionary principle; the customer demands for TFA-free drinking water) • mixing of different raw waters necessary not to exceed 10 µg/L in the produced drinking water
TFMS	*not stated*
PFPrA	*not stated*
PFAS in general	• difficult to eliminate • new regulations (DWD, EFSA) may result in very low limit values
1,4-dioxane	• PMT substance • carcinogenic • difficult to eliminate
1*H*-benzotriazole	• persistent • potential groundwater contaminant • potential endocrine disruptive chemical (EDC)
AMPS	*not stated*
Melamine	• multiple sources (e.g. wastewater, well casing material) • potential carcinogen
Cyanuric acid	• depends on upcoming regulation
DPG	*not stated*
Saccharin	*not stated*

8 Monitoring PMT/vPvM substances in the Sources of Germany's Drinking Water

As part of the Exposure level prioritization category, as presented in Table 1 and will be presented in more detail in Chapter 9, actual monitoring data is needed. To obtain additional monitoring data for some of the selected 176 substances considered in this study (see Chapter 3 for details about which of the 176 substances), an extensive sampling campaign was conducted in Germany's drinking water sources.

8.1 Sampling Campaign

To monitor the presence of selected substances in the sources of Germany's drinking water, drinking water suppliers (DWS) with a significant influence of surface water (bank filtrates, reservoirs) were chosen, covering various regions/rivers in Germany.

For the monitoring, two sampling campaigns were designed to each answer specific questions and complement each other. The first sampling campaign included 46 samples covering the rivers Danube, Elbe, Ems, Havel, Main, Neckar, Rhine, Sieg, and the lakes Constance and Tegel and included surface waters, bank filtrate, ground water, and raw waters (surface water/ bank filtrate at the point of entry into the drinking water treatment plant). This initial broad-scope sampling was conducted to generate extensive occurrence and concentration data and gain insight into environmental entrance pathways, which is required to obtain a better understanding for scarcely analysed PMT/vPvM substances. Based on the results of the first monitoring campaign, the second more focussed monitoring campaign, was designed by selecting the samples which contained the most PMT/vPvM substances and / or where high concentrations were observed (30 samples). The second monitoring campaign complemented the first by adding temporal information that allows a differentiation between locally elevated concentrations (e.g. through point sources) or temporally high concentrations (e.g. tied to specific events) and improve data quality for the assessment of environmental behaviour. Drinking water suppliers, their source waters, and their involvement in the second sampling campaign are listed in Table 13.

Table 13: Drinking water suppliers (DWS) ID numbers, the river basin they are located in, and whether they were chosen for the second sampling campaign

Water supplier	Raw water source	Included in the 2nd sampling campaign
DWS 1	Lake Constance	No
DWS 2	Danube	No
DWS 3	Elbe	No
DWS 4	Elbe	No
DWS 5	Ems	Yes
DWS 6	Ems	No
DWS 7	Havel Lake Tegel	Yes
DWS 8	Main	Yes
DWS 9	Neckar	Yes
DWS 10	Neckar	Yes
DWS 11	Rhine	Yes
DWS 12	Rhine	Yes
DWS 13	Sieg	Yes

Detailed information for each DWS including soil composition, travel time from the respective surface water to wells, distance between sampling points, and raw water composition are summarised in Table 14.

Table 14: Sampling points chosen for the first sampling campaign and their characteristics

Water supplier	Sampling point	Bank soil composition	Travel time from surface water to wells	Distance between sampling points	Raw water composition
DWS 5	SW2	The measuring points are located in the area of the Ur-Ems-Gully or in the area of the low terrace sands (gravel, sand) of the Ur-Ems-Gully	-	210 m south of SW1	100% Surface water
DWS 5	SW1		-	210 m north of SW2 and 160 m south of SW3	100% Surface water
DWS 5	BF1		-	95 m south of SW1and 110 m north of SW2	Up to 80% bank filtrate from the Ems (depending on the damming situation)
DWS 5	SW3		-	160 m north of SW1	100% Surface water
DWS 3	SW4	Sand	-	-	100% surface water
DWS 3	RW1	Sand	-	-	-
DWS 11	BF2	Fine/medium sand	On average 35 days at 15 million m^3/a (27 to >50 days)	~60 m distance between the wells ~35-40 m distance between well and Rhine	~88% bank filtrate, rest surface water the amount of bank filtrate will be smaller in the centre of the gallery
DWS 11	BF3	Fine/medium sand	On average 35 days at 15 million m^3/a (27 to >50 days)	~60 m distance between the wells ~35-40 m distance between well and Rhine	~88% bank filtrate, rest surface water the amount of bank filtrate will be smaller in the centre of the gallery
DWS 11	SW5	Fine/medium sand	On average 35 days at 15 million m^3/a (27 to >50 days)	~35-40 m distance between wells and Rhine	100% surface water
DWS 11	BF4	Fine/medium sand	On average 35 days at 15 million m^3/a (27 to >50 days)	~60 m distance between the wells	~88% bank filtrate, rest surface water

Water supplier	Sampling point	Bank soil composition	Travel time from surface water to wells	Distance between sampling points	Raw water composition
				~35-40 m distance between well and Rhine	the amount of bank filtrate will be smaller in the centre of the gallery
DWS 6	SW6				
DWS 6	RW3	Ground passage gravel, sand	~ 50 days		
DWS 6	RW2				60-70 % infiltration water
DWS 6	RW4				80-90 % infiltration water
DWS 6	SW7				
DWS 6	RW5	Ground passage gravel, sand	~50 days		
DWS 13	BF5				
DWS 13	GW1	Gravel	The travel time depends on delivery rates, water level and ground water level. At high flow rates (3600 m^3/h) it is ~50 days. With lower delivery rates, 50 days are clearly exceeded	~625 m	~30% new ground water formation through precipitation ~ 70% ground water recharge via infiltration from surface waters (The term bank filtrate is inappropriate here)
DWS 8	BF6	-	-	-	
DWS 8	BF7	Mainly gravely sand	~100 days between Rhine bank and well at a medium water level	~520 m	15 – 20 % ground water 10 – 20 % seeped Rhine water 60 – 70 % bank filtrate
DWS 8	SW8	-	-	-	100% surface water

Water supplier	Sampling point	Bank soil composition	Travel time from surface water to wells	Distance between sampling points	Raw water composition
DWS 12	BF8	Topsoil, loam, sand, gravel, shell limestone, calcareous marl, again shell limestone	approx. 27 h		ca. 95-98% BF
DWS 12	BF9	Topsoil, silt, sand, gravel, limestone, clay	approx. 45 h		ca. 95-98% BF
DWS 12	BF10	Topsoil, loam, sand, gravel, clay, limestone	approx. 48 h		ca. 95-98% BF
DWS 12	BF11	Topsoil, gravel, sand	-		ca. 95-98% BF
DWS 12	BF12	Topsoil, loam, sand, gravel, limestone, clay, calcareous marl, clay again, limestone, clay again	approx. 30 h		ca. 95-98% BF
DWS 12	SW9	-	-	-	100 % raw water
DWS 2	SW10	-	-	-	-
DWS 2	RW7	-	-	-	-
DWS 2	RW6	-	-	-	-
DWS 7	BF13	sand	In the range> 10,000 h	500 m	BF: 50% GW: 50%
DWS 7	SW11	-	-	-	-
DWS 7	SW12	-	-	-	-
DWS 7	BF14	sand	Approx. 1800 hours	120 m	BF: 80% GW: 20%

Water supplier	Sampling point	Bank soil composition	Travel time from surface water to wells	Distance between sampling points	Raw water composition
DWS 9	GW4	Sandy to gravelly, partly clayey and silty inclusions, heterogeneous distribution	The mean residence time of the ground water is 12 to 18 years		Ground water with 20 – 30% bank filtrate (Neckar) (according to flow model lowest Neckar influence of the 3 wells)
DWS 9	GW3				Ground water with 20 – 30% bank filtrate (Neckar)
DWS 9	GW2				Ground water with 20 – 30% bank filtrate (Neckar) (according to flow model largest Neckar influence of the 3 wells)
DWS 9	SW13				100% surface water
DWS 10	BF16	Fluviatile deposits, sandy-gravelly	4 – 5 a (i.e., around 35-44.000 h)	The sampling point SW14 is located about 10 km upstream from the relevant infiltration area of the Neckar river into the aquifer	75 ± 5% bank filtrate, 20 ± 5 infiltrated ground water
DWS 10	BF15	Colmatized streambed, partly cohesive sands and gravels of the gravel terrace, fissured porous zechstone	~48 – 600 h depending on ground water/well and Neckar level (The well is rendered inoperative when high water arrives)	The sampling point SW14 is located about 260 m upstream from BF15	Relatively young land-based upland water, old deep water (>40 a) and bank filtrate (30 – 80% depending on the varying hydrogeological situation)
DWS 10	SW14				100% surface water
DWS 1	SW15				100% surface water
DWS 4	GW5				100% ground water

Water supplier	Sampling point	Bank soil composition	Travel time from surface water to wells	Distance between sampling points	Raw water composition
DWS 4	GW6	Glacial sands and gravels			<10% surface water
DWS 4	GW7				100% ground water
DWS 4	SW16				100% surface water

DWS = drinking water supplier, SW = surface water, GW = groundwater, RW = raw water, BF = bank filtrate.

Additional information for each sampling point with respect to the specific sampling dates are presented in Table 15.

Table 15: Metadata collected for each sampling point on the specific sampling date

Water supplier	Sampling point	Sampling date	EC [µS/cm]	T [°C]	Discharge [m³/h]	Water level [cm]	Precipitation [mm] (Σ 7 days before sampling)*[2]
DWS5	SW2	27.10.2020	561	9.8		225	17.6
DWS5	SW1	27.10.2020	730	11.8		330	17.6
DWS5	BF1	27.10.2020	808	15.2		370	17.6
DWS5	SW3	27.10.2020	766	10.0		325	17.6
DWS5	BF1	19.07.2021	686	13.0			25.8
DWS5	SW1	19.07.2021	672	19.8			25.8
DWS5	SW2	19.07.2021	546	18.0			25.8
DWS5	SW3	19.07.2021	718	17.0		85*[1]	25.8
DWS3	SW4	28.10.2020	738	11.2	<1		12.6
DWS3	RW1	28.10.2020	580	10.5			12.6
DWS11	BF2	29.10.2020	465	17.5	175		12.0
DWS11	BF3	29.10.2020	540	16.1	217		12.0
DWS11	SW5	29.10.2020	381	13.6	1489	227	12.0
DWS11	BF4	29.10.2020	501	14.6	205		12.0
DWS11	BF4	27.07.2021	537	15.3			22.1
DWS11	BF3	27.07.2021	530	14.1			22.1
DWS11	BF2	27.07.2021	472	14.4			22.1
DWS11	SW5	27.07.2021	328	21.3	2722	431	22.1
DWS6	SW6	29.10.2020	480	11.3			22.2
DWS6	RW3	29.10.2020	480	11.3			22.2
DWS6	RW2	29.10.2020	656	14.2			22.2
DWS6	RW4	29.10.2020	568	16.0			22.2
DWS6	SW7	29.10.2020	569	11.5			22.2
DWS6	RW5	29.10.2020	570	12.0			22.2
DWS13	BF5	04.11.2020	396	11.4			20.4
DWS13	GW1	04.11.2020	268	11.4		50*[1]	20.4

Water supplier	Sampling point	Sampling date	EC [µS/cm]	T [°C]	Discharge [m³/h]	Water level [cm]	Precipitation [mm] (Σ 7 days before sampling)*2
DWS13	GW1	26.07.2021	284	18.3			9.6
DWS13	BF5	26.07.2021	38500	12.1		210*1	9.6
DWS8	BF6	04.11.2020	712	14.0			25.1
DWS8	BF7	04.11.2020	737	13.9			25.1
DWS8	SW8	04.11.2020	574	14.4		116*1	25.1
DWS8	BF6	21.07.2021	769	12.4			0.6
DWS8	BF7	21.07.2021	737	11.9			0.6
DWS8	SW8	21.07.2021	424	18.9		167*1	0.6
DWS12	BF8	04.11.2020					18.3
DWS12	BF9	04.11.2020					18.3
DWS12	BF10	04.11.2020					18.3
DWS12	BF11	04.11.2020					18.3
DWS12	BF12	04.11.2020					18.3
DWS12	SW9	04.11.2020			1410	279	18.3
DWS12	SW9	27.07.2021			2890	445	22.1
DWS12	BF11	27.07.2021					22.1
DWS12	BF8	27.07.2021					22.1
DWS12	BF12	27.07.2021					22.1
DWS12	BF10	27.07.2021					22.1
DWS12	BF9	27.07.2021					22.1
DWS2	SW10	02.11.2020	489	12.8	91	175*1	20.8
DWS2	RW7	02.11.2020	517	10.1			20.8
DWS2	Rw6	02.11.2020	520	9.9			20.8
DWS7	BF13	10.11.2020	766	12.2			0.0
DWS7	SW11	10.11.2020	1239	13.6		60	0.0
DWS7	SW12	10.11.2020	728	10.4			0.0
DWS7	BF14	10.11.2020	789	10.3			0.0
DWS7	BF13	23.07.2021	841	11.9			3.3
DWS7	SW11	23.07.2021	1409	19.6		50*1	3.3
DWS7	BF14	23.07.2021	689	10.4			3.3

Water supplier	Sampling point	Sampling date	EC [µS/cm]	T [°C]	Discharge [m³/h]	Water level [cm]	Precipitation [mm] (Σ 7 days before sampling)*2
DWS7	SW12	23.07.2021	590	22.3			3.3
DWS9	GW4	11.11.2020	924	11.6			0.0
DWS9	GW3	11.11.2020	858	11.7			0.0
DWS9	GW2	11.11.2020	895	12.7			0.0
DWS9	SW13	11.11.2020	888	10.6		228*1	0.0
DWS9	GW4	15.07.2021	914	11.5			91.2
DWS9	GW3	15.07.2021	854	11.7			91.2
DWS9	GW2	15.07.2021	913	12.7			91.2
DWS9	SW13	15.07.2021	518	17.6		700*1	91.2
DWS10	BF16	09.11.2020		13.7			0.0
DWS10	BF15	09.11.2020		13.7			0.0
DWS10	SW14	09.11.2020				209*1	0.0
DWS10	SW14	26.07.2021		14.7			2.1
DWS10	BF15	26.07.2021		13.7			2.1
DWS10	BF16	26.07.2021		13.2		220*1	2.1
DWS1	SW15	30.11.2020	339	6.0			0.0
DWS4	GW5	30.11.2020	492	10.1			0.0
DWS4	GW6	30.11.2020	743	7.3			0.0
DWS4	GW7	30.11.2020	419	10.1			0.0
DWS4	SW16	30.11.2020	774	5.9	1,05	58	0.0

*1 Water level were taken from www.pegelonline.wsv.de when not provided by water suppliers

*2 Precipitation data were taken from https://www.wetteronline.de/wetterdaten/

8.2 Results and discussion of the monitoring campaign

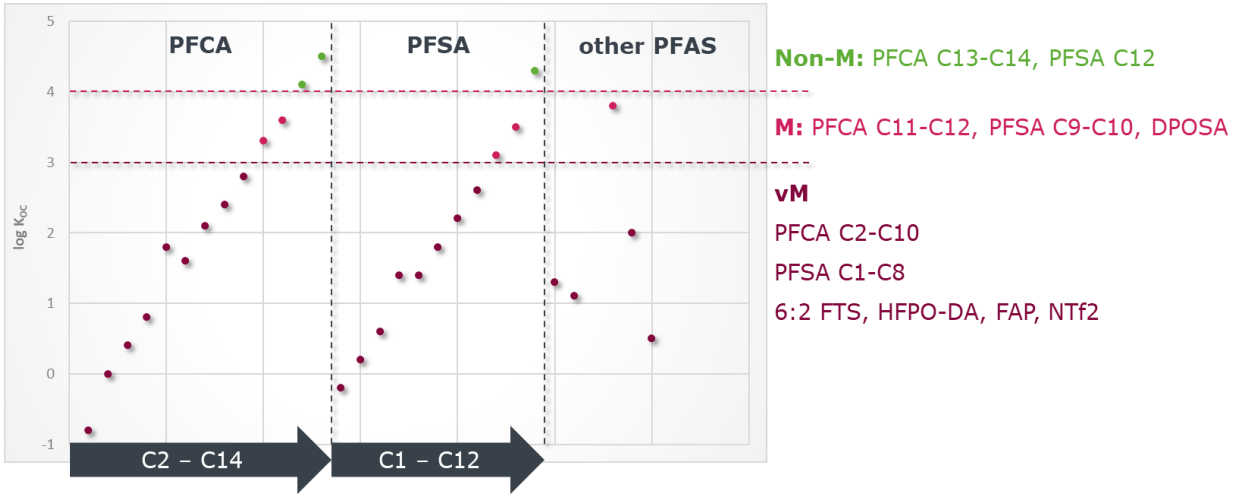
In the following sections the results of the monitoring campaigns are discussed. To facilitate a detailed discussion, the results are split into two groups. The first is the PFAS group (defined by a containing a CF_3-R or R-CF_2-R group, where R is not hydrogen), a well-studied class of persistent environmental pollutants which are not necessarily mobile, and the second is the non-fluorinated PMT/vPvM substances. Raw data for the PFAS group can be found freely online at (Neuwald et al., 2022a) and the raw data for the non-fluorinated PMT/vPvM group can be found at (Neuwald et al., 2022b).

8.2.1. PFAS

Over both sampling campaigns, 30 of the 43 analysed PFAS were detected at least once above their respective LOQ. While only three long-chain PFCA and PFSA were classified as non-mobile (non-M) (log K_{OC} >4), five are mobile (M) (log K_{OC} ≤ 4), and all the others are very mobile (vM) (log K_{OC} ≤ 3) when the definition of M/vM as proposed by the UBA in 2019 is used (Neumann and Schliebner, 2019). This classification demonstrates that most detected PFAS are PMT/vPvM substances, since PFAS are in general considered Persistent and Toxic (Buck et al., 2011) (Figure 9). The term "other PFAS" is then used to describe all PFAS that do not belong to the PFCA or PFSA groups.

Figure 9: Mobility classification of all detected PFAS

Scatterplot of log K_{OC} values of detected PFAS. PFAS are separated into PFCA, PFSA, and other PFAS. Point colours signify the classification as non-M (log K_{OC} >4), M (log K_{OC} ≤ 4), and vM (log K_{OC} ≤ 3). DPOSA: N-(3-(Dimethylamino)propyl)-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulfonamide N-oxide, FAP: Tris(pentafluoroethyl)trifluorophosphate, NTf2: Bis(trifluoromethylsulfonyl)imide



Source: own illustration HSF

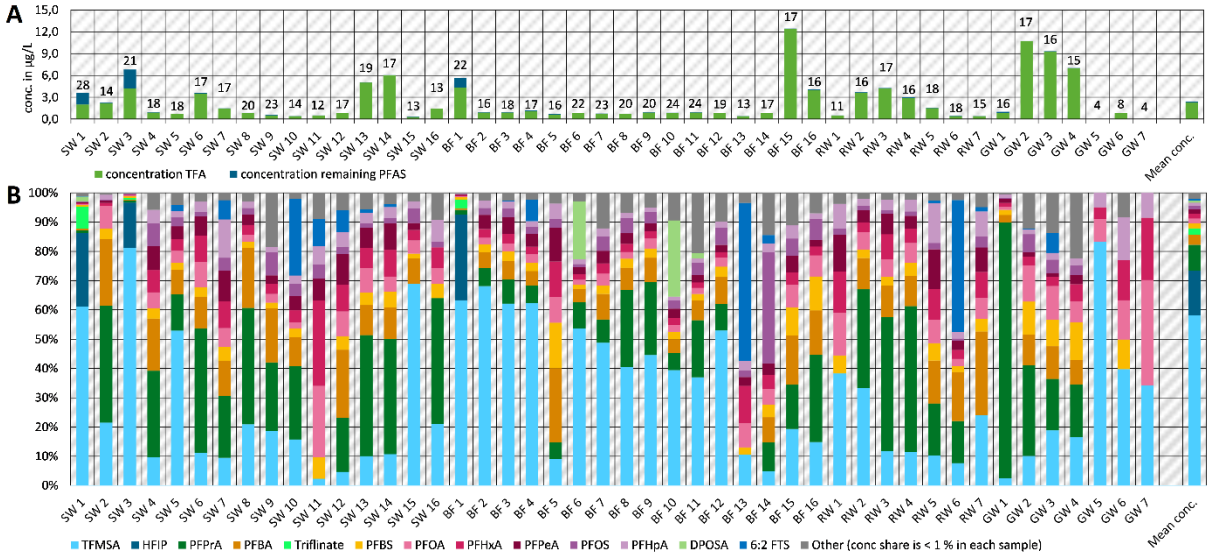
8.2.1.1. First sampling campaign: Environmental occurrence and distribution

Within the first sampling campaign, the number of positive detects per sample ranged from 4 to 28 with a median of 17 (Figure 10). The well-studied PFCA and PFSA with a chain length greater than four were predominantly detected at concentrations below 0.01 µg/L (Figure 11). TFA (median conc. 0.9 µg/L; maximum conc. 12.4 µg/L) accounted for more than 90% of the total PFAS concentration over all samples. This wide-spread occurrence was expected due to TFA's numerous applications and thus multiple entrance pathways into the environment and water cycle (Scheurer et al., 2017). When excluding the highly dominant TFA, the ultra-short-chain PFAS TFMSA (median conc. 8.0 ng/L; maximum conc. 2.1 µg/L; see Figure 11) and PFPrA (median conc. 12.6 ng/L; maximum conc. 0.18 µg/L) accounted for 59% and 9%, respectively, of all non-TFA PFAS. Among other PFAS, the occurrence and distribution of HFIP, NTf_2 and FAP were notable. HFIP, a fluorinated solvent used in polymer chemistry and organic synthesis, was to the best of our knowledge detected for the first time in the aquatic environment during this monitoring campaign. While only detected in three samples, it was present at high concentrations (median and maximum conc. 0.4 µg/L). NTf_2 (median conc. 0.8 ng/L; maximum conc. 2.0 ng/L) and FAP (median conc. 0.5 ng/L; maximum conc. 0.7 ng/L) are fluorinated anions used in ionic liquids, which have only recently been detected in the aquatic environment as a novel group of PFAS (Neuwald et al., 2021, 2020; Zahn et al., 2020). The three ultra-short-

chain PFAS: TFA, PFPrA, and TFMSA account for 98% of the total PFAS concentration in all samples, clearly demonstrating their dominance in the sources of German drinking water.

Figure 10: Total concentrations of PFAS and their distribution in the samples

A) Bar plot of total concentration of all analysed PFAS (blue) and concentration of TFA (green). The number above the bars depict the total amount of detected PFAS per sample. B) Stacked bar plot of relative abundance of all PFAS except for TFA. Blue and green colours represent PFCA and PFSA <C4 and other PFAS while yellow, orange and pink colours represent legacy PFAS. Detects <LOQ were included with half the LOQ value for each substance. TFMSA: Trifluoromethanesulfonic acid, HFIP: Hexafluoroisopropanol, DPOSA: N-(3-(Dimethylamino)propyl)-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulfonamide N-oxide



Source: Neuwald et al., 2022

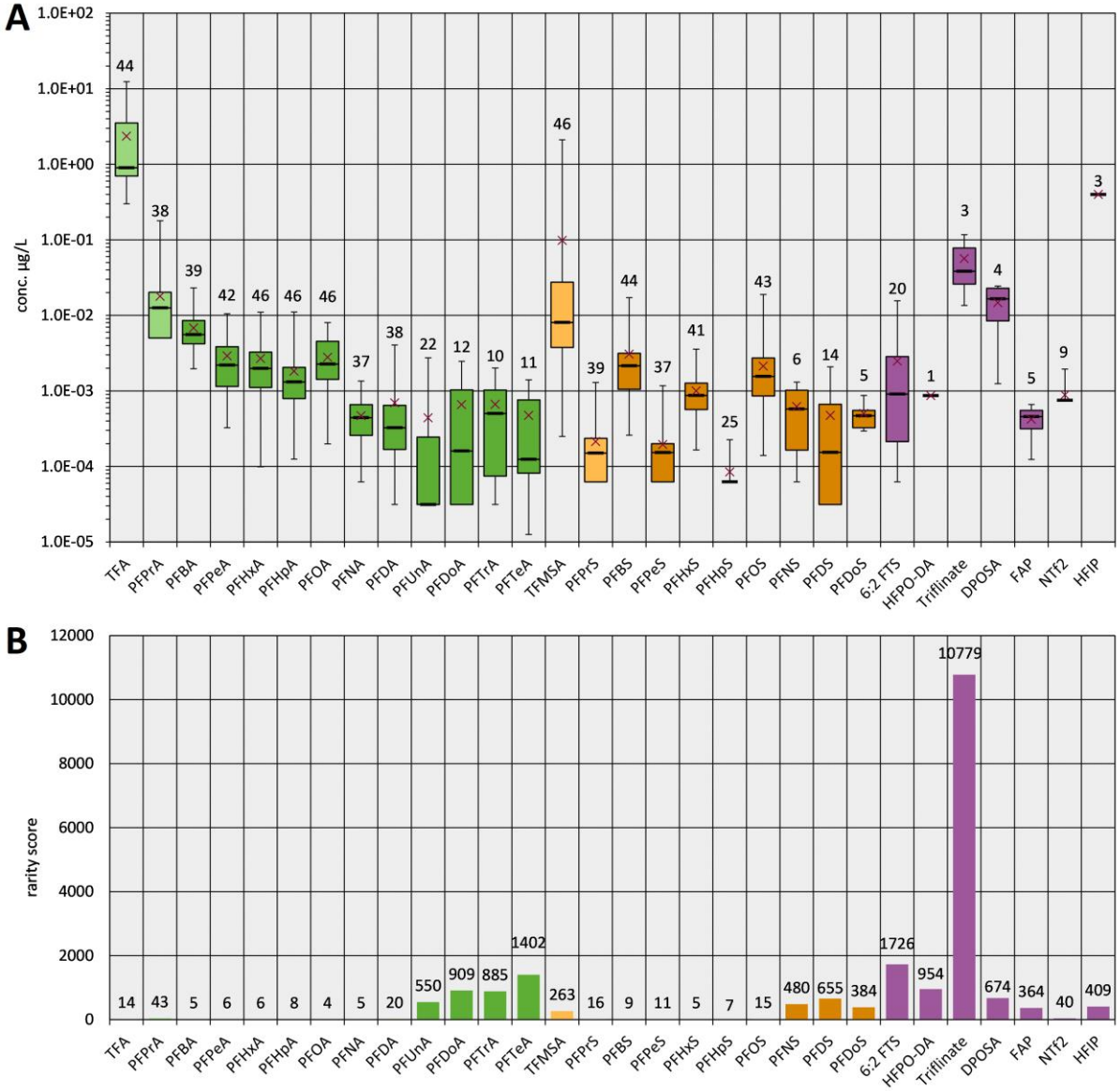
To obtain a better understanding of the environmental distribution of the investigated PFAS, a rarity score (Krauss et al., 2019) was calculated according to equation 1:

$$RS = \frac{maximum\ concentration}{median\ concentration} \cdot \frac{number\ of\ samples}{number\ of\ detects} \qquad \text{equation 1}$$

The rarity score (Figure 11) is an indicator of site-specific contaminations. A high rarity score implies that a substance is not homogeneously distributed within the sample set. For PFCA and PFSA there is an obvious increase in rarity scores between PFDA and PFUnDA and PFOS and PFNS, respectively. Interestingly, this increase coincides exactly with the shift in classification from vM to M. All PFSA and PFCA that are classified as vM have substantially lower rarity scores as the ones that are classified as M, which points towards differences in their environmental behaviour. The one exception here is TFMSA, which is widely present in mostly similar concentrations, but few hot spots with vastly elevated concentration raise the rarity score up to almost 300. This indicates the presence of yet unknown point sources near these sampling locations. Except for 6:2 FTS all other PFAS where infrequently detected, resulting in higher rarity scores.

Figure 11: Concentration range of PFAS and rarity score

A) Boxplots of PFAS concentrations over all samples. The number above the bars depict the number of detects. <LOQ was included as half its value for each substance. B) Rarity score of all detected PFAS. <LOQ and <LOD were included as half their value for each substance. PFCA are shown in green, PFSA in orange, and other PFAS in purple. TFMSA: Trifluoromethanesulfonic acid, Triflinate: Trifluoromethanesulfinic acid, DPOSA: N-(3-(Dimethylamino)propyl)-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulfonamide N-oxide, FAP: Tris(pentafluoroethyl)trifluorophosphate, NTf2: Bis(trifluoromethylsulfonyl)imide, HFIP: Hexafluoroisopropanol



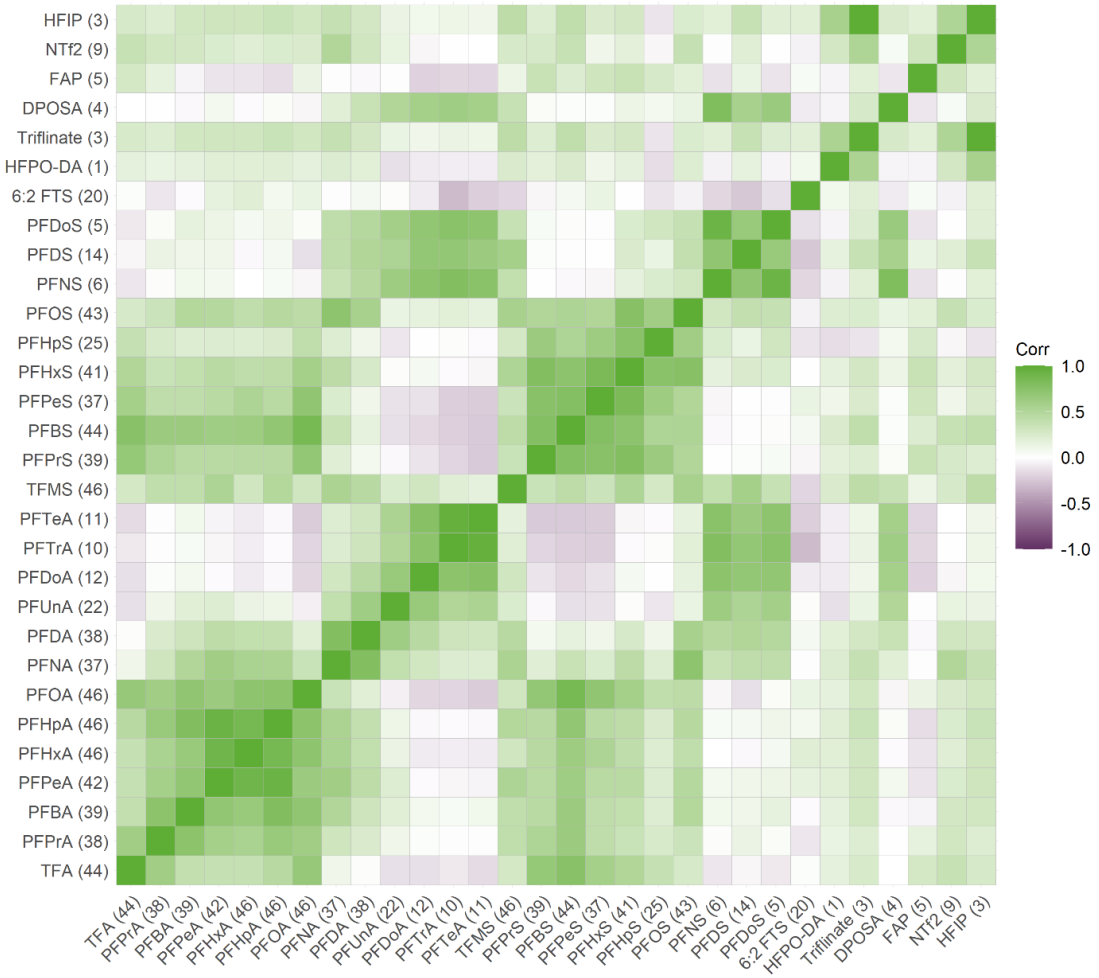
Source: Neuwald et al., 2022

To investigate the distribution of PFAS further and reveal co-occurrences, their correlation amongst each other was plotted (Figure 12). Positive correlations were observed for the PFCA ≤ C8 and the PFSA ≤ 7. Due to the homogenous distribution of these PFAS throughout the sample set this correlation was expected. The longer chain PFCA (≥ C9) and PFSA (≥ C8) homologues also correlate with each other. Given that these substances were classified as site-specific by

their rarity score this is a clear indicator of common sources. For most of the other PFAS, detection frequencies were too low for a meaningful correlation analysis.

Figure 12: Correlation plot of all detected PFAS

Spearman correlation plot of PFAS sorted by type and chain length. Numbers in brackets depict the number of samples where the substances was detected. <LOQ was included as half its value for each substance. TFMSA: Trifluoromethanesulfonic acid, Triflinate: Trifluoromethane-sulfinic acid, DPOSA: N-(3-(Dimethylamino)propyl)-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulfonamide N-oxide, FAP: Tris(pentafluoroethyl)trifluorophosphate, NTf2: Bis(trifluoromethylsulfonyl)imide, HFIP: Hexafluoroisopropanol



Source: Neuwald et al., 2022

8.2.1.2. First sampling campaign: The analytical gap for ultra-short-chain PFAS

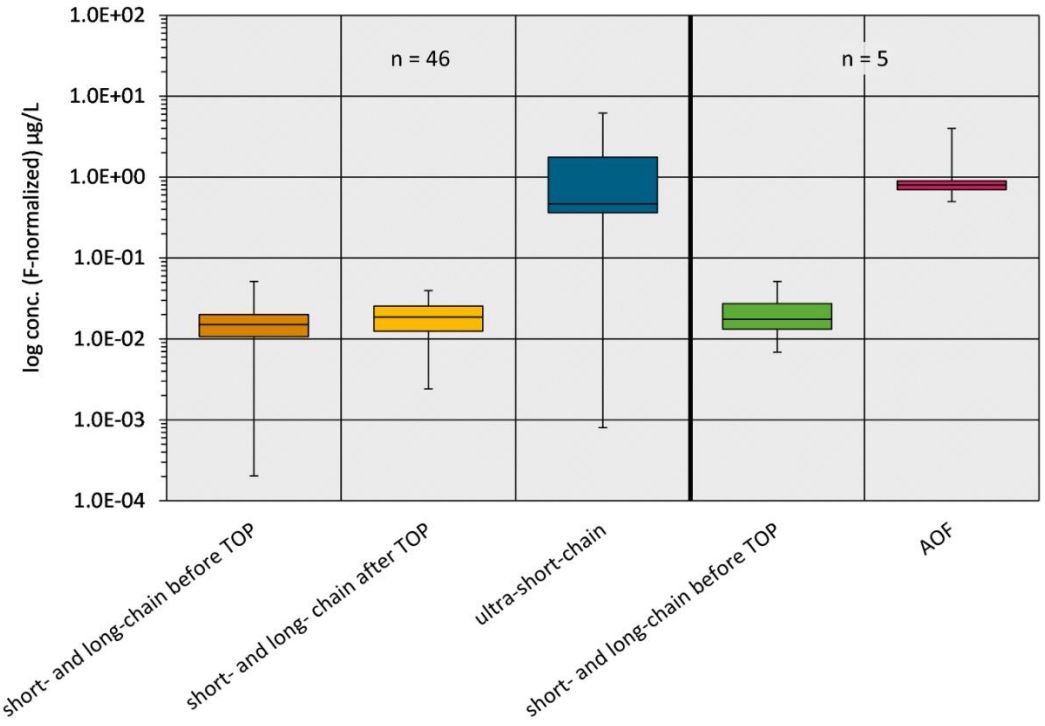
To support regulatory work that considers PFAS as a group, analytical methods are needed that are able to measure total PFAS parameters. The adsorbable organic fluorine (AOF) method which covers all F-containing chemicals that are adsorbed to AC and the total oxidizable precursor (TOP) Assay, which includes precursors that can be transformed into PFCA, are the

two most widely used methods to represent such a total PFAS parameter. Neither of these methods represent a true total PFAS approach and thus their limitations have to be considered. One key limitation for both methods is their omission of ultra-short-chain PFAS. For the AOF, chemicals that cannot be adsorbed to the AC are omitted; while, for the TOP Assay it becomes increasingly difficult to analyse shorter-chain homologues in the high ionic strength reaction mixture. To assess the relevance of these gaps, target analysis, AOF, and TOP Assay results are compared in Figure 13. When comparing the F-normalized results for short- and long-chain PFAS before and after TOP Assay (median 0.015 µg/L and 0.019 µg/L, respectively) it becomes clear that concentration changes are minimal, underpinning the reduced relevance of oxidizable precursors at remote locations where oxidation may have already occurred. The AOF, which was only analysed in five samples shows more pronounced differences to the results of the target analysis in the respective samples (median F-normalized sum of short- and long-chain PFAS from target analysis: 0.015 µg/L; median AOF: 0.8 µg/L), showing that even in these remote locations there is still a substantial PFAS "dark matter" that is neither PFCA, PFSA, or a precursor thereof.

The F-normalized sum of the four ultra-short-chain PFAS TFA, TFMSA, PFPrA, and PFPrS (median 0.4 µg/L) exceeds is in the same order of magnitude than the AOF, showing that a polarity extension of the AOF towards more mobile PFAS would lead to a substantial increase (ca. 50%) from these four target analytes alone. Further increases due to yet unknown very mobile PFAS are at best speculative. When using the AOF and TOP assay, it must be kept in mind that these methods may miss the PFAS most prevalent in the sources of drinking water and most difficult to remove during its preparation.

Figure 13: F normalized sum of all PFAS

Stacked bar plot showing PFCA ≥ C4 and < C4 from target analysis (F normalized) and TOP assay (for PFCA ≥ C4) for all samples. AOF results are shown for five prioritized samples.



Source: Neuwald et al., 2022

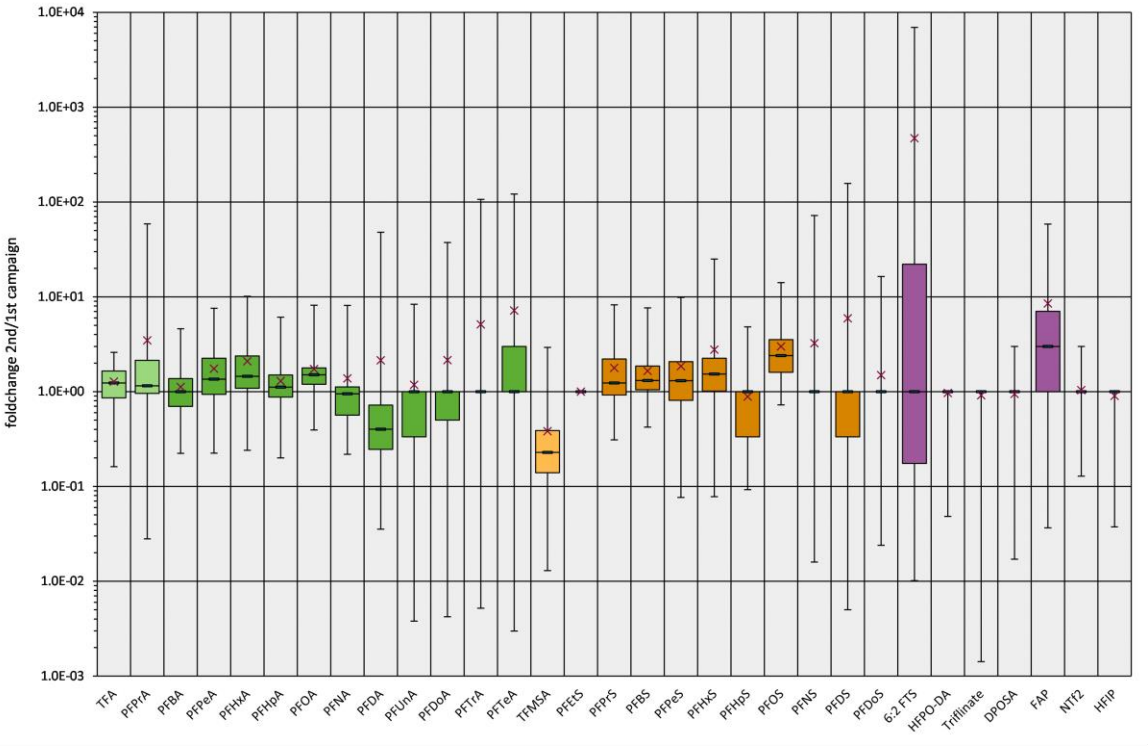
8.2.1.3. Second sampling campaign: Assessment of temporal trends

The second sampling campaign was conducted to reveal temporal trends for the substances in the sample set to provide integral information for the assessment of sources and the environmental behaviour of the substances. To facilitate such a comparison, fold changes between both sampling campaigns were calculated by dividing the concentration of each analyte in each sample during the second sampling campaign by the respective concentration during the first sampling campaign. Resulting fold changes below 1 indicate higher concentrations in the first sampling campaign and values above one indicates higher concentration in the second sampling campaign. The fold changes for all samples per analyte are plotted as box plots in Figure 14. The majority of the analytes have a median fold change near one with a narrow interquartile range, which indicates only small changes between both sampling campaigns, thus the conclusions drawn from the first campaign can be easily transferred to the second campaign for these substances.

A clear exception to this trend is 6:2 FTS which shows a much wider spread of fold change values and the highest mean fold change, indicating a pronounced concentration increase in some of the investigated samples. A more detailed investigation of the behaviour of 6:2 FTS revealed that strong concentration increases are solely limited to bank filtrate and groundwater samples. 6:2 FTS has been shown to reach ground water through contaminated soil (Dauchy et al., 2019), and thus the heavy rain events in Germany in the Summer of 2021 may be the reason for this pronounced increase in this subset of the samples.

Figure 14: Fold changes of PFAS concentrations between both sampling campaigns

Boxplots of the fold changes in concentrations between the first and second sampling campaign (second campaign/first campaign). PFCA are shown in green, PFSA in orange, and other PFAS in purple. TFMSA: Trifluoromethanesulfonic acid, Triflinate: Trifluoromethanesulfinic acid, DPOSA: N-(3-(Dimethylamino)propyl)-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulfonamide N-oxide, FAP: Tris(pentafluoroethyl)trifluorophosphate, NTf2: Bis(trifluoromethylsulfonyl)imide, HFIP: Hexafluoroisopropanol



Source: Neuwald et al., 2022

8.2.2. Non-fluorinated PMT/vPvM substances

There were 26 of the 34 non-fluorinated PMT/vPvM substances that were detected at least once above their respective LOQ over both of the sampling campaigns. For simplicity and for the remainder of this chapter, these substances are referred to as PMT/vPvM substances.

8.2.2.1. First sampling campaign: environmental occurrence and distribution

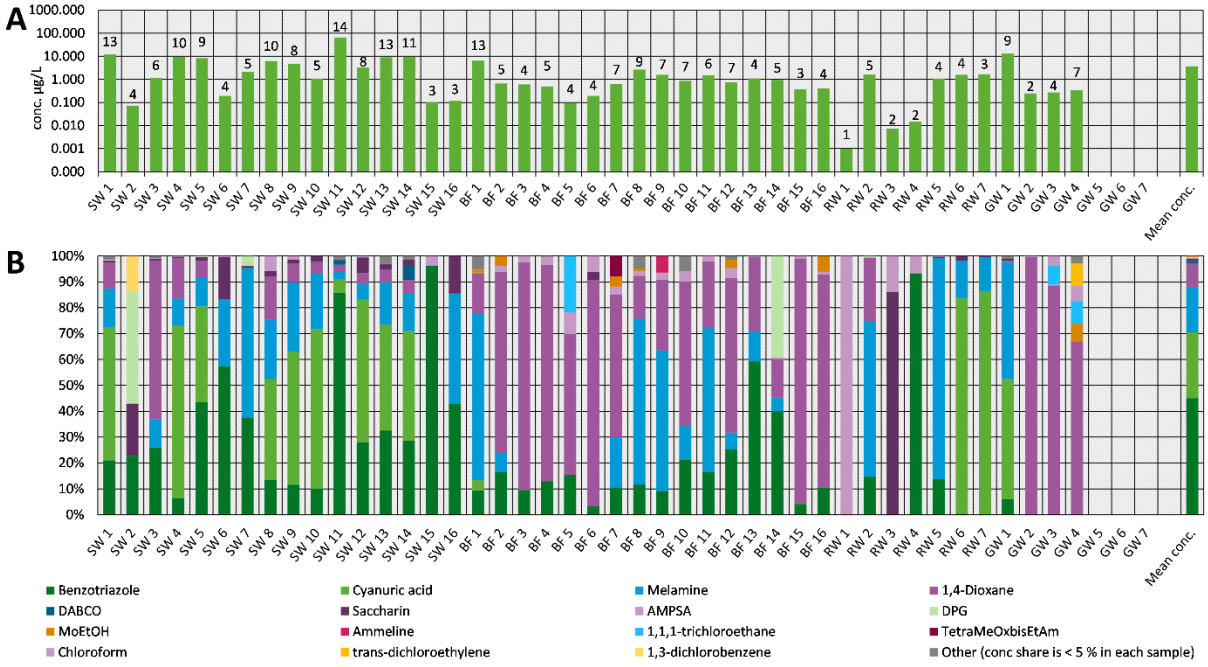
During the first sampling campaign, the total concentration of PMT/vPvM substances in the samples varied greatly between <LOQ and 56.1 µg/L (see Figure 15) with a median of 0.9 µg/L. To take in to consideration the large number of non-detects, mean and median values were calculated using the Kaplan-Meier approach, where appropriate (Helsel, 2010). The median number of detected PMT/vPvM substances per samples was 5. Four analytes dominated in most samples, being responsible for more than 95% of the total PMT/vPvM substance concentration:

- Benzotriazole, a well-known PMT/vPvM substance with a production volume of 1000-10000 tpa. Benzotriazole is mostly used as a corrosion inhibitor in a multitude of consumer products such as dishwasher detergents (Vetter and Lorenz, 2013). In this study benzotriazole was detected in 80% of all samples with a median of 0.11 µg/L and a maximum concentration of 56.1 µg/L was detected (Figure 16), which highlights the potential of elevated local concentrations of PMT/vPvM substances and indicates the presence of a point source.
- Melamine and cyanuric acid, two triazine derivatives, were detected in 63% and 30% of all samples, respectively, with median concentrations of 0.12 µg/L and 0.17 µg/L. Both are high production volume substances (melamine 100000-1000000 t/a; cyanuric acid 10000-100000 t/a) with diverse consumer and product use (Schulze et al., 2019; Zhu and Kannan, 2020). Melamine was one of the 16 PMT/vPvM substances added to the SIN List in 2019.
- 1,4-dioxane, a cyclic diether, was detected in 70% of all samples with a median concentration of 0.29 µg/L. 1,4 dioxane is an industrial chemical (Tanabe et al., 2006) and was found to cause problems in US drinking water production (Broughton et al., 2019). In 2021, 1,4 dioxane was identified as a substance of very high concern under REACH based on the equivalent level of concern it displays when compared to PBT/vPvB substances.

Besides these four rather well-studied chemicals, two scarcely studied PMT/vPvM substances were of significant interest here: AMPSA (80% of samples, median conc. 3.6 ng/L) and DPG (17% of samples, median conc. 0.2 ng/L). The widely detected hydrogel monomer AMPSA was first reported by Schulze et al (2019) in similar concentration ranges as in this study. Despite its low concentrations, AMPSA was one of the most frequently detected PMT/vPvM substances herein. The vulcanization accelerator DPG has been shown to leach from tires (Müller et al., 2022). While monitoring studies are so far scarce, DPG has been found to be widely present in surface waters but varies significantly in its concentration (Schulze et al., 2019; Zahn et al., 2019).

Figure 15: Total concentrations of PMT/vPvM substances and their distribution in the samples

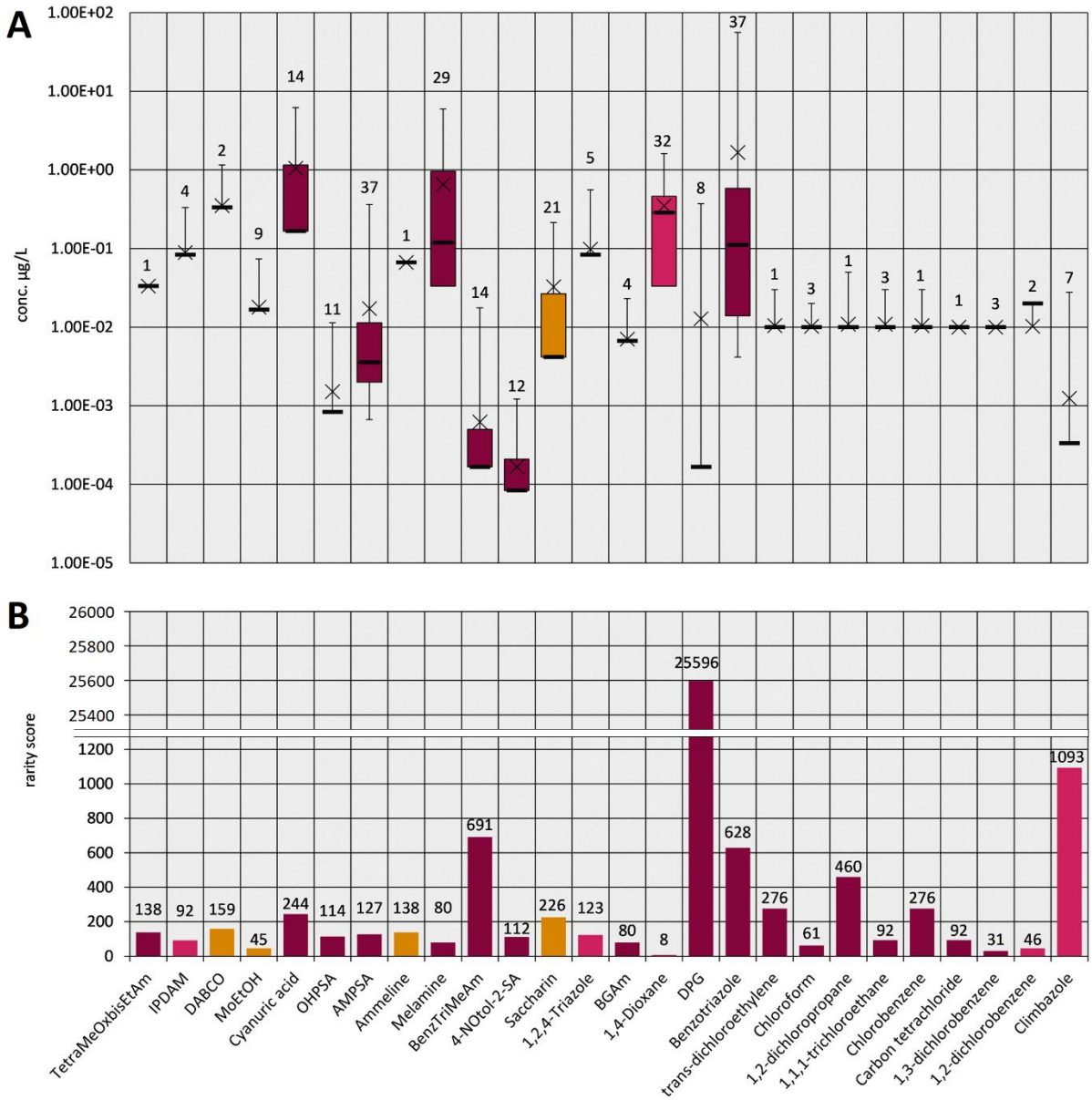
A) Bar plot of total concentration of all analysed PMT/vPvM substances. The number above the bars depict the total amount of detected PMT/vPvM substances per sample. B) Stacked bar plot for relative abundance of all analysed PMT/vPvM substances in all samples. <LOQ was included as half its value for each substance. DABCO: 1,4-Diazabicyclo[2.2.2]octane, AMPSA:2- Acrylamido-2-methyl-1-propanesulfonic acid, DPG: 1,3-Diphenylguanidine, MoEtOH: 2-Morpholinoethanol, TetraMeOxbisEtAm: N,N,N',N'-Tetramethyl-2,2'-oxybis(ethylamine)



Source: Neuwald et al., 2022b

Figure 16: Concentration range of PMT/vPvM substances and rarity score

A) *Boxplots of PMT/vPvM substance concentrations over all samples. Mean, median, minimum, maximum and interquartile ranges were calculated using the Kaplan-Meier approach to consider the large amount of non-detects. The number above the bars depict the number of detects. B) Rarity score of all detected PMT/vPvM substances. Colours reflect the classification of chemicals as PMT/vPvM (dark red), PMT (pink), and potential PM (orange). TetraMeOxbisEtAm: N,N,N',N'-Tetramethyl-2,2'-oxybis(ethylamine), IPDAM: Isoprohonediamine, DABCO: 1,4-Diazabicyclo[2.2.2]octane, MoEtOH: 2-Morpholinoethanol, OHPSA: 3-(allyloxy)-2-hydroxypropanesulfonic acid, AMPSA:2- Acrylamido-2-methyl-1-propanesulfonic acid, BenzTriMeAm: Benzyltrimethylammonium, 4-NOtol-2-SA: 4-Nitrotoluenesulfonic acid, BGAm: Benzoguanamine, DPG: 1,3-Diphenylguanidine*



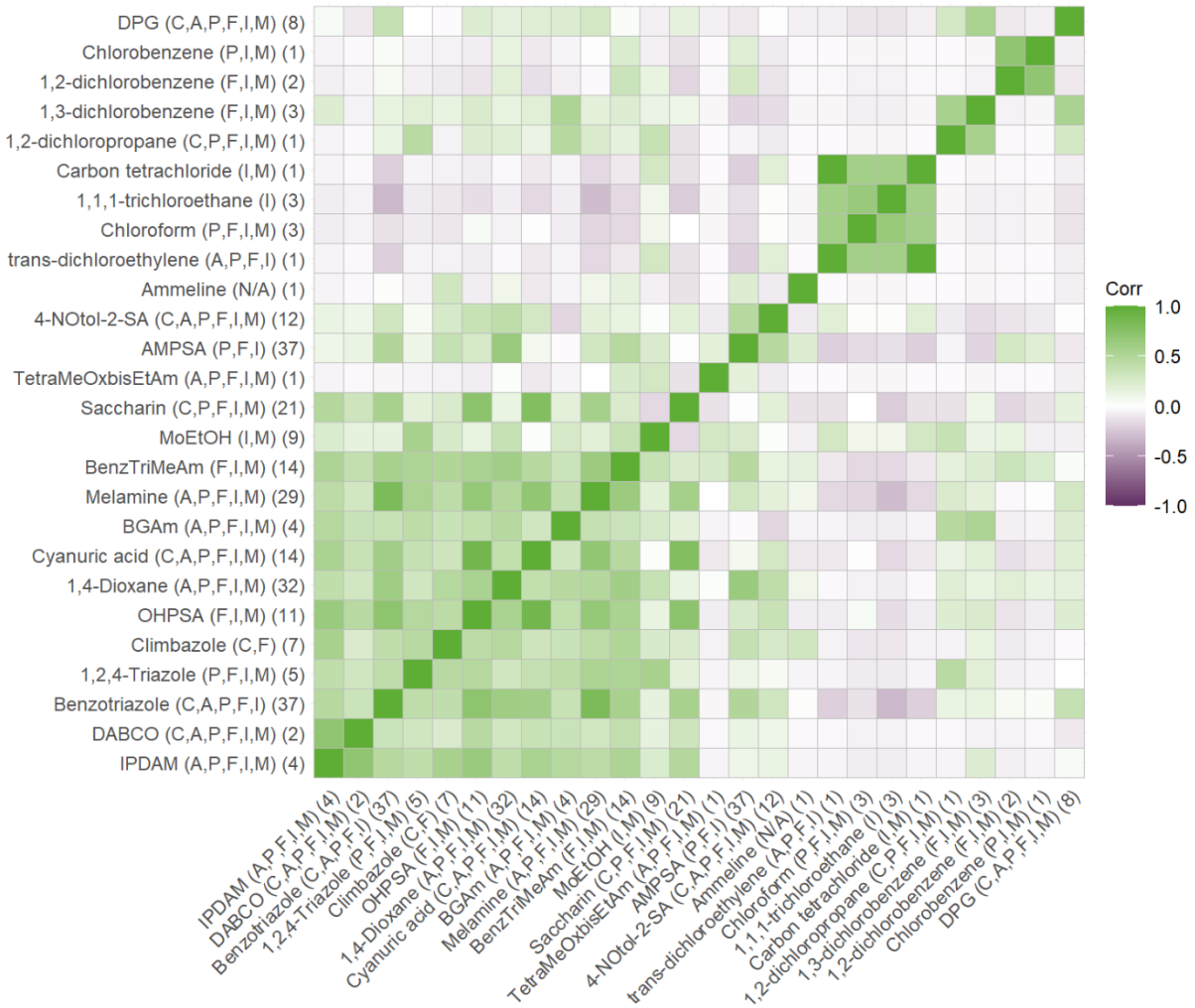
Source: Neuwald et al., 2022b

To investigate the distribution of PMT/vPvM substances within the sample set, the rarity score was calculated analogously to chapter 7.2.1.1. Rarity scores for PMT/vPvM substances were found to be generally higher than for many PFAS, which is also in line with the lower detection frequencies observed for most of them. This points towards the fact that there are a few diffusely distributed PMT/vPvM substances and many local contaminations. Generally, PMT/vPvM substances seem less diffusely distributed than legacy PFAS, which is likely caused by emission patters and not environmental behaviour. DPG was the only PMT/vPvM substance with an exceptionally high rarity score, which indicates a pronounced site-specificity. However, since the main entrance pathway of DPG is assumed to be through road run-off during rain events, it is likely that DPG concentrations are highly dependent on the sampling time as well.

For a more detailed evaluation of environmental occurrence patterns, the correlation of all PMT/vPvM substances was plotted against each other (Figure 17). Low detection frequencies for many PMT/vPvM substances hamper the interpretation of the results but general trends are evident. The plot shows that substances in the lower left corner correlate well, while the correlation decreases towards the upper right side. Generally, the analytes are sorted by decreasing public access based on REACH registered uses from left to right, with substances with pronounced consumer use like benzotriazole on the left, followed by substances which are used in products/have a professional use and finally industrial chemicals like AMPSA towards the right. The increasing correlation that seems tied to a more pronounced public access is likely caused by urban effluent as common environmental entrance pathway. The more industrially used substances on the right sometimes correlate among each other in small groups but rarely with substances with consumer uses, which implies separate sources that are tied to industrial use or production. With the exception of the widely detected AMPSA, chemicals with pronounced consumer uses exhibited higher detection frequencies than those assumed to be released by industrial use. The large only slightly correlating section of industrial uses of PMT/vPvM substances, which encompasses more than half of the substances detected, might points towards very specific sources for many PMT/vPvM substances and may explain the observed inhomogeneity of the data. Missing correlations for DPG to any other PMT/vPvM substance are ascribed to its rather unique environmental entry pathway through road runoff during rain events.

Figure 17: Correlation plot of all detected PMT/vPvM substances

PMT/vPvM substances sorted by type and chain length. Number in brackets depict the number of detects. <LOQ was included with half its value for each substance. Analytes are sorted by REACH registered use. Abbreviations: C: by consumers, A: in articles, P: by professionals, F: in formulation or re-packing, I: at industrial sites, M: in manufacturing.4-NOtol-2-SA: 4-Nitrotoluenesulfonic acid, AMPSA:2- Acrylamido-2-methyl-1-propanesulfonic acid, OHPSA: 3-(allyloxy)-2-hydroxypropanesulfonic acid, IPDAM: Isoprohonediamine, DEMAEtOH: 2-((2-(2-(Dimethylamino)ethoxy)ethyl)(methyl)amino)-ethanol, MoEtOH: 2-Morpholinoethanol, DABCO: 1,4-Diazabicyclo[2.2.2]octane, BGAm: Benzoguanamine, DPG: 1,3-Diphenylguanidine, B2DiMeAmEtMeAm: Bis(2-dimethylaminoethyl)-(methyl)amine, TetraMeOxbisEtAm: N,N,N‘,N‘-Tetramethyl-2,2‘-oxybis(ethylamine), BenzTriMeAm: Benzyltrimethylammonium



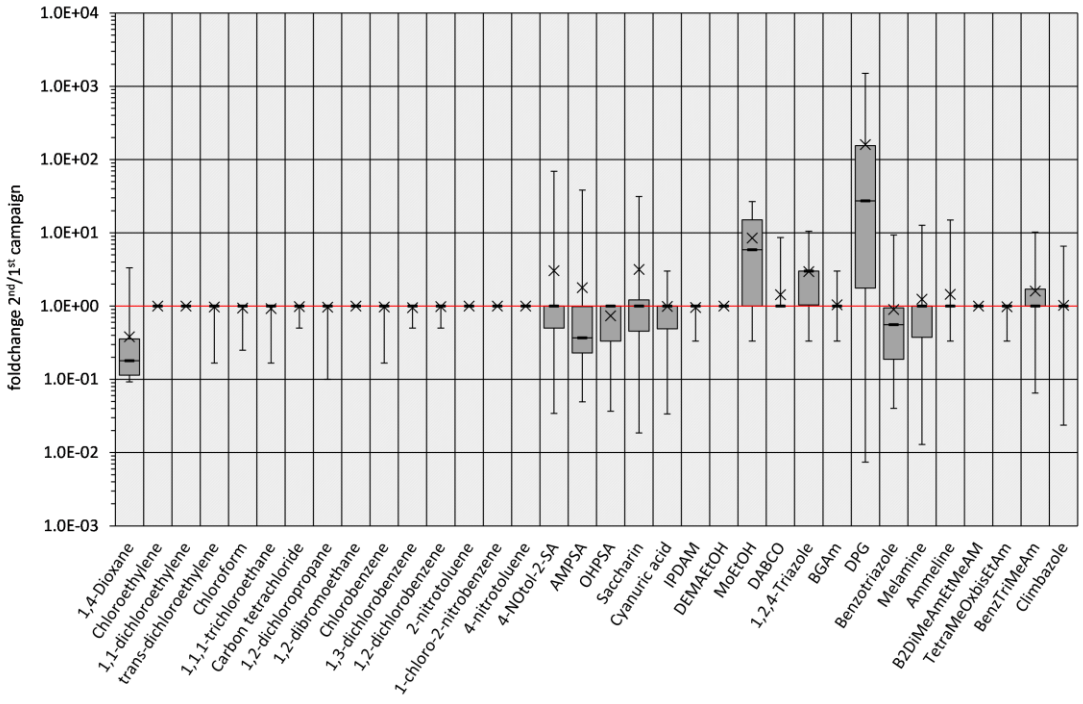
Source: Neuwald et al., 2022b

8.2.2.2. Second sampling campaign: Assessment of temporal trends

The second sampling campaign was conducted to reveal temporal trends for the substances to provide integral information for the assessment of sources and environmental behaviour. Analogous to chapter 7.2.1.3, the fold changes were calculated by dividing concentrations in the second sampling campaign by concentrations in the first sampling campaign (Figure 18). Similar to PFAS, most PMT/vPvM substances have a median fold change close to 1 with a narrow interquartile range, indicating only minor changes between both sampling campaigns and hint towards a low time dependency for most PMT/vPvM substances. DPG, however, is subject to a pronounced increase in detection frequency from 5 during the initial sampling to 26 during the second sampling campaign, which resulted in elevated fold changes. In contrast to 6:2 FTS, which showed elevated concentrations in bank filtrate and groundwater but not in surface water in the second sampling campaign, increased detection frequencies and concentrations for DPG are predominantly observed in surface water. For DPG that leaches from tires and tire wear particles, concentrations of up to 300 µg/L have been detected in storm water (Challis et al., 2021) and thus the heavy rain fall in the summer of 2021 may be mainly responsible for the increased DPG concentrations observed here. This demonstrates that the environmental occurrence of DPG is strongly time dependent, and while median concentrations might be low over a long period of time, short-term high concentrations are present. The environmental impact of such reoccurring peak concentrations is so far largely unexplored.

Figure 18: Fold changes of PMT/vPvM substance concentrations between both sampling campaigns

Boxplots of the fold changes in concentrations between the first and second sampling campaign (second campaign/first campaign). 4-NOtol-2-SA: 4-Nitrotoluenesulfonic acid, AMPSA:2- Acrylamido-2-methyl-1-propanesulfonic acid, OHPSA: 3-(allyloxy)-2-hydroxypropanesulfonic acid, IPDAM: Isoprohonediamine, DEMAEtOH: 2-((2-(2-(Dimethylamino)ethoxy)ethyl)(methyl)amino)-ethanol, MoEtOH: 2-Morpholinoethanol, DABCO: 1,4-Diazabicyclo[2.2.2]octane, BGAm: Benzoguanamine, DPG: 1,3-Diphenylguanidine, B2DiMeAmEtMeAm: Bis(2-dimethylaminoethyl)-(methyl)amine, TetraMeOxbisEtAm: N,N,N‘,N‘-Tetramethyl-2,2‘-oxybis(ethylamine), BenzTriMeAm: Benzyltrimethylammonium



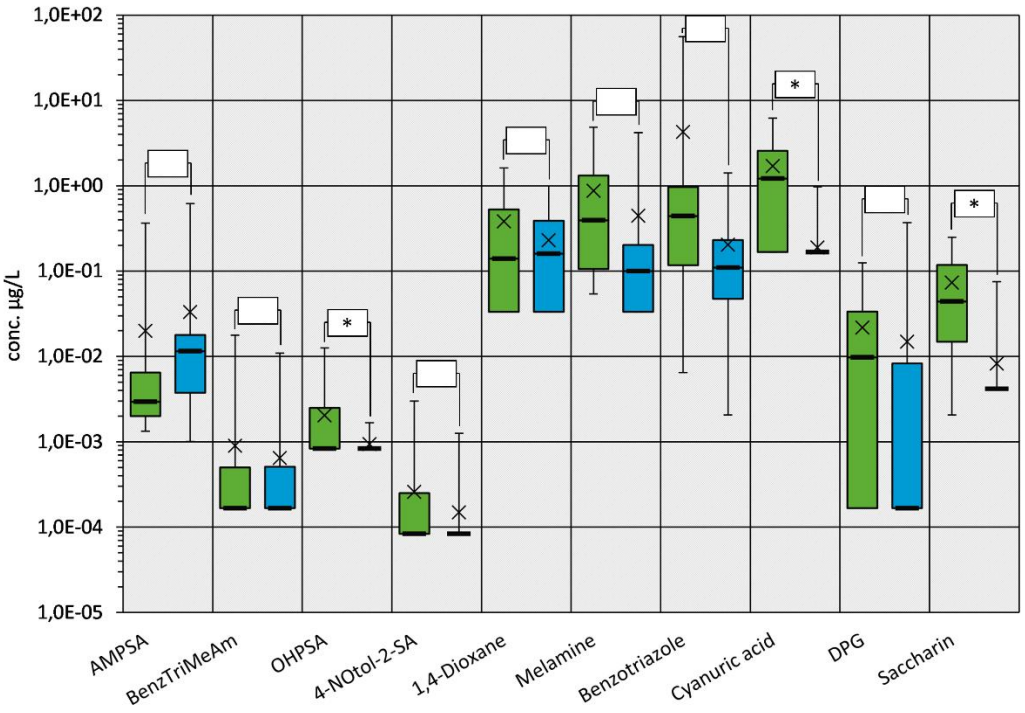
Source: Neuwald et al., 2022b

8.2.2.3. First and second sampling campaign: Assessment of environmental behaviour

Combining the data from both sampling campaigns gives a dataset that can be used for the assessment of the environmental behaviour of PMT/vPvM substances. This dataset was used to compare the occurrence of high detection frequency PMT/vPvM substances in surface water and bank filtrate (Figure 19). A large difference in observed concentrations for these two water types is a first indicator that a substance is (partially) removed during bank filtration. Where concentrations are similar, this implies that a substance reaches bank filtrate without any form of removal. Such results can only be seen as a general trend however, since local conditions may vary significantly. A t-test was used to compare both data sets that revealed statistically significant reduction of cyanuric acid, saccharin and OHPSA concentration between surface water and bank filtrate. For cyanuric acid and saccharin, it is assumed that biological degradation, and not mobility, is the driving force in the concentration reduction. Generally, the data suggests that most of the tested substances do reach bank filtrate without a significant concentration reduction, and thus support the connection between establishing regulatory criteria for mobility and protecting the environment.

Figure 19: Comparison of selected PMT/vPvM substances in surface water and bank filtrate

Boxplots of PMT/vPvM substance concentrations in surface water (green) and bank filtrate (blue). Mean, median, minimum, maximum and interquartile ranges were calculated using the Kaplan-Meier approach to consider non-detects. No star: p-value of t-test > 0.05, 1 star: p-value of t-test <0.05. AMPSA:2- Acrylamido-2-methyl-1-propanesulfonic acid, BenzTriMeAm: Benzyltrimethylammonium, OHPSA: 3-(allyloxy)-2-hydroxypropanesulfonic acid, 4-NOtol-2-SA: 4-Nitrotoluenesulfonic acid, DPG: 1,3- Diphenylguanidine



P (dt50)	19	21	15	66	44	100	27	10	68	27
M (LogDoc/Koc) *: predicted	-2.7* ow	-2.2* ow	-1.5* ow	-1.5* ow	-0.4* ow	1.1	1.5	1.7	2.5	3.3

Source: Neuwald et al., 2022b

9. Category: Exposure Level

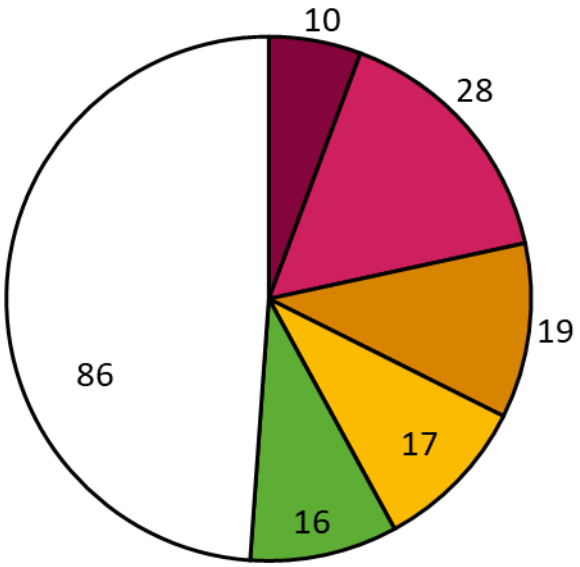
The Analytical and Monitoring Gap, described in Chapter 6, is focussed on if the substance *can be* monitored (analytical gap) or *is being* monitored (monitoring gap). The Exposure Level prioritization category (Table 1) is an extension of the monitoring gap, in that it prioritizes based on the actual exposure level. The categories for Exposure Level are presented in Table 16.

Table 16: Classes of the Exposure Level Prioritization Category

Criteria or PMT/vPvM conclusion	Explanation
No monitoring data currently available	Substances with unknown/unavailable monitoring data
Ubiquitous, high conc.	Ubiquitously detected and occasionally at high concentrations in drinking water sources (greater than 0.1 µg/L or the PNEC if known)
Ubiquitous, low conc.	Ubiquitous but generally at low concentrations in drinking water sources (less than 0.1 µg/L or the PNEC if known)
Local, high conc.	Local contamination in drinking water sources, but at high concentrations
Local, low conc.	Local contamination in drinking water sources but at trace concentrations
Monitored commonly, not found	Monitored often, but not yet detected

To assess the Exposure Level of the 176 selected substances, two approaches were used. The original monitoring study using samples from the sources of Germany's drinking water, as presented in Chapter 8, and a literature review, as presented in Arp et al. (2023a). Due to the availability of analytical methods used in the monitoring campaign, only 76 of the selected 176 substances could be monitored for. From the literature review in Arp et al. (2023a), monitoring data for 58 of the 176 substances could be identified, and 44 of these 58 substances were also included in the monitoring study. The Exposure Level could only be assigned for 90 of the 176 selected substances. For the 44 substances that were included in both the monitoring study and the literature review, the greatest Exposure Level in Table 16 was chosen. For example, if the literature review said a substance had an exposure level of "local, low conc.", and the German monitoring study resulted in a substance having an exposure level of "ubiquitous, lo conc.", then "ubiquitous, low conc." would be selected. The final conclusions of the exposure level distribution for the 176 substances are present in Figure 20.

Figure 20: Distribution of the Exposure Level classes amongst the 176 substances



Ubiquitous, high conc.: Ubiquitously detected and occasionally at high concentrations in drinking water sources (greater than 0.1 µg/L or the PNEC if known) (10 substances)
Ubiquitous, low conc.: Ubiquitous but generally at low concentrations in drinking water sources (less than 0.1 µg/L or the PNEC if known) (28 substances)
Local, high conc.: Local contamination in drinking water sources, but at high concentrations (19 substances)
Local, low conc.: Local contamination in drinking water sources but at trace concentrations (17 substances)
Monitored commonly, not found: Monitored often, but not detected (16 substances).
White: No monitoring data currently available (86 substances)

Source: Original Figure

There were 16 substances that were detected in the German monitoring campaign in Chapter 8, but were not found in the literature review (Arp et al., 2023a). Thus this is one the first times that a study has reported these substances in the sources of drinking water, to the best of our knowledge. These 16 substances are presented in Table 17. The list includes PFAS that were either too mobile for many existing analytical methods (e.g. PFPrS, Lithium bis(trifluoromethylsulfonyl)imide) as well as some of the non-fluorinated PMT/vPvM substances like triazenes (ammeline and 6-phenyl-1,3,5-triazine-2,4-diyldiamine) as well as others (e.g. 1,4-diazabicyclooctane, N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine), Sodium 3-(allyloxy)-2-hydroxypropanesulphonate and 2-morpholinoethanol). Also inTable 17 are some PFAS that are non PMT/vPvM substances, which were added to the monitoring campaign and detected here for the first time (e.g. Perfluorotridecanoic acid (PFTrDA) and Perfluorotetradecanoic acid (PFTetrA)).

Table 17: The 16 substances that were detected here for either the first time or amongst the first times in the sources of German drinking water

EC	CAS	Substance	Analytical & Monitoring gap	German monitoring study
202-095-6	91-76-9	6-phenyl-1,3,5-triazine-2,4-diyldiamine	Major monitoring gap	Local, low conc
415-300-0	90076-65-6	Lithium bis(trifluoromethylsulfonyl)imide	Major monitoring gap	Local, low conc
211-455-1	211-455-1	ammeline	Minor monitoring gap	Local, low conc
279-481-6	80475-32-7	N-[3-(dimethylamino)propyl]-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonamide N-oxide	Minor monitoring gap	Local, low conc
911-467-3	2926-29-6	trifluoromethanesulfinate (triflinate)	not included	Local, low conc
205-999-9	280-57-9	1,4-diazabicyclooctane	Major monitoring gap	Local, low conc
221-220-5	3033-62-3	N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	Major monitoring gap	Local, low conc
258-004-5	52556-42-0	Sodium 3-(allyloxy)-2-hydroxypropanesulphonate	Major monitoring gap	Local, low conc
210-734-5	622-40-2	2-morpholinoethanol	Major monitoring gap	Ubiquitous, low conc
213-059-4	920-66-1	1,1,1,3,3,3-hexafluoropropan-2-ol	not included	Local, low conc
204-445-3	121-03-9	4-nitrotoluene-2-sulphonic acid	Major monitoring gap	Ubiquitous, low conc
276-745-2	72629-94-8	Perfluorotridecanoic acid (PFTrDA)	not included	Ubiquitous, low conc
207-021-6	422-64-0	Perfluoropropanoic acid (PFPrA)	not included	Ubiquitous, low conc
206-803-4	376-06-7	Perfluorotetradecanoic acid (PFTetrA)	not included	Ubiquitous, low conc
-	423-41-6	Perfluoropropanesulfonic acid (PFPrS)	not included	Ubiquitous, low conc
477-710-6	377739-43-0	tris(pentafluoroethyl)trifluorophosphate (FAP)	not included	Local, low conc

10. Category: Overall Prioritization Level

Two of the overall prioritization level classes were previously defined in Arp et al. (2023b). the "High-Priority" class and the "Moderate-Priority" class. These are PMT/vPvM substances registered under REACH with registration volumes > 10 tpa or between 1-10 tpa, respectively. The "Moderate-Priority" class can also include substances that are potential transformation products or impurities of REACH registered substances that meet the PMT/vPvM criteria, as often their tonnages are uncertain and difficult to quantify. The other Overall Prioritization levels are extensions of these two categories and are presented in Table 18.

The "Highest-Priority" substances can be thought of as the "High-Priority" REACH registered substances that have something warranting additional prioritization, such as an analytical gap, unavailability of remediations methods, or ubiquitous detection at high concentrations.

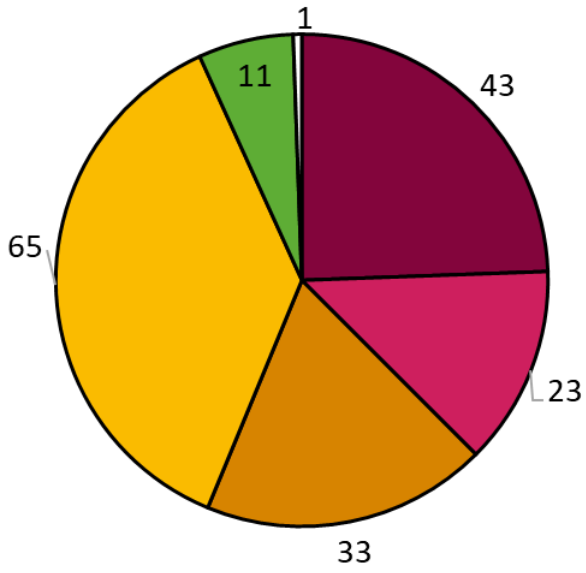
The "Potential-Priority" substances are those that could meet the PMT/vPvM criteria if more data becomes available, such as PM substances where toxicity has not yet been demonstrated or "Potential PMT/vPvM substances" where more weight-of-evidence is needed to confirm if the substances meets the PMT/vPvM criteria or not. The "Lowest-Priority" class refers to those substances that do not meet the PMT/vPvM criteria. It is important to note that the "Lowest-Priority" class does not mean the substance is not hazardous based on another reason than PMT/vPvM substance properties (e.g. toxicity or meeting the PBT/vPvB criteria).

Table 18: Classes of the Overall prioritization level Category

Criteria or PMT/vPvM conclusion	Explanation
Unknown/insufficient data	Substances with unknown/insufficient data to make a PMT/vPvM hazard assessment
Highest-Priority	PMT/vPvM substance with registration volumes > 10 tpa, very high or high emission likelihood, and at least one other dark red category
High-Priority	PMT/vPvM substance with registration volumes > 10 tpa
Moderate-Priority	PMT/vPvM substances with registration volumes < 10 tpa or is a impurity/transformation product of a REACH registered substance
Potential-Priority	All other cases, except if Not PMT/vPvM substance
Lowest-Priority	Substance is Not PMT/vPvM

The distribution of the Overall prioritization level of the 176 selected substances is presented in Figure 21. The outcome of the prioritization framework for all 176 substances considered in this study, organized in order of priority is presented in Table 19.

Figure 21: Overall prioritization level of the 176 substances considered in this study



Highest-Priority: PMT/vPvM substance with registration volumes > 10 tpa, very high or high emission likelihood, and two other dark red categories (43 substances)
High-Priority: PMT/vPvM substance with registration volumes > 10 tpa (23 substances)
Moderate-Priority: PMT/vPvM substances with registration volumes < 10 tpa, or is suspected impurity/transformation product (33 substances)
Potential-Priority: All other cases, except if "Not PMT/vPvM" (65 substances)
Lowest-Priority: Substances is "Not PMT/vPvM" (11 substances).
White: Unknown/insufficient data (1 substance)

Source: Original Figure

There are 43 of the 176 selected substances that met the "Highest-Priority" class level, the most common reason for this was that they could not be remediated with AC filtration or ozonation (40 out of 43 substances), there were also 6 of these 40 that had ubiquitous, high concentrations (1,4-dioxane, benzotriazole, melamine, cyanuric acid, trifluoroacetic acid and trifluoromethanesulfonic acid, all of which are also not efficiently removed by AC filtration and ozonation).

Of the 24 "High-Priority" PMT/vPvM substances, 8 of them can be removed by ozonation only, and the rest of them can be removed by activated carbon; nevertheless, 15 of them have been detected in drinking water sources.

The 33 "Moderate-Priority" PMT/vPvM substances contained several of the PFAS that were included in the monitoring study (and therefore only present as small volumes under REACH, often as impurities or transformation products), but the majority of the substances investigated in the Remediation Gap cannot be removed by ozonation or AC filtration. Twenty-two of these substances have been detected in drinking water sources.

The 65 selected substances falling into the "Potential-priority" class consisted mostly of substances that fulfilled the PM criteria, with no high-quality consensus conclusions that the T criteria is met (38 substances, two of which are also known precursors of PFAS meeting the PMT/vPvM criteria). The remainder met the "Potential PMT/vPvM" criteria (27 substances, of which 7 are suspected precursors of PFAS meeting the PMT/vPvM criteria). Of the 11 "Lowest-Priority" substances, there were 4 that were detected in the environment, of which 3 were long-chain PFAS that meet the PBT/vPvB criteria, and one was a mass-produced flame retardant (Tris(2-butoxyethyl) phosphate).

Table 19: Outcome of PMT/vPvM prioritization framework for all 176 substances considered in this study, organized in order of priority

EC	CAS	Substance	PMT/vPvM hazard	Emission Index	Analytical & Monitoring Gap	Remediation Gap	Exposure level	Overall Prioritization Level
203-618-0	108-80-5	cyanuric acid	vPvM & PMT	very high	Minor monitoring gap	No O3&AC	Ubiquitous, high conc	Highest-priority
203-615-4	108-78-1	Melamine	vPvM & PMT	very high	Monitored frequently	No O3&AC	Ubiquitous, high conc	Highest-priority
249-616-3	29420-49-3	PFBS	vPvM & PMT	very high	Monitored frequently	No O3&AC	Ubiquitous, low conc	Highest-priority
204-661-8	123-91-1	1,4-dioxane	vPvM & PMT	very high	Monitored frequently	No O3&AC	Ubiquitous, high conc	Highest-priority
202-394-1	95-14-7	Benzotriazole	vPvM & PMT	very high	Monitored frequently	Both O3&AC	Ubiquitous, high conc	Highest-priority
244-479-6	21615-47-4	Ammonium undecafluorohexanoate (PFHxA)	vPvM & PMT	very high	Minor monitoring gap	No O3&AC	Ubiquitous, low conc	Highest-priority
200-929-3	76-05-1	Trifluoroacetic acid	vPvM	very high	Monitored frequently	No O3&AC	Ubiquitous, high conc	Highest-priority
200-300-3	56-93-9	Benzyltrimethylammonium chloride	vPvM	very high	Major monitoring gap	No O3&AC	Ubiquitous, low conc	Highest-priority
222-823-6	3622-84-2	N-butylbenzenesulphonamide	vPvM	very high	Major monitoring gap	No O3&AC	Ubiquitous, low conc	Highest-priority
204-445-3	121-03-9	4-nitrotoluene-2-sulphonic acid	vPvM	very high	Major monitoring gap	No O3&AC	Ubiquitous, low conc	Highest-priority
248-580-6	27619-97-2	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonic acid	vPvM	very high	Monitored frequently	No O3&AC	Ubiquitous, low conc	Highest-priority
200-087-7	51-28-5	2,4-dinitrophenol	vPvM & PMT	very high	Minor monitoring gap	No O3&AC	Local, high conc	Highest-priority
200-915-7	75-91-2	tert-butyl hydroperoxide	vPvM & PMT	high	Major monitoring gap	No O3&AC	no detections known	Highest-priority
203-444-5	106-93-4	1,2-dibromoethane	vPvM & PMT	very high	Monitored frequently	No O3&AC	Local, high conc	Highest-priority
201-152-2	78-87-5	1,2-dichloropropane	vPvM & PMT	very high	Monitored frequently	No O3&AC	Local, high conc	Highest-priority
202-808-0	99-99-0	4-nitrotoluene	vPvM & PMT	high	Monitored frequently	No O3&AC	monitored commonly, not found	Highest-priority
203-639-5	109-01-3	1-methylpiperazine	vPvM & PMT	very high	Major monitoring gap	No O3&AC	no detections known	Highest-priority
200-864-0	75-35-4	1,1-dichloroethylene	vPvM & PMT	very high	Monitored frequently	No O3&AC	Local, high conc	Highest-priority
200-663-8	67-66-3	Chloroform	vPvM & PMT	very high	Monitored frequently	No O3&AC	Local, high conc	Highest-priority
200-927-2	76-03-9	Trichloroacetic acid	vPvM & PMT	high	Minor monitoring gap	No O3&AC	no detections known	Highest-priority
204-500-1	121-82-4	Perhydro-1,3,5-trinitro-1,3,5-triazine	vPvM	very high	Minor monitoring gap	No O3&AC	Local, high conc	Highest-priority
811-523-6	88992-45-4	2-hydroxy-N,N,N-trimethyl-3-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)thio]propan-1-aminium chloride	vPvM	high	Major monitoring gap	No O3&AC	no detections known	Highest-priority
200-893-9	75-71-8	Dichlorodifluoromethane	vPvM	very high	Minor monitoring gap	No O3&AC	Local, high conc	Highest-priority
201-114-5	78-40-0	Triethyl phosphate	vPvM	very high	Monitored frequently	No O3&AC	Local, low conc	Highest-priority
682-238-0	1190931-27-1	Ammonium difluoro{[2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	vPvM	high	Major monitoring gap	No O3&AC	no detections known	Highest-priority

EC	CAS	Substance	PMT/vPvM hazard	Emission Index	Analytical & Monitoring Gap	Remediation Gap	Exposure level	Overall Prioritization Level
252-046-8	34455-29-3	Carboxymethyldimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulphonyl]amino] propylammonium hydroxide	vPvM	high	Minor monitoring gap	No O3&AC	no detections known	Highest-priority
236-740-8	13472-08-7	2,2'-azobis[2-methylbutyronitrile]	vPvM	high	Not Monitored; analytical development feasible	No O3&AC	no detections known	Highest-priority
244-751-4	22042-96-2	Diethylenetriaminepenta(methylenephosphonic acid), sodium salt	vPvM	high	Minor monitoring gap	No O3&AC	no detections known	Highest-priority
263-212-4	61792-09-4	Pentasodium diethylenetriaminepentamethylene phosphonate	vPvM	high	Not Monitored; analytical development feasible	No O3&AC	no detections known	Highest-priority
221-220-5	3033-62-3	N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	vPvM	very high	Major monitoring gap	No O3&AC	Local, low conc	Highest-priority
277-242-0	73037-34-0	Disodium oxybis[methylbenzenesulphonate]	vPvM	high	Not Monitored; analytical development feasible	No O3&AC	no detections known	Highest-priority
811-522-0	62880-93-7	sodium 2-methyl-2-({3-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)thio]propanoyl}amino)propane-1-sulfonate	vPvM	high	Major monitoring gap	No O3&AC	no detections known	Highest-priority
203-509-8	107-66-4	Dibutyl hydrogen phosphate	vPvM	very high	Major monitoring gap	No O3&AC	no detections known	Highest-priority
216-087-5	1493-13-6	Trifluoromethanesulphonic acid	vPvM	very high	Minor monitoring gap	No O3&AC	Ubiquitous, high conc	Highest-priority
205-860-2	156-60-5	trans-dichloroethylene	vPvM	very high	Monitored frequently	No O3&AC	Local, high conc	Highest-priority
201-132-3	78-67-1	2,2'-dimethyl-2,2'-azodipropiononitrile	vPvM	high	Not Monitored; analytical development feasible	No O3&AC	no detections known	Highest-priority
221-201-1	3030-47-5	Bis(2-dimethylaminoethyl)(methyl)amine	vPvM	high	Major monitoring gap	No O3&AC	monitored commonly, not found	Highest-priority
202-905-8	100-97-0	Methenamine	vPvM	very high	Minor monitoring gap	No O3&AC	Local, high conc	Highest-priority
203-560-6	108-20-3	Diisopropyl ether	vPvM	very high	Monitored frequently	No O3&AC	Local, high conc	Highest-priority
201-279-3	80-43-3	Bis(α,α-dimethylbenzyl) peroxide	PMT	high	Not Monitored; analytical development challenging	AC only	no detections known	Highest-priority
220-666-8	2855-13-2	3-aminomethyl-3,5,5-trimethylcyclohexylamine	PMT	very high	Minor monitoring gap	No O3&AC	Local, low conc	Highest-priority
223-772-2	4065-45-6	Sulisobenzone	PMT	high	Minor monitoring gap	No O3&AC	no detections known	Highest-priority
212-634-7	834-12-8	Ametryn	vPvM & PMT	very high	Monitored frequently	Both O3&AC	Ubiquitous, low conc	High-priority
237-159-2	13674-87-8	Tris(2-chloro-1-methylethyl) phosphate	vPvM & PMT	very high	Monitored frequently	AC only	Ubiquitous, low conc	High-priority
203-002-1	102-06-7	1,3-diphenylguanidine	vPvM & PMT	very high	Minor monitoring gap	Both O3&AC	Ubiquitous, low conc	High-priority
202-577-6	97-39-2	1,3-di-o-tolylguanidine	vPvM	very high	Major monitoring gap	O3 only	Ubiquitous, low conc	High-priority

EC	CAS	Substance	PMT/vPvM hazard	Emission Index	Analytical & Monitoring Gap	Remediation Gap	Exposure level	Overall Prioritization Level
225-948-4	5165-97-9	Sodium 2-methyl-2-[(1-oxoallyl)amino]propanesulphonate	vPvM	very high	Major monitoring gap	O3 only	Ubiquitous, low conc	High-priority
209-967-5	599-61-1	3,3'-sulphonyldianiline	vPvM & PMT	high	Major monitoring gap	O3 only	no detections known	High-priority
400-600-6	71868-10-5	2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one	vPvM & PMT	high	Minor monitoring gap	AC only	no detections known	High-priority
200-831-0	75-01-4	Chloroethylene	vPvM & PMT	very high	Monitored frequently	O3 only	Local, high conc	High-priority
204-340-2	119-64-2	1,2,3,4-tetrahydronaphthalene	vPvM & PMT	high	Minor monitoring gap	AC only	no detections known	High-priority
204-077-3	115-27-5	Chlorendic anhydride	vPvM & PMT	high	Not Monitored; analytical development feasible	AC only	no detections known	High-priority
203-492-7	107-46-0	Hexamethyldisiloxane	vPvM & PMT	high	Minor monitoring gap	AC only	no detections known	High-priority
204-337-6	119-61-9	Benzophenone	vPvM & PMT	very high	Minor monitoring gap	AC only	Local, high conc	High-priority
200-262-8	56-23-5	Carbon tetrachloride	vPvM & PMT	very high	Monitored frequently	AC only	Local, high conc	High-priority
208-792-1	541-73-1	1,3-dichlorobenzene	vPvM & PMT	very high	Monitored frequently	AC only	Local, high conc	High-priority
201-248-4	80-08-0	Dapsone	vPvM & PMT	very high	Monitored frequently	O3 only	Local, low conc	High-priority
203-628-5	108-90-7	Chlorobenzene	vPvM	very high	Monitored frequently	AC only	Local, high conc	High-priority
290-824-9	90268-24-9	Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(4-chloro-2,5-dimethoxyphenyl and 2,4-xylyl) derivs.	vPvM	high	Major monitoring gap	Both O3&AC	no detections known	High-priority
202-095-6	91-76-9	6-phenyl-1,3,5-triazine-2,4-diyldiamine	vPvM	very high	Major monitoring gap	O3 only	Local, low conc	High-priority
258-004-5	52556-42-0	Sodium 3-(allyloxy)-2-hydroxypropanesulphonate	vPvM	very high	Major monitoring gap	O3 only	Local, low conc	High-priority
219-006-1	2312-35-8	Propargite	PMT	high	Minor monitoring gap	Both O3&AC	no detections known	High-priority
202-425-9	95-50-1	1,2-dichlorobenzene	PMT	very high	Monitored frequently	AC only	Local, high conc	High-priority
253-775-4	38083-17-9	Climbazole	PMT	very high	Minor monitoring gap	AC only	Local, low conc	High-priority
206-466-3	345-92-6	Bis(4-fluorophenyl) ketone	PMT	high	Major monitoring gap	AC only	no detections known	High-priority
204-616-2	123-30-8	4-aminophenol	PMT	high	Major monitoring gap	O3 only	no detections known	High-priority
206-402-4	335-67-1	Perfluorooctanoic acid (PFOA)	vPvM & PMT	not REACH	not included	not included	Ubiquitous, high conc	Moderate-priority
217-179-8; 260-375-3	1763-23-1, 56773-42-3	Perfluorooctane sulfonic acid (PFOS)	vPvM & PMT	medium	not included	not included	Ubiquitous, high conc	Moderate-priority
206-587-1	3871-99-6, 355-46-4	Perfluorohexanesulfonic acid (PFHxS)	vPvM & PMT	not REACH	not included	not included	Ubiquitous, high conc	Moderate-priority
220-300-7	2706-90-3	Perfluoropentanoic acid (PFPA)	vPvM & PMT	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
206-798-9	375-85-9	Perfluoroheptanoic acid (PFHpA)	vPvM & PMT	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
206-801-3	375-95-1	Perfluorononanoic acid (PFNA)	vPvM & PMT	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority

EC	CAS	Substance	PMT/vPvM hazard	Emission Index	Analytical & Monitoring Gap	Remediation Gap	Exposure level	Overall Prioritization Level
206-400-3	335-76-2	Perfluorodecanoic acid (PFDA)	vPvM & PMT	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
220-301-2	2706-91-4	Perfluoropentanesulfonic acid (PFPS)	vPvM & PMT	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
206-800-8	375-92-8	Perfluoroheptane sulfonic acid (PFHpS)	vPvM & PMT	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
206-786-3	375-22-4	Perfluorobutanoic acid (PFBA)	vPvM	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
207-021-6	422-64-0	Perfluoropropanoic acid (PFPrA)	vPvM	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
206-203-2	307-55-1	Perfluorododecanoic acid (PFDoDA)	PMT	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
-	68259-12-1	Perfluorononane sulfonic acid (PFNS)	PMT	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
218-165-4	2058-94-8	Perfluoroundecanoic acid (PFUnDA)	PMT	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
206-022-9	288-88-0	1,2,4-triazole	PMT	medium	Monitored frequently	No O3&AC	Ubiquitous, low conc	Moderate-priority
206-401-9	67906-42-7, 335-77-3	Perfluorodecane sulfonic acid (PFDS)	PMT	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
700-242-3	62037-80-3	Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate	vPvM & PMT	medium	Minor monitoring gap	No O3&AC	Local, low conc	Moderate-priority
201-853-3	88-72-2	2-nitrotoluene	vPvM & PMT	low	Monitored frequently	No O3&AC	monitored commonly, not found	Moderate-priority
201-854-9	88-73-3	1-chloro-2-nitrobenzene	vPvM & PMT	low	Minor monitoring gap	AC only	monitored commonly, not found	Moderate-priority
203-581-0	108-42-9	3-chloroaniline	vPvM & PMT	low	Monitored frequently	O3 only	no detections known	Moderate-priority
430-550-0	1671-49-4	4-mesyl-2-nitrotoluene	vPvM & PMT	low	Major monitoring gap	No O3&AC	no detections known	Moderate-priority
700-323-3	908020-52-0	Ammonium difluoro[1,1,2,2-tetrafluoro-2-(pentafluoroethoxy)ethoxy]acetate	vPvM & PMT	low	Major monitoring gap	No O3&AC	no detections known	Moderate-priority
700-413-2	6331-96-0	2-amino-4,5-dichlorobenzenesulfonic acid	vPvM & PMT	low	Major monitoring gap	O3 only	no detections known	Moderate-priority
204-473-6	121-47-1	3-aminobenzenesulphonic acid	vPvM & PMT	low	Major monitoring gap	O3 only	no detections known	Moderate-priority
405-800-7	27955-94-8	4,4',4''-(ethan-1,1,1-triyl)triphenol	vPvM & PMT	low	Major monitoring gap	AC only	no detections known	Moderate-priority
411-280-2	74091-64-8	2,5-bis-isocyanatomethyl-bicyclo[2.2.1]heptane	vPvM & PMT	low	Not Monitored; analytical development feasible	No O3&AC	no detections known	Moderate-priority
-	423-41-6	Perfluoropropanesulfonic acid (PFPrS)	vPvM	not REACH	not included	not included	Ubiquitous, low conc	Moderate-priority
477-710-6	-	tris(pentafluoroethyl)trifluorophosphate (FAP)	vPvM	not REACH	not included	not included	Local, low conc	Moderate-priority
-	354-88-1	Perfluoroethanesulfonic acid (PFEtS)	vPvM	not REACH	not included	not included	no detections known	Moderate-priority
200-756-3	71-55-6	1,1,1-trichloroethane	vPvM	medium	Monitored frequently	No O3&AC	Local, high conc	Moderate-priority

EC	CAS	Substance	PMT/vPvM hazard	Emission Index	Analytical & Monitoring Gap	Remediation Gap	Exposure level	Overall Prioritization Level
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	vPvM	low	Not Monitored; analytical development feasible	No O3&AC	no detections known	Moderate-priority
213-059-4	920-66-1	1,1,1,3,3,3-hexafluoropropan-2-ol	vPvM	medium	not included	not included	Local, low conc	Moderate-priority
201-758-7	87-62-7	2,6-xylidine	PMT	medium	Minor monitoring gap	O3 only	Local, low conc	Moderate-priority
210-734-5	622-40-2	2-morpholinoethanol	PM	very high	Major monitoring gap	No O3&AC	Ubiquitous, low conc	Potential-priority
221-111-2	3006-86-8	Cyclohexylidenebis[tert-butyl] peroxide	PM	high	Not Monitored; analytical development challenging	AC only	no detections known	Potential-priority
207-074-5	431-47-0	Methyl trifluoroacetate	PM	high	Major monitoring gap	No O3&AC	no detections known	Potential-priority
615-064-0	700874-87-9	{difluoro[(1,2,2-trifluoroethenyl)oxy]methoxy}trifluoromethane	PM	high	Major monitoring gap	O3 only	no detections known	Potential-priority
205-999-9	280-57-9	1,4-diazabicyclooctane	PM	very high	Major monitoring gap	No O3&AC	Local, low conc	Potential-priority
220-237-5	2680-03-7	N,N-dimethylacrylamide	PM	high	Minor monitoring gap	O3 only	no detections known	Potential-priority
202-605-7	97-74-5	Tetramethylthiuram monosulphide	PM	high	Major monitoring gap	No O3&AC	no detections known	Potential-priority
273-066-3	68937-41-7	Phenol, isopropylated, phosphate (3:1)	PM	high	Not Monitored; analytical development feasible	AC only	no detections known	Potential-priority
201-052-9	77-73-6	3a,4,7,7a-tetrahydro-4,7-methanoindene	PM	high	Minor monitoring gap	Both O3&AC	no detections known	Potential-priority
206-596-0	355-93-1	2,2,3,3,4,4,5,5-octafluoropentyl methacrylate	PM and precursor of vPvM PFAS	high	Major monitoring gap	Both O3&AC	monitored commonly, not found	Potential-priority
252-043-1	34454-97-2	1,1,2,2,3,3,4,4,4-nonafluoro-N-(2-hydroxyethyl)-N-methylbutane-1-sulphonamide	PM	high	Major monitoring gap	No O3&AC	monitored commonly, not found	Potential-priority
206-841-1	382-28-5	2,2,3,3,5,5,6,6-octafluoro-4-(trifluoromethyl)morpholine	PM	high	Major monitoring gap	AC only	monitored commonly, not found	Potential-priority
201-321-0	81-07-2	1,2-benzisothiazol-3(2H)-one 1,1-dioxide	PM	very high	Minor monitoring gap	No O3&AC	Local, high conc	Potential-priority
203-004-2	102-08-9	1,3-diphenyl-2-thiourea	PM	high	Major monitoring gap	Both O3&AC	no detections known	Potential-priority
207-586-9	482-89-3	2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	PM	high	Major monitoring gap	Both O3&AC	no detections known	Potential-priority
225-716-2	5026-74-4	p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	PM	high	Not Monitored; analytical development challenging	O3 only	no detections known	Potential-priority
226-109-5	5281-04-9	Calcium 3-hydroxy-4-[(4-methyl-2-sulphonatophenyl)azo]-2-naphthoate	PM	high	Major monitoring gap	O3 only	no detections known	Potential-priority

EC	CAS	Substance	PMT/vPvM hazard	Emission Index	Analytical & Monitoring Gap	Remediation Gap	Exposure level	Overall Prioritization Level
201-254-7	80-15-9	α,α-dimethylbenzyl hydroperoxide	PM	high	Not Monitored; analytical development challenging	No O3&AC	no detections known	Potential-priority
207-050-4	428-59-1	Trifluoro(trifluoromethyl)oxirane	PM	high	Major monitoring gap	No O3&AC	no detections known	Potential-priority
436-710-6	756-13-8	1,1,1,2,2,4,5,5,5-nonafluoro-4-(trifluoromethyl)-3-pentanone	PM and precursor of vPvM PFAS	high	Major monitoring gap	AC only	no detections known	Potential-priority
252-044-7	34455-00-0	1,1,2,2,3,3,4,4,4-nonafluoro-N,N-bis(2-hydroxyethyl)butane-1-sulphonamide	PM	high	Major monitoring gap	No O3&AC	no detections known	Potential-priority
279-481-6	80475-32-7	N-[3-(dimethylamino)propyl]-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonamide N-oxide	PM	very high	Minor monitoring gap	No O3&AC	Local, low conc	Potential-priority
911-467-3	2926-29-6	trifluoromethanesulfinate (triflinate)	PM	high	not included	No O3&AC	Local, low conc	Potential-priority
200-664-3	67-68-5	Dimethyl sulfoxide	PM	high	Minor monitoring gap	No O3&AC	no detections known	Potential-priority
204-809-1	126-86-3	2,4,7,9-tetramethyldec-5-yne-4,7-diol	PM	very high	Minor monitoring gap	Both O3&AC	Local, high conc	Potential-priority
214-703-7	1187-93-5	Trifluoro(trifluoromethoxy)ethylene	PM	high	Major monitoring gap	AC only	no detections known	Potential-priority
275-662-9	71604-74-5	m-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	PM	high	Not Monitored; analytical development challenging	O3 only	no detections known	Potential-priority
253-733-5	37971-36-1	2-phosphonobutane-1,2,4-tricarboxylic acid	PM	high	Minor monitoring gap	No O3&AC	no detections known	Potential-priority
442-390-9	40573-09-9	1,1,2,2,3,3-hexafluoro-1-trifluoromethoxy-3-trifluorovinyloxypropane	PM	high	Major monitoring gap	Both O3&AC	monitored commonly, not found	Potential-priority
223-989-2	4156-21-2	Sodium p-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]benzenesulphonate	PM	high	Not Monitored; analytical development feasible	O3 only	no detections known	Potential-priority
202-870-9	100-61-8	N-methylaniline	PM	high	Minor monitoring gap	O3 only	no detections known	Potential-priority
218-760-9	2226-96-2	4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	PM	high	Major monitoring gap	No O3&AC	no detections known	Potential-priority
223-055-4	3710-84-7	N,N-diethylhydroxylamine	PM	high	Not Monitored; analytical development feasible	No O3&AC	no detections known	Potential-priority
201-286-1	80-51-3	4,4'-oxydi(benzenesulphonohydrazide)	PM	high	Not Monitored; analytical development feasible	No O3&AC	no detections known	Potential-priority
235-166-5	12108-13-3	Tricarbonyl(methylcyclopentadienyl)manganese	PM	high	Not Monitored; analytical development feasible	not included	no detections known	Potential-priority

EC	CAS	Substance	PMT/vPvM hazard	Emission Index	Analytical & Monitoring Gap	Remediation Gap	Exposure level	Overall Prioritization Level
415-300-0	90076-65-6	Lithium bis(trifluoromethylsulfonyl)imide	PM	low	Major monitoring gap	AC only	Local, low conc	Potential-priority
207-012-7	422-05-9	2,2,3,3,3-pentafluoropropanol	PM	low	not included	not included	monitored commonly, not found	Potential-priority
430-710-1	15290-77-4	1,1,2,2,3,3,4-heptafluorocyclopentane	PM	low	not included	not included	monitored commonly, not found	Potential-priority
216-600-2	1623-05-8	1,1,1,2,2,3,3-heptafluoro-3-[(trifluorovinyl)oxy]propane	Potential PMT/vPvM/, but precursor of PFAS	high	Major monitoring gap	AC only	no detections known	Potential-priority
203-614-9	108-77-0	2,4,6-trichloro-1,3,5-triazine	Potential PMT/vPvM	high	Major monitoring gap	No O3&AC	no detections known	Potential-priority
202-852-0	100-43-6	4-vinylpyridine	Potential PMT/vPvM	high	Not Monitored; analytical development feasible	O3 only	no detections known	Potential-priority
229-713-7	6674-22-2	1,8-diazabicyclo[5.4.0]undec-7-ene	Potential PMT/vPvM	high	Major monitoring gap	No O3&AC	no detections known	Potential-priority
222-429-4	3468-63-1	1-[(2,4-dinitrophenyl)azo]-2-naphthol	Potential PMT/vPvM	high	Major monitoring gap	Both O3&AC	no detections known	Potential-priority
252-156-6	34690-00-1	[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methylene)]]tetrakisphosphonic acid	Potential PMT/vPvM	high	Not Monitored; analytical development feasible	No O3&AC	no detections known	Potential-priority
209-544-5	584-84-9	4-methyl-m-phenylene diisocyanate	Potential PMT/vPvM	high	Not Monitored; analytical development feasible	Both O3&AC	no detections known	Potential-priority
266-737-7	67584-59-2	2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl methacrylate	Not PMT/vPvM, but precursor of PFBS	high	Major monitoring gap	Both O3&AC	no detections known	Potential-priority
217-168-8	1761-71-3	4,4'-methylenebis(cyclohexylamine)	Potential PMT/vPvM	high	Not Monitored; analytical development feasible	No O3&AC	no detections known	Potential-priority
258-904-8	53988-10-6	1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione	Potential PMT/vPvM	high	Not Monitored; analytical development feasible	No O3&AC	no detections known	Potential-priority
288-657-1	85857-16-5	Trimethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	Not PMT/vPvM, but precursor of PFHxA	high	Major monitoring gap	AC only	monitored commonly, not found	Potential-priority
278-947-6	78560-45-9	Trichloro(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	Not PMT/vPvM,	high	Major monitoring gap	AC only	monitored commonly, not found	Potential-priority

EC	CAS	Substance	PMT/vPvM hazard	Emission Index	Analytical & Monitoring Gap	Remediation Gap	Exposure level	Overall Prioritization Level
			but precursor of PFHxA					
257-473-3	51851-37-7	Triethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	Not PMT/vPvM, but precursor of PFHxA	high	Major monitoring gap	AC only	monitored commonly, not found	Potential-priority
219-470-5	2440-22-4	2-(2H-benzotriazol-2-yl)-p-cresol	Potential PMT/vPvM	high	Minor monitoring gap	AC only	no detections known	Potential-priority
209-143-5	556-88-7	1-nitroguanidine	Potential PMT/vPvM	high	Minor monitoring gap	No O3&AC	no detections known	Potential-priority
247-722-4	26471-62-5	m-tolylidene diisocyanate	Potential PMT/vPvM	high	Major monitoring gap	Both O3&AC	no detections known	Potential-priority
229-962-1	6864-37-5	2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)	Potential PMT/vPvM	high	Minor monitoring gap	No O3&AC	no detections known	Potential-priority
241-527-8	17527-29-6	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate	Not PMT/vPvM, but precursor of PFHxA	high	Minor monitoring gap	Both O3&AC	monitored commonly, not found	Potential-priority
218-407-9	2144-53-8	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl methacrylate	Not PMT/vPvM, but precursor of PFHxA	high	Major monitoring gap	Both O3&AC	monitored commonly, not found	Potential-priority
266-733-5	67584-55-8	2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl acrylate	Not PMT/vPvM, but precursor of PFBS	high	Major monitoring gap	Both O3&AC	no detections known	Potential-priority
209-813-7	593-85-1	Diguanidinium carbonate	Potential PMT/vPvM	high	Method development not attempted/unknown	No O3&AC	no detections known	Potential-priority
246-835-6	25321-09-9	Diisopropylbenzene	Potential PMT/vPvM	high	Minor monitoring gap	AC only	no detections known	Potential-priority
214-189-4	1112-39-6	Dimethoxydimethylsilane	Potential PMT/vPvM	high	Not Monitored; analytical development feasible	No O3&AC	no detections known	Potential-priority
211-455-1	211-455-1	ammeline	Potential PMT/vPvM	not REACH	Minor monitoring gap	O3 only	Local, low conc	Potential-priority
645-93-2	645-93-2	ammelide	Potential PMT/vPvM	not REACH	Minor monitoring gap	O3 only	no detections known	Potential-priority
428-100-3	94239-04-0	2-fluoro-6-trifluoromethylpyridine	Potential PMT/vPvM	low	Major monitoring gap	No O3&AC	no detections known	Potential-priority

EC	CAS	Substance	PMT/vPvM hazard	Emission Index	Analytical & Monitoring Gap	Remediation Gap	Exposure level	Overall Prioritization Level
230-625-6	7226-23-5	Tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one	Potential PMT/vPvM	low	Not Monitored; analytical development feasible	No O3&AC	no detections known	Potential-priority
217-157-8	1758-73-2	Aminoiminomethanesulphinic acid	Not PMT/vPvM	high	Major monitoring gap	No O3&AC	no detections known	Lowest-priority
402-860-6	110553-27-0	4,6-bis(octylthiomethyl)-o-cresol	Not PMT/vPvM	high	Minor monitoring gap	AC only	no detections known	Lowest-priority
273-501-7	68987-63-3	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, chlorinated	Not PMT/vPvM	high	Major monitoring gap	not included	no detections known	Lowest-priority
406-080-7	83016-70-0	2-[(2-[2-(dimethylamino)ethoxy]ethyl)methylamino]ethanol	Not PMT/vPvM	high	Major monitoring gap	No O3&AC	monitored commonly, not found	Lowest-priority
500-033-5	25068-38-6	4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane	Not PMT/vPvM	very high	Not Monitored; analytical development feasible	AC only	no detections known	Lowest-priority
219-863-1	2554-06-5	2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane	Not PMT/vPvM	high	Not Monitored; analytical development feasible	Both O3&AC	no detections known	Lowest-priority
423-340-5	162881-26-7	Phenyl bis(2,4,6-trimethylbenzoyl)-phosphine oxide	Not PMT/vPvM	high	Minor monitoring gap	AC only	no detections known	Lowest-priority
201-122-9	78-51-3	Tris(2-butoxyethyl) phosphate	Not PMT/vPvM	very high	Monitored frequently	AC only	Ubiquitous, high conc	Lowest-priority
276-745-2	72629-94-8	Perfluorotridecanoic acid (PFTrDA)	Not PMT/vPvM	not REACH	not included	not included	Ubiquitous, low conc	Lowest-priority
279-259-9	79780-39-5	Perfluorododecane sulfonic acid (PFDoDS)	Not PMT/vPvM	not REACH	not included	not included	Local, low conc	Lowest-priority
206-803-4	376-06-7	Perfluorotetradecanoic acid (PFTetrA)	Not PMT/vPvM	not REACH	not included	not included	Ubiquitous, low conc	Lowest-priority
241-749-5	17766-26-6	1,3,5-triazine-2,4,6(1H,3H,5H)-trithione, trisodium salt	No data	high	Major monitoring gap	No O3&AC	no detections known	Insufficient information

11. Conclusions

The prioritization framework for PMT/vPvM substances presented here has two major applications. The first function is to prioritize PMT/vPvM substances registered under REACH for immediate follow up action. Results of the prioritization of 176 substances here, showed that 43 substances met the highest-priority category. The second function is to highlight data gaps, particularly as to which substances lack analytical methods, monitoring data, remediation methods or an assessment of the exposure level. It is of importance for PMT/vPvM substances and substances detected in drinking water sources, that these data gaps are filled. Further investigating high-priority and especially highest-priority PMT/vPvM substances with respect to risk mitigation, as well as filling key data gaps for all potential-priority to highest-priority substances, should be enacted upon by REACH registrants, regulators, researchers and the water sector.

This study utilized the 176 substances presented; however, this prioritization framework could be applied to a larger group of substances. In future studies, this prioritization framework could be applied to the 344 PMT/vPvM substances registered under REACH and detailed in Arp et al. (2023b).

The prioritization framework was developed explicitly for REACH registered substances, particularly the REACH emission likelihood category. Since the hazard classes for PMT/vPvM substances have recently been introduced in the CLP regulation (European Commission, 2022a) a variation or extension of this framework could be developed for pesticides, biocides or other substance groups not registered under REACH. Further categories could also be introduced such as the likelihood of chronic toxicity, considering the long exposure times to PMT/vPvM substances. In addition, existing categories could be modified , such as the REACH Emission Likelihood or Exposure Level by including environmental exposure modelling based parameters.

Though a large part of the prioritization framework was developed to prioritize follow-up actions for REACH registered substances that present a long term threat to the sources of our drinking water, the broader future aim of such a prioritization framework is to prevent emissions of PMT/vPvM substances to the sources of our drinking water.

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List of Annexes

Annexes A and B present supplementary information directly related to the main text of this report.

Annexes C-E present additional work that was conducted as part of project FKZ 3719 65 408.

- Annex A. PMT/vPvM hazard assessment of the 176 selected substances.
- Annex B. Analysis Methods from the monitoring study.
- Annex C. Workshop and summary of gaps
- Annex D. Overview of project dissemination activities
- Annex E. Factsheets for 10 selected PMT/vPvM substances

A PMT/vPvM assessment of the 176 substances

The German Environment Agency (UBA) began scientifically and technically developing criteria under REACH for substances considered persistent, mobile and toxic (PMT) or very persistent and very mobile (vPvM) in 2009 (Neumann and Schliebner, 2019). The European Commission (EC) stated in 2020 that they aimed to adopt the PMT/vPvM criteria for use in REACH for the identification of SVHCs and for use in the CLP Regulation as new hazard classes (European Commission, 2020). More background about the PMT/vPvM assessment can be found in Arp and Hale (2023). Table A1 presents the PMT/vPvM hazard assessment of the 176 substances following Arp and Hale (2023), which uses the criteria proposed in 2019 by UBA. In 2021 the EC published a first draft proposal for PMT/vPvM criteria as new hazard classes in the CLP Regulation (European Commission, 2021), which were similar to those included in the draft CLP amendment released September 2022 (European Commission, 2022b). These criteria are less stringent regarding mobility than the PMT/vPvM criteria proposed in 2019 by UBA, but have identical criteria for persistent (P) and very persistent (vP) and similar criteria for toxicity (T). Differences in the assessment of mobile (M) and very mobile (vM) between the 2019 criteria by and the 2021 criteria by EC are provided in Table A1 under the column "M rationale". Potential changes in the outcome of the assessment between the use of the criteria proposed in 2019 by UBA (and used in this report) and the criteria proposed in 2021 by the EC are as follows:

- vM -> M: the substance is “vM” according to the criteria proposed in 2019 by UBA, but only “M” according to the criteria proposed in 2021 by the EC.
- M -> not M: the substance is “M” according to the criteria proposed in 2019 by UBA, but only "not M" according to the criteria proposed in 2021 by the EC.
- M -> potential M/vM: the substance is “M” based on weight-of-evidence assessment and using the criteria proposed in 2019 by UBA, but the same weight-of-evidence is insufficient to conclude “M” or “not M” using the criteria proposed in 2021 by the EC; and consequently, only the category “potential M/vM” can be assigned.

For further information about how the PMT/vPvM assessment was conducted, including for these 176 substances, please refer to Arp and Hale (2023).

Table A1. Outcome of the PMT/vPvM hazard assessment for the 176 substances using the updated guideline (Arp and Hale, 2023)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
108-78-1	203-615-4	Melamine	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	vP: No degradation in a OECD TG 309 (Hofman-Caris and Claßen, 2020). Calculated half-life melamine in water: >10.000 days; measured max t1/2.max(d) in soil = 913 days (eChemPortal database)	UBA: vM EC: vM exp log Koc=1.1	STOTE RE (nephrotoxic in combination with cyanuric acid)T
80-08-0	201-248-4	Dapsone	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	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)	UBA: vM EC: vM exp log Koc=1.8	(EDC_UnderAssess)(Pro.S.P._ED)
37640-57-6	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)	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	vP: same as melamine (CAS RN 108-78-1)	UBA: vM EC: vM exp log Koc=1.1	STOTE RE (nephrotoxic in combination with cyanuric acid)T
3622-84-2	222-823-6	N-butylbenzenesulphonamide	Arp and Hale (2019)	vPvM	vPvM & PMT	vP: measured max t1/2.max(d):w=985(vP);s=n.d.;sed=n.d.	UBA: vM EC: M min Dow=2.0 (2a)	Cramer Cl.III
95-50-1	202-425-9	1,2-dichlorobenzene	Arp and Hale (2019)	PMT	vPvM	vP: measured max t1/2.max(d):w=n.d.;s=191(vP);sed=n.d.	UBA: M EC: Pot.M/vM min Dow=3.3 (2a)	(SINlist:1,2-dichlorobenzene is very toxic to aquatic species, it is potentially very persistant and very bioaccumulative and has been detected in environmental and human samples. Therefore ChemSec considers this to be of equivalent level of concern according to the 57f criteria.)
123-91-1	204-661-8	1,4-dioxane	Arp and Hale (2019)	vPvM & PMT	PMT	vP: No degradation in a OECD TG 309 (Hofman-Caris and Claßen, 2020), calculated half-life 1,4-dioxane: >10.000 days. No significant biodegradation in 301F test.	UBA: vM EC: vM min Dow=-0.4 (2a)	(Carc2)
126-86-3	204-809-1	2,4,7,9-tetramethyldec-5-yne-4,7-diol	Arp and Hale (2019)	PM	PMT	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)	UBA: M EC: Not M exp log Koc=3.2	Cramer Cl.III
288-88-0	206-022-9	1,2,4-triazole	Arp and Hale (2019)	PMT	PMT	P: All biodegradation results in 301A and 302B tests imply no	UBA: vM EC: vM min Dow=-0.7 (2a)	(Rep2)(EDC_UnderAssess)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						significant biodegradation. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)		
834-12-8	212-634-7	Ametryn	Arp and Hale (2019)	vPvM & PMT	PMT	vP: measured max t1/2.max(d):w=n.d.;s=150(P);sed=1 780(vP)	UBA: vM EC: M exp log Koc=2.1	(Ecotox_PMT2019)(Ecotox_Envirotox)
2855-13-2	220-666-8	3-aminomethyl-3,5,5-trimethylcyclohexylamine	Arp and Hale (2019)	PMT	PMT	P: No significant biodegradation in 301A tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: vM EC: vM min Dow=-6.6 (2a)	(Pro.S.P._ED)
51-28-5	200-087-7	2,4-dinitrophenol	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: this is not persistent in soil, but data in some REACH dossiers suggests the vP criteria in fresh water is met. Further, evidence of persistency is its discovery in monitoring studies (UBA, 2019), consistent indications of P across all tested QSARs, and this substances was also considered prioritized by Nödler et al. (2019) as resistent to drinking water treatment.	UBA: vM EC: vM exp log Koc=1.1	(DNEL)(Pro.S.P._ED)
56-23-5	200-262-8	Carbon tetrachloride	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 172d, weight-of-evidence by discovery in monitoring studies (UBA, 2019), and consistent indications of P across tested QSARs	UBA: vM EC: vM exp log Koc=1.9	(Carc2)
56-93-9	200-300-3	Benzyltrimethylammonium chloride	Arp and Hale (2019)	vPvM	vPvM & PMT	Potential P/vP++: Reach dossiers all conclude not P, yet screening tests are ambiguous showing both P and not P, QSARs are consistnently pointing to P, and this substance seems frequent in monitoring data of bank filtrate and drinking water	UBA: vM EC: vM min Dow=-2.2 (2c)	Cramer Cl.III
67-66-3	200-663-8	Chloroform	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 55d, weight-of-evidence by discovery in monitoring studies (UBA, 2019), available QSARs and no biodeg. observed in majority of biodegradation screen tests e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: M exp log Koc=2.0	(Carc2)(Rep2)
75-35-4	200-864-0	1,1-dichloroethylene	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 36d, weight-of-evidence by discovery in monitoring studies (UBA, 2019), available QSARs and no biodeg. observed in majority of biodegradation screen tests e.g. OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: vM EC: vM exp log Koc=1.4	(Carc2)
75-71-8	200-893-9	Dichlorodifluoromethane	Arp and Hale (2019)	vPvM	vPvM	Potential P/vP++: apolar PFAS, estimated t1/2 (error factor 10) = 70d, weight-of-	UBA: vM EC: vM exp log Koc=1.2	Cramer Cl.III

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						evidence by discovery in monitoring studies (UBA, 2019), and consistent indications of P across tested QSARs		
76-05-1	200-929-3	Trifluoroacetic acid	Arp and Hale (2019)	vPvM	vPvM	Potential P/vP++: TFA, estimated t1/2 (error factor 10) = 53d, weight-of-evidence by discovery in monitoring studies (UBA, 2019), available QSARs and no biodeg. observed in majority of biodegradation screen tests e.g. OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: vM EC: vM exp log Koc=-0.8	Cramer Cl.III
78-51-3	201-122-9	Tris(2-butoxyethyl) phosphate	Arp and Hale (2019)	Not PMT/vPvM	vPvM	Not P: Not P (readily biodeg): EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Cited as Directive 84/449/EEC, C.5;EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Cited as Directive 84/449/EEC, C.5;EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Cited as Directive 92/69/EEC, C.4-C;OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) 1992;EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Cited as Directive 92/69/EEC, C.4-C;OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) 1992	UBA: vM EC: M exp log Koc=2.5	Cramer Cl.III
78-87-5	201-152-2	1,2-dichloropropane	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential 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.	UBA: vM EC: vM exp log Koc=1.7	(Carc1ab)(SINlist:Classified CMR according to Annex VI of Regulation 1272/2008)
95-14-7	202-394-1	Benzotriazole	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	vP: No degradation in a OECD TG 309 (Hofman-Caris and Claßen, 2020). Calculated half-life was 1Hbenzotriazole: >10.000 days and majority of biodegradation screen tests, e.g. OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: vM EC: vM exp log Koc=1.5	(EDC_UnderAssess)
97-39-2	202-577-6	1,3-di-o-tolylguanidine	Arp and Hale (2019)	vPvM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 236d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM min Dow=-4.0 (2a)	(Carc_MinorOpinion)Cramer Cl.III
102-06-7	203-002-1	1,3-diphenylguanidine	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 194d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability:	UBA: vM EC: M exp log Koc=2.5	(Rep2)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)		
106-93-4	203-444-5	1,2-dibromoethane	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 30d, weight-of-evidence by discovery in monitoring studies (UBA, 2019), and consistent indications of P across tested QSARs	UBA: vM EC: vM exp log Koc=0.1	(Carc1ab)(SINlist:Classified CMR according to Annex VI of Regulation 1272/2008)(Pro.S.P._ED)
108-20-3	203-560-6	Diisopropyl ether	Arp and Hale (2019)	vPvM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 59d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: vM EC: M min Dow=1.6 (2a)	Cramer Cl.III
108-80-5	203-618-0	Cyanuric acid	Arp and Hale (2019)	vPvM & PMT	vPvM	vP: vP Assessment for EC 253-575-7, consistent indicators of P, montored extensively in the environment (Schulze et al. 2019) and in this study in bank filtrate, raw water and drinking water	UBA: vM EC: vM exp log Koc=1.7	STOTE RE (nephrotoxic in combination with melamine)T
108-90-7	203-628-5	Chlorobenzene	Arp and Hale (2019)	vPvM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 28d, weight-of-evidence by discovery in monitoring studies (UBA, 2019), and consistent indications of P across tested QSARs	UBA: vM EC: M exp log Koc=2.5	Cramer Cl.III
119-61-9	204-337-6	Benzophenone	Arp and Hale (2019)	vPvM & PMT	PMT	Potential P/vP++: P discussion has no current consensus, REACH dossier evaluations favour screening tests showing readily biodegradation, but results from screening tests are wide spread. There is more discussion on this from IARC-WHO (https://monographs.iarc.who.int/wp-content/uploads/2018/06/mono101-007.pdf) . From this study, estimated t1/2 (error factor 10) = 35d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	UBA: vM EC: M exp log Koc=2.7	(SINlist:For Benzophenone carcinogenic effects have been reported. It is potentially persistent and has been found in the environment. Its derivates are potential endocrine disruptors.)(Pro.S.P._ED)
121-47-1	204-473-6	3-aminobenzenesulphonic acid	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 119d, found in several water samples in Schulze et al. (2019) and consistent indications of P across tested QSARs	UBA: vM EC: vM min Dow=-2.8 (2a)	(Pro.S.P._ED)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
121-82-4	204-500-1	Perhydro-1,3,5-trinitro-1,3,5-triazine	Arp and Hale (2019)	vPvM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 72d, weight-of-evidence by discovery in monitoring studies (UBA, 2019), and consistent indications of P across tested QSARs. REACH dossiers claim not P due to anaerobic degradation or alkaline hydrolysis, but these are rare environments for RDX contamination (Lapointe et al., 2017).	UBA: vM EC: M exp log Koc=2.0	Cramer Cl.III
156-60-5	205-860-2	trans-dichloroethylene	Arp and Hale (2019)	vPvM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 36d, weight-of-evidence by discovery in monitoring studies (UBA, 2019), and consistent indications of P across tested QSARs	UBA: vM EC: M min Dow=1.9 (2a)	Cramer Cl.III
280-57-9	205-999-9	1,4-diazabicyclooctane	Arp and Hale (2019)	PM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 57d, found in several water samples in Schulze et al. (2019) and consistent indications of P across tested QSARs	UBA: M EC: Not M exp log Koc=3.4	Cramer Cl.III
541-73-1	208-792-1	1,3-dichlorobenzene	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 131d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: M exp log Koc=2.4	(Pro.S.P._ED)
1493-13-6	216-087-5	Trifluoromethanesulphonic acid	Arp and Hale (2019)	vPvM	vPvM	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 67d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-E (Determination of the "Ready" Biodegradability - Closed Bottle Test);EU Method C.4-E (Determination of the "Ready" Biodegradability - Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: vM EC: vM exp log Koc=-0.2	Cramer Cl.III
5165-97-9	225-948-4	Sodium 2-methyl-2-[(1-oxoallyl)amino]propanesulphonate	Arp and Hale (2019)	vPvM	vPvM	Potential P/vP++: estimated t1/2 (error factor 10) = 33d, found in several water samples in Schulze et al. (2019) and consistent indications of P across tested QSARs	UBA: vM EC: vM min Dow=-2.7 (2b)	Cramer Cl.III
13674-87-8	237-159-2	Tris[2-chloro-1-(chloromethyl)ethyl] phosphate	Arp and Hale (2019)	vPvM & PMT	PMT	vP: estimated t1/2 (error factor 10) = 617d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.6 (Degradation: Chemical Oxygen Demand);EU Method C.5 (Degradation: Biochemical Oxygen Demand);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);EU Method C.6 (Degradation: Chemical Oxygen Demand);EU Method C.5 (Degradation: Biochemical Oxygen Demand);OECD Guideline 301 B (Ready Biodegradability: CO2	UBA: vM EC: M exp log Koc=2.2	(Carc2)(SINlist:This substance has been detected in children who are exposed to the chemical through house dust. It is a suspected carcinogen. The substance shows experimental and estimated P and T properties. It is considered to be of equivalent level of concern.)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						Evolution Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 302 C (Inherent Biodegradability: Modified MITI Test (II));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))		
52556-42-0	258-004-5	Sodium 3-(allyloxy)-2-hydroxypropanesulphonate	Arp and Hale (2019)	vPvM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 34d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM min Dow=-1.5 (2a)	Cramer Cl.III
6331-96-0	700-413-2	2-amino-4,5-dichlorobenzenesulfonic acid	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 334d, found in several water samples in Schulze et al. (2019) and consistent indications of P across tested QSARs	UBA: vM EC: vM min Dow=-1.0 (2b)	(Pro.S.P._ED)
29420-49-3	206-793-1	1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulphonic acid	Arp and Hale (2019)	vPvM & PMT	vPvM	vP: short-chain PFAS, on SVHC list - vPvB substance	UBA: vM EC: vM exp log Koc=1.4	(SVHC:Equivalent level of concern having probable serious effects to human health (Article 57(f) - human health)#Equivalent level of concern having probable serious effects to the environment (Article 57(f) - environment))
75-01-4	200-831-0	Chloroethylene	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 24d, weight-of-evidence by discovery in monitoring studies (UBA, 2019), and consistent indications of P across tested QSARs	UBA: vM EC: vM exp log Koc=0.9	(Carc1ab)(SINlist:Classified CMR according to Annex VI of Regulation 1272/2008)
81-07-2	201-321-0	1,2-benzisothiazol-3(2H)-one 1,1-dioxide	Arp and Hale (2019)	PM	vPvM & PMT	Potential P/vP++: the reported t1/2 in soil is 30d; however, it is found in several water samples in Schulze et al. (2019) and consistent indications of P across tested QSARs. Thus it is considered sufficiently P in the environment	UBA: M EC: Not M exp log Koc=3.3	Cramer Cl.III
78-67-1	201-132-3	2,2'-dimethyl-2,2'-azodipropiononitrile	Arp and Hale (2019)	vPvM	vPvM	vP: measured max t1/2.max(d):w=950(vP);s=n.d.;sed=n.d.	UBA: vM EC: vM min Dow=1.1 (2a)	Cramer Cl.III
91-76-9	202-095-6	6-phenyl-1,3,5-triazine-2,4-diyldiamine	Arp and Hale (2019)	vPvM	vPvM	vP: No significant biodegradation in 301C and E tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: vM EC: vM exp log Koc=1.4	Cramer Cl.III
121-03-9	204-445-3	4-nitrotoluene-2-sulphonic acid	Arp and Hale (2019)	vPvM	vPvM	vP: No significant biodegradation in 301E and C tests. The PBT assessment evaluates the substance to be persistent. Therefore	UBA: vM EC: vM min Dow=-1.5 (2a)	(PBT_MinorityOpinion)Cramer Cl.III

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						this substance is assessed to be persistent in water. (Berger et al. 2018)		
382-28-5	206-841-1	2,2,3,3,5,5,6,6-octafluoro-4-(trifluoromethyl)morpholine	Arp and Hale (2019)	PM	vPvM	vP: short-chain PFAS, REACH dossier P evaluatin (2020), SINlist evaluation (2019)	UBA: M EC: Not M exp log Koc=3.6	Cramer Cl.III
115-27-5	204-077-3	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	vP: estimated t1/2 (error factor 10) = 2 923d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 302 C (Inherent Biodegradability: Modified MITI Test (II));OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 302 C (Inherent Biodegradability: Modified MITI Test (II));OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 302 C (Inherent Biodegradability: Modified MITI Test (II));OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 302 C (Inherent Biodegradability: Modified MITI Test (II));OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	UBA: vM EC: vM min Dow=-1.6 (2a)	(PBT_UnderAssess)
556-88-7	209-143-5	1-nitroguanidine	Arp and Hale (2019)	Potential PMT/vPvM	vPvM	Pot.P/vP: estimated t1/2 (error factor 10) = 28d, and consistency across all tested QSARs	UBA: vM EC: vM min Dow=-3.2 (2a)	Cramer Cl.III
593-85-1	209-813-7	Diguanidinium carbonate	Arp and Hale (2019)	Potential PMT/vPvM	vPvM	Pot.P/vP: weight-of-evidence (this study) based on all known QSARs and no biodeg. observed in majority of biodegradation screen tests, e.g. EU Method C.4-B (Determination of the "Ready" Biodegradability - Modified OECD Screening Test) according to EEC guideline 92/69 of December 29, 1992;EU Method C.4-B (Determination of the "Ready" Biodegradability - Modified OECD Screening Test) according to EEC guideline 92/69 of December 29, 1992;OECD Guideline 301 E (Ready biodegradability: Modified OECD Screening Test) (1992);OECD Guideline 301 E (Ready biodegradability: Modified OECD Screening Test) (1992)	UBA: vM EC: vM min Dow=-1.4 (2a)	-
3033-62-3	221-220-5	N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)	Arp and Hale (2019)	vPvM	vPvM	vP: All biodegradation results in 301F and 302B imply no significant biodegradation. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: vM EC: vM min Dow=-5.5 (2a)	Cramer Cl.III
41583-09-9	203-615-4	Melamine	Arp and Hale (2019)	vPvM & PMT	vPvM	vP: No degradation in a OECD TG 309 (Hofman-Caris and Claßen, 2020). Calculated half-life melamine in water: >10.000 days; measured max t1/2.max(d) in soil = 913 days (eChemPortal database)	UBA: vM EC: vM exp log Koc=1.1	STOTE RE (nephrotoxic in combination with cyanuric acid)T

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
68987-63-3	273-501-7	Copper, [29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-, chlorinated	Arp and Hale (2019)	Not PMT/vPvM	vPvM	Pot.P/vP: IFS QSAR results in P, no biodeg. observed in other QSARs or majority of biodegredation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	UBA: Not M EC: Not M min Dow=6.7 (2a)	-
73037-34-0	277-242-0	Disodium oxybis[methylbenzenesulphonate]	Arp and Hale (2019)	vPvM	vPvM	vP: No significant biodegradation in 301F and C tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: vM EC: vM min Dow=-1.9 (2b)	Cramer Cl.III
90268-24-9	290-824-9	Butanamide, 2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-, N,N'-bis(4-chloro-2,5-dimethoxyphenyl and 2,4-xylyl) derivs.	Arp and Hale (2019)	vPvM	vPvM	vP: estimated t1/2 (error factor 10) = 12 894d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM min Dow=1.3 (2a)	Cramer Cl.III
83016-70-0	406-080-7	2-[(2-[2-(dimethylamino)ethoxy]ethyl)methylamino]ethanol	Arp and Hale (2019)	Not PMT/vPvM	vPvM	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)	UBA: Not M EC: Not M exp log Koc=4.1	Cramer Cl.III
1671-49-4	430-550-0	4-mesyl-2-nitrotoluene	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	vP: All biodegradation results in 301F and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: vM EC: M exp log Koc=2.3	(Rep2)
3030-47-5	221-201-1	Bis(2-dimethylaminoethyl)(methyl)amine	Arp and Hale (2019)	vPvM	vPvM	vP: All biodegradation results in 301C and E and 302B imply no significant biodegradation. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: vM EC: vM min Dow=-7.2 (2a)	Cramer Cl.III
107-46-0	203-492-7	Hexamethyldisiloxane	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	vP: measured max t1/2.max(d):w=n.d.;s=408(vP);sed=192(vP)	UBA: vM EC: M exp log Koc=2.9	(PBT_UnderAssess)(Ecotox_PMT2019)
22042-96-2	244-751-4	[[(phosphonomethyl)imino]bis[(ethylenenitrilo)bis(methylene)]]tetrakisphosphonic acid, sodium salt	Arp and Hale (2019)	vPvM	vPvM	vP: estimated t1/2 (error factor 10) = 4 685d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 E (Ready biodegradability:	UBA: vM EC: vM min Dow=-16.3 (2b)	(PBT_MinorityOpinion)Cramer Cl.III

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						Modified OECD Screening Test);OECD Guideline 301 E (Ready biodegradability: Modified OECD Screening Test)		
34690-00-1	252-156-6	[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methylene)]]tetrakisphosphonic acid	Arp and Hale (2019)	Potential PMT/vPvM	vPvM & PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 5 690d, and BIOWIN screen tool as recommended in the PBT guideline	UBA: vM EC: vM min Dow=-15.9 (2b)	Cramer Cl.III
61792-09-4	263-212-4	Pentasodium pentahydrogen [[(phosphonatomethyl)imino]bis[ethane-2,1-diylnitrilobis(methylene)]]tetrakisphosphonate	Arp and Hale (2019)	vPvM	vPvM	vP: estimated t1/2 (error factor 10) = 4 685d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 E (Ready biodegradability: Modified OECD Screening Test);OECD Guideline 301 E (Ready biodegradability: Modified OECD Screening Test)	UBA: vM EC: vM min Dow=-16.3 (2b)	(PBT_MinorityOpinion)Cramer Cl.III
129909-90-6	603-373-3	4-amino-N-(1,1-dimethylethyl)-4,5-dihydro-3-(1-methylethyl)-5-oxo-1H-1,2,4-triazole-1-carboxamide	Arp and Hale (2019)	vPvM	vPvM	vP: 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)	UBA: vM EC: vM exp log Koc=1.4	-
2312-35-8	219-006-1	Propargite	Arp and Hale (2019)	PMT	PMT	vP: measured max t1/2.max(d):w=128(vP);s=234(vP);sed=n.d.	UBA: M EC: Not M exp log Koc=3.9	(Carc2)(EDC_UnderAssess)(Ecotox_PMT2019)(Ecotox_Envirotox)
12108-13-3	235-166-5	Tricarbonyl(methylcyclopentadienyl)manganese	Arp and Hale (2019)	PM	PMT	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)	UBA: M EC: Not M exp log Koc=3.4	-
87-62-7	201-758-7	2,6-xylidine	Arp and Hale (2019)	PMT	PMT	P: No significant biodegradation in 301F tests. 302B tests not reliable. Registrant evaluates this substance to be persistent. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: vM EC: vM exp log Koc=1.6	(Carc2)
123-30-8	204-616-2	4-aminophenol	Arp and Hale (2019)	PMT	PMT	P: No significant biodegradation in 301C tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: vM EC: vM exp log Koc=0.5	(Mut2)
622-40-2	210-734-5	2-morpholinoethanol	Arp and Hale (2019)	PM	PMT	P: No significant biodegradation in 302B test. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: vM EC: vM exp log Koc=1.3	Cramer Cl.III
2226-96-2	218-760-9	4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	Arp and Hale (2019)	PM	PMT	P: No significant biodegradation in 301A tests. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: M EC: Not M exp log Koc=3.2	Cramer Cl.III
4065-45-6	223-772-2	Sulisobenzone	Arp and Hale (2019)	PMT	PMT	P: All biodegradation results in 301F and 302B tests imply no significant biodegradation. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: vM EC: vM exp log Koc=2.0	(Pro.S.P._ED)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
5281-09-4	226-109-5	Calcium 3-hydroxy-4-[(4-methyl-2-sulphonatophenyl)azo]-2-naphthoate	Arp and Hale (2019)	PM	PMT	P: Biodegradation results in 301 C test <20% and persistence due to PBT assessment. Therefore this substance is assessed to be persistent in water. (Berger et al. 2018)	UBA: M EC: Not M exp log Koc=3.6	Cramer Cl.III
13472-08-7	236-740-8	2,2'-azobis[2-methylbutyronitrile]	Arp and Hale (2019)	vPvM	PMT	vP: SINList vPvM (Chemsec, 2019), "No significant biodegradation in 301D test. The PBT assessment evaluates the substance to be persistent. Therefore this substance is assessed to be persistent in water."	UBA: vM EC: M min Dow=2.1 (2a)	Cramer Cl.III
37971-36-1	253-733-5	2-phosphonobutane-1,2,4-tricarboxylic acid	Arp and Hale (2019)	PM	PMT	P: measured max t1/2.max(d):w=n.d.;s=142(P);sed=n.d.	UBA: vM EC: vM min Dow=-19.2 (2b)	Cramer Cl.III
98362-33-5	500-281-4	2,3-Epoxypropyl neodecanoate, oligomeric reaction products with toluene-4-sulfonic acid	Arp and Hale (2019)	Potential PMT/vPvM	PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 218d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	UBA: vM EC: M exp log Koc=2.8	Cramer Cl.III
67-68-5	200-664-3	Dimethyl sulfoxide	Arp and Hale (2019)	PM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 22d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: vM EC: vM exp log Koc=-2.1	Cramer Cl.III
75-91-2	200-915-7	tert-butyl hydroperoxide	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 31d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: vM EC: vM exp log Koc=-0.3	(Mut2)
76-03-9	200-927-2	Trichloroacetic acid	Arp and Hale (2019)	vPvM & PMT	vPvM	vP: concluded in the dossier with vP assessment, soil half-life found at 120 half days	UBA: vM EC: vM exp log Koc=0.0	(Ecotox_ NOEC = 8.6 µg/L to Algae)T
77-73-6	201-052-9	3a,4,7,7a-tetrahydro-4,7-methanoindene	Arp and Hale (2019)	PM	PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 26d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: M exp log Koc=2.5	Cramer Cl.III

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
78-40-0	201-114-5	Triethyl phosphate	Arp and Hale (2019)	vPvM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 20d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM exp log Koc=-0.3	Cramer Cl.III
80-15-9	201-254-7	α,α-dimethylbenzyl hydroperoxide	Arp and Hale (2019)	PM	PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 40d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) (1981);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) (1981)	UBA: vM EC: M min Dow=1.6 (2a)	Cramer Cl.III
80-43-3	201-279-3	Bis(α,α-dimethylbenzyl) peroxide	Arp and Hale (2019)	PMT	PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 139d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: M EC: Not M exp log Koc=4.0	(PBT_UnderAssess)
80-51-3	201-286-1	4,4'-oxydi(benzenesulphonohydrazide)	Arp and Hale (2019)	PM	vPvM & PMT	P: estimated t1/2 (error factor 10) = 519d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM min Dow=1.2 (2a)	Cramer Cl.III
88-72-2	201-853-3	2-nitrotoluene	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 66d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM exp log Koc=1.9	(Carc1ab)(Mut1)(Rep2)(SINlist:Classified CMR according to Annex VI of Regulation 1272/2008)
88-73-3	201-854-9	1-chloro-2-nitrobenzene	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 115d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 D	UBA: vM EC: vM exp log Koc=2.0	(Carc_BroadConsensus)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						(Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)		
97-74-5	202-605-7	Tetramethylthiuram monosulphide	Arp and Hale (2019)	PM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 98d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	UBA: vM EC: vM min Dow=1.2 (2a)	Cramer Cl.III
99-99-0	202-808-0	4-nitrotoluene	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 66d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: M min Dow=2.4 (2a)	(Pro.S.P._ED)
100-43-6	202-852-0	4-vinylpyridine	Arp and Hale (2019)	Potential PMT/vPvM	vPvM & PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 33d, and consistency across all tested QSARs	UBA: vM EC: vM exp log Koc=0.5	Cramer Cl.III
100-61-8	202-870-9	N-methylaniline	Arp and Hale (2019)	PM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 44d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	UBA: vM EC: vM exp log Koc=1.7	Cramer Cl.III
100-97-0	202-905-8	Methenamine	Arp and Hale (2019)	vPvM	vPvM & PMT	vP: No degradation in a OECD TG 309 (Hofman-Caris and Claßen, 2020), calculated half-life urotropin: >128 days. EU Method C.4-E (Determination of the "Ready" Biodegradability - Closed Bottle Test);EU Method C.4-E (Determination of the "Ready" Biodegradability - Closed Bottle Test);EU Method C.6 (Degradation: Chemical Oxygen Demand) 1984;EU Method C.6 (Degradation: Chemical Oxygen Demand) 1984;OECD Guideline 301 A (Ready Biodegradability: DOC Die Away Test)	UBA: vM EC: vM min Dow=-6.6 (2a)	Cramer Cl.III
102-08-9	203-004-2	1,3-diphenyl-2-thiourea	Arp and Hale (2019)	PM	PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 46d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	UBA: vM EC: vM exp log Koc=1.6	Cramer Cl.III
107-66-4	203-509-8	Dibutyl hydrogen phosphate	Arp and Hale (2019)	vPvM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 25d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-E (Determination of the "Ready"	UBA: vM EC: vM exp log Koc=0.5	-

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						Biodegradability - Closed Bottle Test) Cited as RG Directive 79/831/ Annex V;EU Method C.4-E (Determination of the "Ready" Biodegradability - Closed Bottle Test) Cited as RG Directive 79/831/ Annex V;OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)		
108-42-9	203-581-0	3-chloroaniline	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: From data in the dossier, the water half-life is near the criteria for P, and the sediment vP criteria is met in a water-sediment system,	UBA: vM EC: vM exp log Koc=1.6	(Ecotox_PMT2019)
109-01-3	203-639-5	1-methylpiperazine	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 29d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: vM EC: M exp log Koc=2.9	(StotRE_MinorOpinion)
119-64-2	204-340-2	1,2,3,4-tetrahydronaphthalene	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 41d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: vM EC: M exp log Koc=2.7	(Pro.S.P._ED)
345-92-6	206-466-3	Bis(4-fluorophenyl) ketone	Arp and Hale (2019)	PMT	PMT	vP: estimated t1/2 (error factor 10) = 1 369d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	UBA: M EC: Pot.M/vM min Dow=3.4 (2a)	(Pro.S.P._ED)
482-89-3	207-586-9	2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	Arp and Hale (2019)	PM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 189d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: M exp log Koc=2.9	Cramer Cl.III
584-84-9	209-544-5	4-methyl-m-phenylene diisocyanate	Arp and Hale (2019)	Potential PMT/vPvM	PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 44d, and consistency across all tested QSARs	UBA: vM EC: M exp log Koc=2.1	(Carc2)(STOTRE_1_2)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
599-61-1	209-967-5	3,3'-sulphonyldianiline	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 343d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM exp log Koc=1.8	(Pro.S.P._ED)
1758-73-2	217-157-8	Aminoiminomethanesulphinic acid	Arp and Hale (2019)	Not PMT/vPvM	vPvM & PMT	Not P: Not P (readily biodeg): OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM min Dow=-1.0 (2b)	Cramer Cl.III
1761-71-3	217-168-8	4,4'-methylenebis(cyclohexylamine)	Arp and Hale (2019)	Potential PMT/vPvM	vPvM & PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 26d, and consistency across all tested QSARs	UBA: vM EC: vM min Dow=-4.7 (2a)	(Pro.S.P._ED)
2440-22-4	219-470-5	2-(2H-benzotriazol-2-yl)-p-cresol	Arp and Hale (2019)	Potential PMT/vPvM	PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 54d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	UBA: Pot.M/vM EC: Not M min Dow=4.2 (2a)	(Pro.S.P._ED)
2554-06-5	219-863-1	2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane	Arp and Hale (2019)	Not PMT/vPvM	PMT	Potential P/vP++: The P conclusion remains controversial; currently D4 is being considered as SVHC based on vPvB and PMT properties (https://echa.europa.eu/documents/10162/50488161-546d-2048-828a-b6d9ef29f310)	UBA: Not M EC: Not M exp log Koc=4.7	(Ecotox_PMT2019)
284-95-7, 2680-03-7		N,N-dimethylacrylamide	Arp and Hale (2019)	PM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 15d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM exp log Koc=1.3	Cramer Cl.III
3006-86-8	221-111-2	Cyclohexylidenebis[tert-butyl] peroxide	Arp and Hale (2019)	PM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 157d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) 31st July 1992;OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) 17th July 1992;EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) 31st July 1992;OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) 17th July 1992	UBA: vM EC: M exp log Koc=2.7	Cramer Cl.III
3468-63-1	222-429-4	1-[(2,4-dinitrophenyl)azo]-2-naphthol	Arp and Hale (2019)	Potential PMT/vPvM	PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 1 152d, and BIOWIN screen tool as recommended in the PBT guideline	UBA: vM EC: M min Dow=2.5 (2a)	(Ecotox_PMT2019)(Pro.S.P._ED)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
3710-84-7	223-055-4	N,N-diethylhydroxylamine	Arp and Hale (2019)	PM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 20d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	UBA: vM EC: M min Dow=-0.3 (2c)	-
5026-74-4	225-716-2	p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	Arp and Hale (2019)	PM	vPvM & PMT	P: estimated t1/2 (error factor 10) = 415d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) July 17, 1992;EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) July 17, 1992	UBA: vM EC: vM exp log Koc=1.9	Cramer Cl.III
6674-22-2	229-713-7	1,8-diazabicyclo[5.4.0]undec-7-ene	Arp and Hale (2019)	Potential PMT/vPvM	vPvM & PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 27d, and consistency across all tested QSARs	UBA: vM EC: vM min Dow=-9.8 (2a)	Cramer Cl.III
6864-37-5	229-962-1	2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)	Arp and Hale (2019)	Potential PMT/vPvM	vPvM & PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 37d, and consistency across all tested QSARs	UBA: vM EC: M exp log Koc=2.6	(EDC_UnderAssess)(Pro.S.P._ED)
7226-23-5	230-625-6	Tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one	Arp and Hale (2019)	Potential PMT/vPvM	vPvM & PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 29d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 E (Ready biodegradability: Modified OECD Screening Test);OECD Guideline 301 E (Ready biodegradability: Modified OECD Screening Test)	UBA: vM EC: vM min Dow=0.1 (2a)	(Rep2)
25321-09-9	246-835-6	Diisopropylbenzene	Arp and Hale (2019)	Potential PMT/vPvM	PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 48d, and consistency across all tested QSARs	UBA: M EC: Not M exp log Koc=3.8	-
26471-62-5	209-544-5	m-tolylidene diisocyanate	Arp and Hale (2019)	Potential PMT/vPvM	PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 44d, and consistency across all tested QSARs	UBA: vM EC: M exp log Koc=2.1	(Carc2)(STOTRE_1_2)
38083-17-9	253-775-4	Climbazole	Arp and Hale (2019)	PMT	PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 95d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	UBA: M EC: Not M exp log Koc=3.8	(EDC_UnderAssess)(Ecotox_PMT2019)
53988-10-6	258-904-8	1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione	Arp and Hale (2019)	Potential PMT/vPvM	vPvM & PMT	Pot.P/vP: IFS QSAR results in P, no biodeg. observed in other QSARs or majority of biodegredation screen tests, e.g. OECD Guideline 301 C	UBA: vM EC: vM exp log Koc=1.9	(Rep_BroadConsensus)(EDC_UnderAssess)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						(Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))		
68937-41-7	273-066-3	Phenol, isopropylated, phosphate (3:1)	Arp and Hale (2019)	PM	PMT	P: estimated t1/2 (error factor 10) = 504d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EPA OPPTS 835.3110 (Ready Biodegradability);EPA OPPTS 835.3110 (Ready Biodegradability);EU Method C.4-E (Determination of the "Ready" Biodegradability - Closed Bottle Test);EU Method C.4-E (Determination of the "Ready" Biodegradability - Closed Bottle Test);OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test)	UBA: M EC: Not M exp log Koc=3.4	Cramer Cl.III
71604-74-5	275-662-9	m-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline	Arp and Hale (2019)	PM	vPvM & PMT	P: estimated t1/2 (error factor 10) = 415d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EPA OPPTS 835.3110 (Ready Biodegradability);EPA OPPTS 835.3110 (Ready Biodegradability);EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	UBA: vM EC: vM exp log Koc=1.9	Cramer Cl.III
71868-10-5	400-600-6	2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 214d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	UBA: vM EC: M exp log Koc=2.5	(SVHC:Toxic for reproduction (Article 57c))(Rep1)(EDC_UnderAssess)(SI Nlist:Classified CMR according to Annex VI of Regulation 1272/2008)
110553-27-0	402-860-6	4,6-bis(octylthiomethyl)-o-cresol	Arp and Hale (2019)	Not PMT/vPvM	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 53d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.5 (Degradation: Biochemical Oxygen Demand);EU Method C.5 (Degradation: Biochemical Oxygen Demand);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	UBA: Not M EC: Not M min Dow=10.0 (2a)	(Ecotox_PMT2019)
27955-94-8	405-800-7	4,4',4''-(ethan-1,1,1-triyl)triphenol	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 73d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Annex V;OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);EU	UBA: vM EC: M exp log Koc=2.2	(Pro.S.P._ED)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Annex V;OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)		
74091-64-8	411-280-2	2,5-bis-isocyanatomethyl-bicyclo[2.2.1]heptane	Arp and Hale (2019)	vPvM & PMT	vPvM & PMT	Potential P/vP++: estimated t1/2 (error factor 10) = 38d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM min Dow=1.3 (2a)	(STOTRE_1_2)
162881-26-7	423-340-5	Phenyl bis(2,4,6-trimethylbenzoyl)-phosphine oxide	Arp and Hale (2019)	Not PMT/vPvM	PMT	vP: estimated t1/2 (error factor 10) = 614d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test);EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test);EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test);EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test);EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test)	UBA: Not M EC: Not M min Dow=5.8 (2a)	(Ecotox_PMT2019)
94239-04-0	428-100-3	2-fluoro-6-trifluoromethylpyridine	Arp and Hale (2019)	Potential PMT/vPvM	vPvM & PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 1 086d, and BIOWIN screen tool as recommended in the PBT guideline	UBA: vM EC: vM exp log Koc=1.7	Cramer Cl.III
25068-38-6	500-033-5	4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane	Arp and Hale (2019)	Not PMT/vPvM	vPvM & PMT	no conclusion/data: only limited QSAR data, estimated t1/2 (error factor 10) = 29d	UBA: vM EC: M exp log Koc=2.6	(SVHC:Toxic for reproduction (Article 57c)#Endocrine disrupting properties (Article 57(f) - environment)#Endocrine disrupting properties (Article 57(f) - human health))(Rep1)(EDC_UnderAssess)(SINlist:Bisphenol A is classified as being toxic to reproduction and has been identified as an SVHC due to its endocrine disrupting properties for human health and the environment.)(Pro.S.P._ED)
1112-39-6	214-189-4	Dimethoxydimethylsilane	Arp and Hale (2019)	Potential PMT/vPvM	vPvM & PMT	Pot.P/vP: estimated t1/2 (error factor 10) = 32d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test);OECD Guideline 310 (Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)	UBA: vM EC: vM exp log Koc=-0.7	Cramer Cl.III

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
90076-65-6	415-300-0	Lithium bis(trifluoromethylsulfonyl)imide	short-chain PFAS-REACH	PM	not assessed	P: short-chain PFAS, estimated t1/2 (error factor 10) = 531d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM exp log Koc=0.5	Cramer Cl.III
27619-97-2	248-580-6	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonic acid	short-chain PFAS-REACH	**vPvM**	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 2 937d, 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. -	UBA: vM EC: vM exp log Koc=1.3	Cramer Cl.III
431-47-0	207-074-5	Methyl trifluoroacetate	short-chain PFAS-REACH	PM	not assessed	Potential P/vP++: TFA, estimated t1/2 (error factor 10) = 54d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. -	UBA: vM EC: vM exp log Koc=-0.1	Cramer Cl.III
62037-80-3	700-242-3	Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate	short-chain PFAS-REACH	**vPvM & PMT**	not assessed	vP: short-chain PFAS, on SVHC list - vPvB substance	UBA: vM EC: vM exp log Koc=1.1	(SVHC:Equivalent level of concern having probable serious effects to human health (Article 57(f) - human health)#Equivalent level of concern having probable serious effects to the environment (Article 57(f) - environment))(PBT_UnderAssess)
17527-29-6	241-527-8	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate	short-chain PFAS-REACH	Not PMT/vPvM	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 4 136d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: Not M EC: Not M exp log Koc=4.2	(PBT_UnderAssess)(EDC_UnderAssess) (DNEL)
2144-53-8	218-407-9	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl methacrylate	short-chain PFAS-REACH	Not PMT/vPvM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 4 214d, 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. -	UBA: Not M EC: Not M exp log Koc=4.2	(PBT_UnderAssess)(EDC_UnderAssess)(Ecotox_PMT2019)
428-59-1	207-050-4	Trifluoro(trifluoromethyl)oxirane	short-chain PFAS-REACH	PM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 656d, 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. -	UBA: vM EC: M min Dow=1.8 (2a)	Cramer Cl.III

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
1187-93-5	214-703-7	Trifluoro(trifluoromethoxy)ethylene	short-chain PFAS-REACH	PM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 198d, 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. -	UBA: vM EC: vM min Dow=1.3 (2a)	Cramer Cl.III
700874-87-9	615-064-0	{difluoro[(1,2,2-trifluoroethenyl)oxy]methoxy}trifluoromethane	short-chain PFAS-REACH	PM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 934d, 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. -	UBA: vM EC: vM min Dow=1.2 (2a)	Cramer Cl.III
1623-05-8	216-600-2	1,1,1,2,2,3,3-heptafluoro-3-[(trifluorovinyl)oxy]propane	short-chain PFAS-REACH	Potential PMT/vPvM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 929d, 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. -	UBA: Pot.M/vM EC: Not M min Dow=4.0 (2a)	Cramer Cl.III
756-13-8	436-710-6	1,1,1,2,2,4,5,5,5-nonafluoro-4-(trifluoromethyl)-3-pentanone	short-chain PFAS-REACH	PM	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 13 525d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: M EC: Pot.M/vM min Dow=3.4 (2a)	Cramer Cl.III
355-93-1	206-596-0	2,2,3,3,4,4,5,5-octafluoropentyl methacrylate	short-chain PFAS-REACH	PM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 114d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. -	UBA: M EC: Pot.M/vM min Dow=3.0 (2a)	Cramer Cl.III
85857-16-5	288-657-1	Trimethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	short-chain PFAS-REACH	Not PMT/vPvM	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 6 740d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Modified sturm test;EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Modified sturm test;OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: Not M EC: Not M min Dow=5.9 (2a)	Cramer Cl.III
78560-45-9	278-947-6	Trichloro(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	short-chain PFAS-REACH	Not PMT/vPvM	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 6 206d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide	UBA: Not M EC: Not M min Dow=7.4 (2a)	Cramer Cl.III

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						Evolution Test) Modified sturm test;OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))		
51851-37-7	257-473-3	Triethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane	short-chain PFAS-REACH	Not PMT/vPvM	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 8 399d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) Modified sturm test;OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: Not M EC: Not M min Dow=7.5 (2a)	Cramer Cl.III
1190931-27-1	682-238-0	Ammonium difluoro{[2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	short-chain PFAS-REACH	vPvM	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 18 579d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-A (Determination of the "Ready" Biodegradability - Dissolved Organic Carbon (DOC) Die-Away Test);OECD Guideline 301 A (Ready Biodegradability: DOC Die Away Test);EU Method C.4-A (Determination of the "Ready" Biodegradability - Dissolved Organic Carbon (DOC) Die-Away Test);OECD Guideline 301 A (Ready Biodegradability: DOC Die Away Test)	UBA: vM EC: vM exp log Koc=1.0	Cramer Cl.III
908020-52-0	700-323-3	Ammonium difluoro[1,1,2,2-tetrafluoro-2-(pentafluoroethoxy)ethoxy]acetate	short-chain PFAS-REACH	vPvM & PMT	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 4 214d, 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. -	UBA: vM EC: M min Dow=0.7 (2b)	(PBT_UnderAssess)
34454-97-2	252-043-1	1,1,2,2,3,3,4,4,4-nonafluoro-N-(2-hydroxyethyl)-N-methylbutane-1-sulphonamide	short-chain PFAS-REACH	PM	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 723d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test)	UBA: M EC: Pot.M/vM min Dow=2.7 (2a)	Cramer Cl.III
34455-00-0	252-044-7	1,1,2,2,3,3,4,4,4-nonafluoro-N,N-bis(2-hydroxyethyl)butane-1-sulphonamide	short-chain PFAS-REACH	PM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 595d, 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. -	UBA: M EC: Pot.M/vM min Dow=2.7 (2a)	Cramer Cl.III
67584-55-8	266-733-5	2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl acrylate	short-chain PFAS-REACH	Not PMT/vPvM	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 883d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);EU Method C.4-C (Determination of the "Ready"	UBA: Not M EC: Not M exp log Koc=4.0	Cramer Cl.III

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						Biodegradability - Carbon Dioxide Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);ISO DIS 9439 (Ultimate Aerobic Biodegradability - Method by Analysis of Released Carbon Dioxide);ISO DIS 9439 (Ultimate Aerobic Biodegradability - Method by Analysis of Released Carbon Dioxide)		
67584-59-2	266-737-7	2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl methacrylate	short-chain PFAS-REACH	Not PMT/vPvM	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 1 001d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test);ISO DIS 9439 (Ultimate Aerobic Biodegradability - Method by Analysis of Released Carbon Dioxide)	UBA: Not M EC: Not M min Dow=4.9 (2a)	Cramer Cl.III
80475-32-7	279-481-6	N-[3-(dimethylamino)propyl]-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonamide N-oxide	short-chain PFAS-REACH	PM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 16 855d, 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. -	UBA: M EC: Not M exp log Koc=3.8	Cramer Cl.III
88992-45-4	811-523-6	2-hydroxy-N,N,N-trimethyl-3-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)thio]propan-1-aminium chloride	short-chain PFAS-REACH	**vPvM**	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 4 623d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) (2008);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) (1992);EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) (2008);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) (1992);ISO DIS 9439 (Ultimate Aerobic Biodegradability - Method by Analysis of Released Carbon Dioxide) (1999);ISO DIS 9439 (Ultimate Aerobic Biodegradability - Method by Analysis of Released Carbon Dioxide) (1999)	UBA: vM EC: M min Dow=0.4 (2c)	Cramer Cl.III
34455-29-3	252-046-8	Carboxymethyldimethyl-3-[[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)sulphonyl]amino]propylammonium hydroxide	short-chain PFAS-REACH	**vPvM**	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 4 052d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-D (Determination of the "Ready" Biodegradability - Manometric Respirometry Test);EU Method C.4-D (Determination of the "Ready" Biodegradability - Manometric Respirometry Test);OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	UBA: vM EC: vM exp log Koc=1.3	Cramer Cl.III

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
62880-93-7	811-522-0	sodium 2-methyl-2-({3-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)thio]propanoyl}amino)propane-1-sulfonate	short-chain PFAS-REACH	**vPvM**	not assessed	vP: short-chain PFAS, estimated t1/2 (error factor 10) = 7 198d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) (2008);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) (1992);EU Method C.4-C (Determination of the "Ready" Biodegradability - Carbon Dioxide Evolution Test) (2008);OECD Guideline 301 B (Ready Biodegradability: CO2 Evolution Test) (1992);ISO DIS 9439 (Ultimate Aerobic Biodegradability - Method by Analysis of Released Carbon Dioxide) (1999);ISO DIS 9439 (Ultimate Aerobic Biodegradability - Method by Analysis of Released Carbon Dioxide) (1999)	UBA: vM EC: M min Dow=1.1 (2b)	Cramer Cl.III
2926-29-6		dipotassium trifluoroacetate trifluoromethanesulfinate	short-chain PFAS-REACH	PM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 633d, 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. -	UBA: vM EC: vM min Dow=0.4 (2a)	Cramer Cl.III
40573-09-9	442-390-9	1,1,2,2,3,3-hexafluoro-1-trifluoromethoxy-3-trifluorovinyloxypropane	short-chain PFAS-REACH	PM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 3 660d, 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. -	UBA: M EC: Not M exp log Koc=3.7	Cramer Cl.III
21615-47-4	244-479-6	Ammonium undecafluorohexanoate	short-chain PFAS-REACH	**vPvM & PMT**	not assessed	vP: short-chain PFAS, PFAS read-across and estimated t1/2 (error factor 10) = 1 048d, 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	UBA: vM EC: vM exp log Koc=1.8	(read-across PFAS)
645-92-1	-	Ammeline	triazine	Potential PMT/vPvM	not assessed	Potential P/vP: Zheng et al. (2021)	vM: Zheng et al. (2021)	Cramer Cl.III
645-93-2	-	Ammelide	triazine	Potential PMT/vPvM	not assessed	Potential P/vP: Zheng et al. (2021)	vM: Zheng et al. (2021)	Cramer Cl.III
108-77-0	203-614-9	2,4,6-trichloro-1,3,5-triazine	triazine	Potential PMT/vPvM	not assessed	Pot.P/vP: estimated t1/2 (error factor 10) = 162d, and BIOWIN screen tool as recommended in the PBT guideline	UBA: vM EC: vM min Dow=0.6 (2a)	Cramer Cl.III
4156-21-2	223-989-2	Sodium p-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]benzenesulphonate	triazine	PM	not assessed	P: estimated t1/2 (error factor 10) = 408d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test);OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	UBA: vM EC: vM min Dow=-0.5 (2a)	Cramer Cl.III

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
17766-26-6	241-749-5	1,3,5-triazine-2,4,6(1H,3H,5H)-trithione, trisodium salt	triazine	no data/structure	not assessed	no conclusion/data: only limited QSAR data, estimated t1/2 (error factor 10) = 41d	UBA: vM EC: M min Dow=0.8 (2b)	Cramer Cl.III
2058-94-8	-	PFUnDA	monitoring PFAS	PMT	not assessed	vP: long-chain PFAS, on SVHC list - vPvB substance	UBA: M EC: Not M exp log Koc=3.3	(SVHC:vPvB (Article 57e))
307-55-1	-	PFDoDA	monitoring PFAS	PMT	not assessed	vP: long-chain PFAS, on SVHC list - vPvB substance	UBA: M EC: Not M exp log Koc=3.6	(SVHC:vPvB (Article 57e))
68259-12-1	-	PFNS	monitoring PFAS	Potential PMT/vPvM	not assessed	vP: short-chain PFAS (read-across)	UBA: EC:	SVHC
67906-42-7	-	PFDS	monitoring PFAS	PMT	not assessed	vP: long-chain PFAS, PFAS read-across and estimated t1/2 (error factor 10) = 66 528d, 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. -	UBA: M EC: Not M exp log Koc=3.5	(read-across PFAS)
920-66-1	213-059-4	1,1,1,3,3,3-hexafluoropropan-2-ol	monitoring PFAS	vPvM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 271d, weight-of-evidence (this study) based on all known QSARs and majority of biodegradation screen tests, e.g. OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I));OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test (I))	UBA: vM EC: vM min Dow=0.4 (2b)	Cramer Cl.III
422-05-9	207-012-7	2,2,3,3,3-pentafluoropropanol	monitoring PFAS	PM	not assessed	Potential P/vP++: short-chain PFAS, estimated t1/2 (error factor 10) = 112d, 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. -	UBA: vM EC: vM exp log Koc=0.6	Cramer Cl.III
15290-77-4	430-710-1	1,1,2,2,3,3,4-heptafluorocyclopentane	monitoring PFAS	PM	not assessed	Potential P/vP++: apolar PFAS, estimated t1/2 (error factor 10) = 152d, 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. -	UBA: vM EC: M min Dow=2.4 (2a)	Cramer Cl.III
375-22-4	-	PFBA	monitoring PFAS	vPvM	not assessed	vP: short-chain PFAS, PFAS read-across and estimated t1/2 (error factor 10) = 230d, 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. -	UBA: vM EC: vM exp log Koc=0.4	Cramer Cl.III
2706-90-3	-	PFPeA - Perfluorovaleric acid	monitoring PFAS	vPvM & PMT	not assessed	vP: short-chain PFAS, PFAS read-across and estimated t1/2 (error factor 10) = 486d, weight-of-evidence (this study) based on all	UBA: vM EC: vM exp log Koc=0.8	(read-across PFAS)

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
						used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. -		
375-85-9	-	PFHpA	monitoring PFAS	vPvM & PMT	not assessed	vP: long-chain PFAS, PFAS read-across and estimated t1/2 (error factor 10) = 2 267d, 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. -	UBA: vM EC: vM exp log Koc=1.6	(read-across PFAS)
335-67-1	-	PFOA	monitoring PFAS	vPvM & PMT	not assessed	vP: long-chain PFAS, On SVHC list - PBT substance	UBA: vM EC: M exp log Koc=2.1	(SVHC:Toxic for reproduction (Article 57c)#PBT (Article 57d))
72629-94-8	-	PFTriDA	monitoring PFAS	Not PMT/vPvM	not assessed	vP: long-chain PFAS, on SVHC list - vPvB substance	UBA: Not M EC: Not M exp log Koc=4.1	(SVHC:vPvB (Article 57e))
375-95-1	-	PFNA	monitoring PFAS	vPvM & PMT	not assessed	vP: long-chain PFAS, On SVHC list - PBT substance	UBA: vM EC: M exp log Koc=2.4	(SVHC:Toxic for reproduction (Article 57c)#PBT (Article 57d))
335-76-2	-	PFDA	monitoring PFAS	vPvM & PMT	not assessed	vP: long-chain PFAS, On SVHC list - PBT substance	UBA: vM EC: M exp log Koc=2.8	(SVHC:Toxic for reproduction (Article 57c)#PBT (Article 57d))
2706-91-4	-	PFPS (C5-Sulfonate)	monitoring PFAS	vPvM & PMT	not assessed	vP: short-chain PFAS, PFAS read-across and estimated t1/2 (error factor 10) = 1 158d, weight-of-evidence (this study) based on all used QSARs and no biodeg. observed in majority of biodegradation screen tests for substance/main transformation products, e.g. -	UBA: vM EC: vM exp log Koc=1.4	(read-across PFAS)
3871-99-6	-	PFHxS	monitoring PFAS	vPvM & PMT	not assessed	vP: short-chain PFAS, on SVHC list - vPvB substance	UBA: vM EC: vM exp log Koc=1.8	(SVHC:vPvB (Article 57e))
375-92-8	-	PFHpS	monitoring PFAS	vPvM & PMT	not assessed	vP: long-chain PFAS, PFAS read-across and estimated t1/2 (error factor 10) = 5 746d, 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. -	UBA: vM EC: M exp log Koc=2.2	(read-across PFAS)
1763-23-1	260-375-3	Tetraethylammonium heptadecafluorooctanesulphonate	monitoring PFAS	vPvM & PMT	not assessed	vP: long-chain PFAS, Stockholm Convention	UBA: vM EC: M exp log Koc=2.6	(Rep_BroadConsensus)(PBT_BroadConses)
79780-39-5	-	PFDoS	monitoring PFAS	Potential PMT/vPvM	not assessed	vP: short-chain PFAS (read-across)	UBA: EC:	SVHC
422-64-0	-	PFPrA	monitoring PFAS	vPvM	not assessed	vP: short-chain PFAS (read-across)	UBA: vM EC: vM Read-across, ultra-short-chain PFAS	short-chain PFAS

Cas No.	EC No.	Full Name	Reason for Including	PMT/vPvM conclusion (2022)	PMT/vPvM conclusion (2019)	P Rationale (2022)	M Rationale (2022)	T Rationale (2022)
376-06-7	-	PFTeA	monitoring PFAS	Potential PMT/vPvM	not assessed	vP: short-chain PFAS (read-across)	UBA: EC:	SVHC
354-88-1	-	PFEtS	monitoring PFAS	**vPvM**	not assessed	vP: short-chain PFAS (read-across)	UBA: vM EC: vM Read-across, ultra-short-chain PFAS	short-chain PFAS
423-41-6	-	PFPrS	monitoring PFAS	**vPvM**	not assessed	vP: short-chain PFAS (read-across)	UBA: vM EC: vM Read-across, ultra-short-chain PFAS	short-chain PFAS
377739-43-0	477-710-6	tris(pentafluoroethyl)trifluorophosphate (FAP)	monitoring PFAS	**vPvM**	not assessed	vP: short-chain PFAS (read-across)	UBA: vM EC: vM Read-across	short-chain PFAS

B Analysis methods for the monitoring study

B.1 Gas chromatographic methods

B.1.1 Headspace gas chromatography mass spectrometry (GC-MS)

Trifluoroacetic acid (TFA) was analysed with a GC-MS equipped with an autosampler and a temperature-controlled injection system. To prepare the sample, it is first evaporated to dryness at basic conditions, then methylated with acidic catalysis and finally closed gas tight. A gaseous aliquot of 1000 µL is extracted by means of an autosampler with a heatable, gas tight plunger syringe and injected with a split ratio of 1:7. The temperature-controlled injection system is programmed as follows: start temperature 75 °C, heating rate 2 °C/s, end temperature 80 °C, hold time 4 min. In order to ensure sufficient focussing of the sample at the column head, a temperature program with low start temperature (35 °C) and long hold time (5 min) followed by a heating phase (20°C/min) finally obtaining 250 °C is applied. Helium is used as carrier gas with a flow of 1.0 – 1.3 L/min. As MS settings EI (70 eV) and SIM mode were chosen.

2,2,3,3,5,5,6,6-octafluoro-4-(trifluoromethyl)morpholine, 1,1,2,2,3,3-hexafluoro-1-trifluoromethoxy-3-trifluorovinyloxypropane, 1,1,2,2,3,3,4-heptafluorocyclopentane, 2,2,3,3,3-pentafluoropropanol, 1,1,1,3,3,3-hexafluoropropan-2-ol, 1,2-dibromoethane, 2,2,3,3,4,4,5,5-octafluoropentyl methacrylate, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate, 1,3-dichlorobenzene, Trimethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl methacrylate, 1,2-dichlorobenzene, Triethoxy(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane, 2-nitrotoluene, Dichlorodifluoromethane, Chloroethylene, 1,1-dichloroethylene, trans-dichloroethylene, Chloroform, 1,1,1-trichloroethane, Carbon tetrachloride, 1,2-dichloropropane, and Chlorobenzene are analysed with GC-MS equipped with an autosampler and a temperature-controlled injection system. A gaseous aliquot of 1000 µL is taken from the samples headspace and injected using a split ratio of 10:1. The temperature-controlled injection system is programmed as follows: start temperature 80 °C, heating rate 2 °C/s, end temperature 85 °C, hold time 4 min. The split ratio was set to 5:1. In order to ensure sufficient focussing of the sample at the column head, a temperature program with low start temperature (35 °C) and long hold time (5 min) followed by a heating phase (10°C/min) finally obtaining 220 °C is applied. The final temperature is hold for 1 min. Helium is used as carrier gas with a flow of ~1.0 L/min. As MS settings EI (70 eV) and SIM mode were chosen.

B.1.2 Headspace-solid phase micro extraction (SPME) GC-MS

1,4-Dioxan is analysed with GC-MS, equipped with an autosampler and temperature-controlled injection system. The sample is enriched using a SPME fibre (65 µm, PDMS DBV, 23 Gauge) for 60 min at 45 °C in the incubator. The temperature-controlled injection system is programmed as follows: start temperature 255 °C, heating rate 2 °C/s, end temperature 260 °C, hold time 10 min. In order to ensure sufficient focussing of the sample at the column head, a temperature program with low start temperature (35 °C) and long hold time (5 min) followed by a heating phase (10°C/min) finally obtaining 100 °C is applied. The final temperature is hold for 2 min. Helium is used as carrier gas with a flow of ~1.0 L/min. MS settings EI (70 eV) and SIM mode were chosen.

B.1.3 GC-MS after liquid-liquid extraction

1-chloro-2-nitrobenzene, 1,1,2,2,3,3,4,4,4-Nonafluoro-N-(2-hydroxyethyl)-N-methyl-1-butanesulfonamide, Trichloro(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane, and 4-nitrotoluene are analysed after liquid-liquid-extraction with hexane and liquid injection (splitless). MS settings EI (70 eV) and SIM mode were chosen.

B.2 Liquid-chromatographic methods

B.2.1 Chemicals

The chemicals used were ultrapure water, acetonitrile and methanol (all LiChrosolv® UHPLC-MS grade, Merck KGaA, Darmstadt, Germany). Ammonia (30%) was purchased from Carl Roth GmbH (Karlsruhe, Germany). Ammonium formate (>99% purity) was obtained from Fluka (Munich, Germany) and formic acid was purchased from Fisher Chemical (Schwerte, Germany).

B.2.2 Sample preparation

For HILIC measurements, multi-layer SPE (mlSPE) and evaporative concentration (EC) was used. For RPLC measurements, weak anion-exchange SPE was applied.

Multi-layer solid phase extraction: The mlSPE cartridges contained 60 mg of CHROMABOND sorbens HR-XAW, CHROMABOND sorbents HR-XCW (both 45 µm) and Carbograph graphitized carbon black and were provided by Macherey Nagel (Düren, Germany). The protocol was as follows: 200 g of each water sample was adjusted to pH 5.5 ± 0.1 with formic acid or ammonia solution. Conditioning of the cartridges was performed using 1 mL methanolic ammonia solution (5%), 1 mL methanolic formic acid solution (2%), 1 mL methanol and 3 mL water. The samples were passed through the cartridge at a flow rate of approximately 5 mL/min and the cartridge was dried under a gentle stream of nitrogen for about 15 minutes. Elution was performed sequentially with 3 mL methanolic ammonia solution (5%), followed by evaporation of the extract (50°C; under a gentle stream of nitrogen), addition of 3 mL methanolic formic acid solution (2%) and 1.5 mL methanol, again followed by evaporation of the extract (50°C; under a gentle stream of nitrogen), and reconstitution in 1 mL acetonitrile:water 95:5 (v:v). The eluate was then mixed for 15 s and filtered through a syringe filter (regenerated cellulose, 0.20 µm, GE Healthcare, Little Chalfont, UK) into a 1 mL PP vial (Klaus Ziemer, Langerwehe, Germany).

Evaporative concentration: 10 mL of the samples was pipetted into 15 mL PP vials (Kartell S.p.A, Noviglio, MI, Italy) and evaporated using a Speedvac SPD 111V vacuum centrifuge, an RVT 400 cooling trap (both Thermo Fisher Scientific, Waltham, Massachusetts, USA) and an MZ 2 membrane pump (Vacuubrand, Wertheim, Germany). The samples were reconstituted and filtered as mentioned above.

Weak anion-exchange SPE: 200 g of each water sample was weighed and enriched with Oasis WAX cartridges (Waters, Milford, MA, USA). The SPE protocol was as follows: Conditioning of the cartridges was performed with 2 mL methanolic ammonia solution (1%, v:v), 2x2 mL methanol and 3x2 mL water. After the samples were passed through the cartridges, they were rinsed with 3 mL water:methanol 4:1 (v:v) and dried under a gentle stream of nitrogen for 10 minutes. Elution was performed using 2x1 mL methanolic ammonia solution (1%, v:v). The eluate was

then evaporated to dryness at 50 °C under a gentle stream of nitrogen, reconstituted in 0.5 mL water:methanol 4:1 (v:v), and filtered through a syringe filter into a 0.5 mL PP vial.

B.2.3 LC-MS instrumentation

The LC-MS system used was a Shimadzu Nexera X2, consisting of a degassing unit, four pumps, an autosampler, a communication module and a column oven (Shimadzu, Kyoto, Japan) coupled to a QTrap 5500 (AB Sciex, Darmstadt, Germany).

HILIC measurements: The column used was an Acquity UPLC BEH Amide 1.7 µm, 2.1 x 100 mm (Waters, Milford, MA, USA) and heated to 30 °C. The eluents consist of 95% water and 5% acetonitrile (v:v, eluent A) and 5% water and 95% acetonitrile (v:v, eluent B) with 5 mM ammonium formate, adjusted to pH 3. The injection volume was 5 µL, the total run time was 10 minutes and the flow rate was 500 µL/min. The employed gradient is shown in table B1.

Table B1: Gradient for HILIC measurements

Time in min	% Eluent B
0.0	100
1.0	100
5.0	75
6.0	50
8.0	50
8.1	100
10.0	100

RPLC measurements: The columns used were an Acquity UPLC HSS T3 1.8 µm, 2.1 x 50 mm for the chromatographic run and a Luna C18(2), 5 µm 30 x 2 mm column (Phenomenex, Torrance, California, United States) was installed after the mixing chamber of the eluents and before the injector to retain solvent blank signals for RPLC measurements. The RPLC eluents consist of 95% water and 5% methanol (v:v, eluent A) and 10% water and 90% methanol (v:v, eluent B) with 5 mM ammonium formate. The injection volume was 7.5 µL, the total run time was 8 minutes and the flow rate was 500 µL/min. The gradient used is shown in table B2.

Table B2: Gradient for RPLC measurements

Time in min	% Eluent B
0.0	0
0.5	0
1.0	30
3.5	100
5.1	100
5.5	0
8.0	0

MRM parameters HILIC ESI positive: The parameters for HILIC ESI positive analytes are displayed in table B3.

Table B3: MRM parameters for HILIC ESI positive analytes

CAS-No.	Analyte	Time (min)	Q1 Mass	Q3 Mass	DP	EP	CE	CXP
2855-13-2	IPDAM	6,08	171,164	154,2	70	10	18	15
2855-13-2	IPDAM	6,08	171,164	81,2	70	10	31	12
83016-70-0	DEMAEtOH	6,22	191,161	102,2	66	10	23	12
83016-70-0	DEMAEtOH	6,22	191,161	72,1	66	10	23	12
622-40-2	MoEtOH	3,75	132,076	114,2	86	10	21	12
622-40-2	MoEtOH	3,75	132,076	70,1	86	10	27	10
280-57-9	3EDiAm	5,42	113,075	84,1	236	10	29	10
280-57-9	3EDiAm	5,42	113,075	56,1	236	10	31	8

CAS-No.	Analyte	Time (min)	Q1 Mass	Q3 Mass	DP	EP	CE	CXP
834-12-8	Ametryn	0,59	228,093	186,2	80	11	25	17
834-12-8	Ametryn	0,59	228,093	68,1	80	11	55	10
288-88-0	1,2,4-Triazole	0,92	70	43	120	10	30	7
288-88-0	1,2,4-Triazole	0,92	70	28	120	10	45	7
91-76-9	BGAm	0,78	188,1	104,1	130	10	35	12
91-76-9	BGAm	0,78	188,1	85	130	10	27	11
102-06-7	DPGu	1,46	212	77	96	10	53	10
102-06-7	DPGu	1,46	212	119	96	10	29	12
95-14-7	Benzotriazole	0,66	120,1	92	20	10	16	11
95-14-7	Benzotriazole	0,66	120,1	65	20	10	35	10
108-78-1	Melamine	3,98	127,1	85	90	10	25	10
108-78-1	Melamine	3,98	127,1	42,9	90	10	60	7
645-92-1	Ammeline	4,89	128	86	60	3	22	8
645-92-1	Ammeline	4,89	128	69	60	3	40	8
3030-47-5	B2DiMeAmEtMeAM	5,87	174	129	70	10	17	13
3030-47-5	B2DiMeAmEtMeAM	5,87	174	72	70	10	27	9
3033-62-3	TetraMeOxbisEtAm	6,03	161	116	68	10	16	11
3033-62-3	TetraMeOxbisEtAm	6,03	161	72	68	10	22	12
56-93-9	BenzTriMeAm	1,53	150	91	78	10	27	12
56-93-9	BenzTriMeAm	1,53	150	65	78	10	50	8

CAS-No.	Analyte	Time (min)	Q1 Mass	Q3 Mass	DP	EP	CE	CXP
38083-17-9	Climbazol	0,58	293	197	32	10	21	13
38083-17-9	Climbazol	0,58	293	69	32	10	31	13

MRM parameters HILIC ESI negative: The parameters for HILIC ESI negative analytes are displayed in table B4

Table B4: MRM parameters for HILIC ESI negative analytes

CAS-No.	Analyte	Time (min)	Q1 Mass	Q3 Mass	DP	EP	CE	CXP
1493-13-6	TFMSA	0,48	148,869	80	-80	-10	-30	-9
1493-13-6	TFMSA	0,48	148,869	98,9	-80	-10	-34	-11
15214-89-8	AMPSA	1,37	205,957	80	-100	-10	-42	-9
15214-89-8	AMPSA	1,37	205,957	135	-100	-10	-26	-13
52556-42-0	OHPSA	1,34	194,915	79,9	-85	-10	-44	-9
52556-42-0	OHPSA	1,34	194,915	94,9	-85	-10	-26	-11
81-07-2	Saccharin	0,74	181,885	42,1	-105	-10	-60	-7
81-07-2	Saccharin	0,74	181,885	105,9	-105	-10	-26	-11
108-80-5	Cyanuric acid	1,68	127,914	42,1	-75	-10	-36	-7
108-80-5	Cyanuric acid	1,68	127,914	85	-75	-10	-14	-7
55589-62-3	Acesulfame	0,61	162	82	-70	-10	-20	-9
55589-62-3	Acesulfame	0,61	162	77,9	-70	-10	-42	-9
377739-43-0	FAP	0,43	444,9	118,9	-85	-10	-42	-13
377739-43-0	FAP	0,43	444,9	344,8	-85	-10	-42	-31

CAS-No.	Analyte	Time (min)	Q1 Mass	Q3 Mass	DP	EP	CE	CXP
161401-25-8	NTf2	0,44	279,9	63,9	-70	-10	-110	-10
161401-25-8	NTf2	0,44	279,9	77,9	-70	-10	-65	-8
354-88-1	PFEtS	0,46	199	80	-20	-10	-43	-10
354-88-1	PFEtS	0,46	199	99	-20	-10	-34	-10
422-64-0	PFPrA	0,56	163	119	-20	-10	-13	-10
422-64-0	PFPrA	0,56	163	69	-20	-10	-50	-10
143-66-8	Na-TPheB	0,43	319,2	241	-80	-10	-45	-10
143-66-8	Na-TPheB	0,43	319,2	77,1	-80	-10	-40	-10
17766-26-6	Triazine-Trithione	0,75	175,9	58	-60	-10	-50	-9
17766-26-6	Triazine-Trithione	0,75	175,9	117	-60	-10	-17	-13
1286479-01-3	Saccharin 13C6	0,67	188,1	42	-73	-7	-68	-6
1286479-01-3	Saccharin 13C6	0,67	188,1	106	-73	-7	-26	-6

MRM parameters RPLC ESI negative: The parameters for RPLC ESI negative analytes are displayed in table B5

Table B5: MRM parameters for RPLC ESI negative analytes

CAS-No.	Analyte	Time (min)	Q1 Mass	Q3 Mass	DP	EP	CE	CXP
375-22-4	PFBA	2,48	213	169	-52	-10	-20	-10
2706-90-3	PFPeA	3,19	263	219	-40	-10	-13	-10
307-24-4	PFHxA	3,51	313	269	-60	-10	-13	-10
307-24-4	PFHxA	3,51	313	119	-60	-10	-32	-10

CAS-No.	Analyte	Time (min)	Q1 Mass	Q3 Mass	DP	EP	CE	CXP
375-85-9	PFHpA	3,75	363	319	-60	-10	-15	-10
375-85-9	PFHpA	3,75	363	169	-60	-10	-25	-10
335-67-1	PFOA	3,94	413	369	-60	-10	-15	-10
335-67-1	PFOA	3,94	413	169	-60	-10	-27	-10
375-95-1	PFNA	4,11	463	419	-60	-10	-18	-10
375-95-1	PFNA	4,11	463	169	-60	-10	-29	-10
335-76-2	PFDA	4,25	513	469	-40	-10	-18	-10
335-76-2	PFDA	4,25	513	269	-40	-10	-27	-10
2058-94-8	PFUnA	4,39	563	519	-60	-10	-20	-10
2058-94-8	PFUnA	4,39	563	319	-60	-10	-27	-10
307-55-1	PFDoA	4,53	613	569	-60	-10	-23	-10
307-55-1	PFDoA	4,53	613	219	-60	-10	-29	-10
72629-94-8	PFTrA	4,67	663	619	-80	-10	-23	-10
72629-94-8	PFTrA	4,67	663	169	-80	-10	-41	-10
376-06-7	PFTeA	4,82	713	669	-60	-10	-23	-10
376-06-7	PFTeA	4,82	713	169	-60	-10	-41	-10
375-73-5	PFBS	3,26	299	80	-39	-10	-100	-10
375-73-5	PFBS	3,26	299	99	-39	-10	-66	-10
355-46-4	PFHxS	3,74	399	80	-32	-10	-100	-10
355-46-4	PFHxS	3,74	399	99	-32	-10	-88	-10

CAS-No.	Analyte	Time (min)	Q1 Mass	Q3 Mass	DP	EP	CE	CXP
375-92-8	PFHpS	3,93	449	80	-42	-10	-100	-10
375-92-8	PFHpS	3,93	449	99	-42	-10	-100	-10
1763-23-1	PFOS	4,09	499	80	-35	-10	-100	-10
1763-23-1	PFOS	4,09	499	99	-35	-10	-100	-10
335-77-3	PFDS	4,37	599	80	-52	-10	-130	-10
335-77-3	PFDS	4,37	599	99	-52	-10	-120	-10
	MPFBA	2,48	217	172	-52	-10	-13	-10
	MPFHxA	3,51	315	270	-50	-10	-13	-10
	MPFHxA	3,51	315	119	-50	-10	-34	-10
	MPFOA	3,94	417	372	-60	-10	-16	-10
	MPFOA	3,94	417	169	-60	-10	-34	-10
	MPFNA	4,11	468	423	-55	-10	-16	-10
	MPFNA	4,11	468	219	-55	-10	-34	-10
	MPFDA	4,25	515	470	-35	-10	-16	-10
	MPFDA	4,25	515	270	-35	-10	-29	-10
	MPFUnA	4,39	565	520	-60	-10	-21	-10
	MPFUnA	4,39	565	219	-60	-10	-31	-10
	MPFDoA	4,53	615	570	-60	-10	-18	-10
	MPFDoA	4,53	615	169	-60	-10	-46	-10
	MPFHxS	3,74	403	84	-40	-10	-80	-10

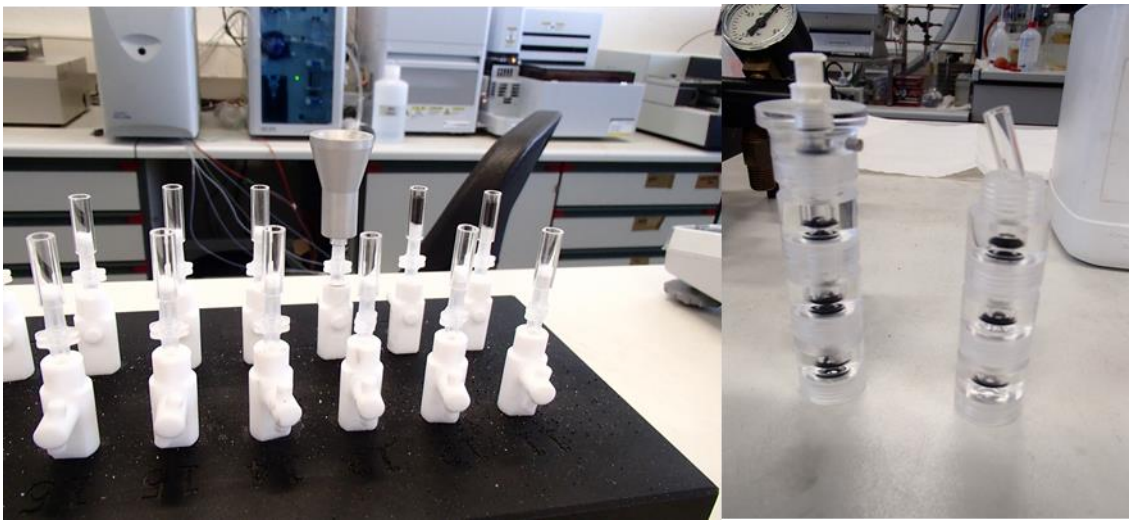
CAS-No.	Analyte	Time (min)	Q1 Mass	Q3 Mass	DP	EP	CE	CXP
	MPFHxS	3,74	403	103	-40	-10	-64	-10
	MPFOS	4,09	503	80	-40	-10	-88	-10
	MPFOS	4,09	503	99	-40	-10	-91	-10
27619-97-2	6:2 FTS	3,92	427	81	-100	-10	-75	-10
	M-6:2 FTS	3,92	429	81	-92	-10	-78	-10
13252-13-6	HFPO-DA	3,59	329	169	-30	-10	-20	-10
13252-13-6	HFPO-DA	3,59	329	285	-30	-10	-10	-10
423-41-6	PFPrS	2,83	249	80	-40	-10	-55	-10
423-41-6	PFPrS	2,83	249	99	-40	-10	-30	-10
121-03-9	4-NOtol-2-SA	2,35	216	80	-100	-10	-56	-10
121-03-9	4-NOtol-2-SA	2,35	216	170	-100	-10	-33	-10
2706-91-4	PFPeS	3,49	348,9	80	-40	-10	-80	-10
2706-91-4	PFPeS	3,49	348,9	99	-40	-10	-40	-10
68259-12-1	PFNS	4,19	548,8	80	-80	-10	-120	-10
68259-12-1	PFNS	4,19	548,8	99	-80	-10	-105	-10
79780-39-5	PFDoS	4,65	698,7	80	-130	-10	-130	-10
79780-39-5	PFDoS	4,65	698,7	99	-130	-10	-120	-10
2926-29-6	Triflinate	0,42	132,9	69	-60	-10	-20	-10
2926-29-6	Triflinate	0,42	132,9	83	-60	-10	-15	-10
80475-32-7	DPOSA	4,05	526,8	64	-170	-10	-105	-10

CAS-No.	Analyte	Time (min)	Q1 Mass	Q3 Mass	DP	EP	CE	CXP
80475-32-7	DPOSA	4,05	526,8	120	-170	-10	-40	-10

B.3 Determination of adsorbable organic fluorine (AOF)

The adsorbable organic fluorine (AOF) was determined as follows: A sample aliquot of 100 mL was mixed with 5 mL aqueous $NaNO_3$ solution (0.2 mol/L) and the AOF was extracted by using 100 mg (2 × 50 mg duplex extraction, Figure B1) of activated carbon (AC) adsorbent (Blücher #100043). The flow rate was adjusted to 3 mL/min, followed by 25 mL of $NaNO_3$ washing solution (0.01 mol/L) at the same flow rate to remove adsorbed F^-.

Figure B1: Photo of the duplex-AC-extraction.



Source: own photos, TZW: DVGW-Technologiezentrum Wasser

Determination of AOF was performed with a modified combustion ion chromatography (CIC) system for ultra-trace fluorine analysis, consisting of an automated boat controller (ABC-100), an automatic quick furnace (AQF-100) with a water supply unit (WS-100), and a gas absorption unit (GA-100) (all from Mitsubishi Chemical Analytech Co., LTD, Kanagawa, Japan). The combustion unit was linked to an IC system (ICS-2100, Thermo Fisher Scientific, Idstein, Germany). For analysis, the adsorbent was transferred to a ceramic sample boat (a1-envirosciences, Düsseldorf, Germany) and combusted in a furnace at 950–1000 °C while delivering 0.1 mL/min of ultrapure water by the solenoid pump of WS 100. Organically bound fluorine from the adsorbed organic substances was converted into hydrogen fluoride (HF) while the addition of excess water into the combustion tube prevents the formation of silicon tetrafluoride. The HF formed was absorbed in an aqueous methane sulfonic acid solution (1 mg/L) and measured as F^- by IC analysis. The adsorbent of the second cartridge of the same sample was analysed in the same way. Both results were corrected for the blank and added together to give AOF. The limit of quantification was 1 µg/L, 0.5 µg/L was set as the qualitative reporting level. All analyses were performed in duplicates.

B.4 Performance of the total oxidizable precursor (TOP) Assay, extraction, and analysis of PFAAs

For the total oxidizable precursor (TOP) assay, a sample aliquot of 50 mL was mixed with 1 g $K_2S_2O_8$ and 0.95 mL NaOH (10 M) in a 50-mL-container (PP). After capping, the batch was incubated at 80 °C for 20 h. After cooling (ice bath), the pH was adjusted to pH 5 with formic acid and a mixture of internal standards (IS; isotopically labelled C4–C13 PFCA, PFBS, PFHxS, and PFOS) and 2 mL MeOH were added. The analytes (C4–C14 PFCA as well as PFPrS, PFBS, PFPS, PFHxS, PFHpS, PFOS, PFNS, and PFDS) were extracted by Strata X-AW (6 mL, 200 mg; Phenomenex) at a flow rate of 0.8 mL/min. The sorbent was preconditioned with 4 mL MeOH containing 0.1% NH_4OH, 4 mL MeOH, and 2 × 5 mL ultrapure water. After extraction, the sorbent was dried for 30 min by N_2 and the analytes were eluted with 2 × 2 mL MeOH and 3 × 2 mL MeOH containing 0.1% NH_4OH. After evaporating the extract to dryness (N_2), the residues were redissolved in 0.25 mL MeOH/H_2O (80/20, v/v) and analysed by high performance liquid chromatography coupled to tandem mass spectrometry (HPLC-MS/MS).

Instrumental analysis was conducted by using the 1260 Infinity II LC System (Agilent) connected to a 6500+ MS/MS instrument (Sciex). The analytical column was a Luna Omega Polar C18 100 × 2.1 mm, 1.6 µm (Phenomenex). Eluent A was 10% MeOH in ultrapure water (+ 0.01 M ammonium acetate) and eluent B was MeOH. Eluent flow was 0.18 mL/min and the injection volume was 10 µL. The gradient was as follows: Starting at 20% B, increasing to 25% B from 0–0.5 min, increasing to 70% B from 0.5–7.0 min, increasing to 98% B from 7.0–14.5 min, holding this condition until minute 21.5 and decreasing to starting conditions within 0.5 min. The equilibration time was 8.0 min. The MS/MS-parameters of the analytes are listed in Table B6

Table B6: MS/MS-parameters (Sciex 6500+) for the determination of PFAAs after the TOP-assay.

[*1] *m/z* in quadrupol 1; [*2] *m/z* in quadrupol 3; [*3] declustering potential in V ; [*4] entrance potential in V; [*5] collision energy in eV ; [*6] collision cell exit potential in V

Analyte	Q1[*1]	Q3[*2]	DP[*3]	EP[*4]	CE[*5]	CXP[*6]
PFBA	212,9	168,9	−14	−11	−15	−10
PFPeA	262,8	219	−12	−19	−20	−10
	262,8	69	−58	−9	−20	−10
PFHxA	312,8	269	−12	−17	−20	−10
	312,8	119	−26	−13	−20	−10
PFHpA	362,8	319	−14	−21	−35	−10
	362,8	169	−24	−11	−35	−10
PFOA	412,9	368,9	−14	−25	−30	−10
	412,9	169	−24	−15	−30	−10
PFNA	462,8	419	−16	−27	−40	−10
	462,8	219	−24	−13	−40	−10
PFDA	512,8	469	−16	−31	−40	−10
	512,8	219	−24	−13	−40	−10

Analyte	Q1[*1]	Q3[*2]	DP[*3]	EP[*4]	CE[*5]	CXP[*6]
PFUdA	562,8	518,9	−16	−37	−55	−10
	562,8	269	−26	−23	−55	−10
PFDoA	612,8	568,9	−18	−37	−50	−10
	612,8	169	−34	−11	−50	−10
PFTrDA	662,8	619	−18	−39	−75	−10
	662,8	169	−36	−13	−75	−10
PFTeDA	712,8	669	−20	−41	−75	−10
	712,8	169	−36	−13	−75	−10
PFPrS	248,9	80	−75	−10	−52	−9
	248,9	98,9	−75	−10	−36	−11
PFBS	298,8	80	−75	−10	−62	−9
	298,8	99	−75	−10	−36	−11
PFPS	348,8	80	−65	−10	−80	−9
	348,8	99	−65	−10	−38	−11
PFHxS	398,8	80	−105	−10	−90	−9
	398,8	99	−105	−10	−80	−11
PFHpS	448,8	80	−125	−10	−104	−9
	448,8	99	−125	−10	−88	−11
PFOS	498,8	99	−125	−10	−98	−11
	498,8	80	−125	−10	−114	−9
PFNS	548,8	80	−115	−10	−122	−9
	548,8	99	−115	−10	−106	−11
PFDS	598,8	80	−110	−10	−132	−9
	598,8	99	−110	−10	−118	−11

C Workshop and summary of gaps

C.1 Third PMT workshop "Getting control of PMT and vPvM substances under REACH"

The third PMT Workshop entitled " Getting control of PMT and vPvM substances under REACH" took place online on the 25th and the 26th of March 2021. Over 700 experts from 32 nations representing water suppliers, the chemical industry, academia, regulators and NGOs registered to participate, and audience numbers peaked at 510. Presentations were held by the following organisations: ChemSec, ECHA, DVGW – Technologiezentrum Wasser, Federal Institute for Occupational Safety and Health, the University of Vienna, Technical University of Munich, Vitens, EAWAG, EurEua, European Commission, European Chemical Industry Council, BSAF, VCI, CHEM Trust, the European Environment Agency, Dutch Water research Institute, National Institute for Public Health and the Environment, Dutch Ministry of Infrastructure and Water Management, Vewin as well as UBA and the Norwegian Geotechnical Institute (NGI) The vast majority of these speakers have since published a scientific peer reviewed article based on the results of the workshop. Details can be found in Appendix E.

The workshop showcased a multitude of perspectives to get control of PMT and vPvM substances under REACH. The latest policy and governance developments related to the proposed inclusion of PMT/vPvM substances to the CLP regulation and to REACH were presented. Furthermore, the reasoning and evidence behind the decision to identify the first two PMT/vPvM substances as SVHC (PFBS and GenX) were presented as well as several national strategies to handle PMT/vPvM substances. NGOs showed how both market and policy mechanisms could be coordinated to drive innovation and transition towards safer alternatives to PMT/vPvM substances. Water suppliers provided case study monitoring data to highlight their concerns related to the presence of PMT/vPvM substances in drinking water sources from around Europe and the lack of practical remedial solutions to remove them. The chemical industry showcased their stewardship initiatives, welcoming an open dialogue with all parties in order to ensure the protection of the environment and human health. Academic research was presented in the form of monitoring and remediation studies, toxicity and persistence screening methods, as well as real world case studies for emerging PMT substances.

At the start of the workshop, participants were asked about the gaps they perceived related to PMT/vPvM substances via live polls. Towards the end of the workshop the audience's opinion was probed again related of the current state of 10 major gaps in getting in control of PMT/vPvM substances. The results of these polls and a discussion is given below.

C.2 Current PMT/vPvM substance gaps

At the start of the workshop a poll was opened for all participants with the following question

- What are the most important gaps for PMT substances ? (Please pick 3)

The answers to choose from were divided in to substance assessment gaps and risk governance gaps as follows:

- Availability of Persistency data?
- Availability of Mobility data?
- Availability for Toxicity data?

- Availability of Analytical methods?
- Availability of Monitoring data?
- Availability of transformation products and mixture composition data?
- Missing risk assessment tools/models?
- Missing water remediation infrastructure?
- Missing chemical legislation?
- Missing safe and sustainable substitutes?

The results from this opening poll were as follows:

Table C1: Results of the opening poll at the third PMT workshop

Name of gap	Percent of votes
Availability of transformation products and mixture composition data	48
Availability of analytical methods	44
Availability of monitoring data	37
Missing safe and sustainable substitutes	29
Missing risk assessment tools/models	28
Missing chemical legislation	26
Availability of toxicity data	24
Availability of mobility data	21
Availability of persistency data	19
Missing water remediation infrastructure	15

NB: Data is corrected for number of unique respondents, the data ignores «no response» and double responses, n=336 meaning 336 workshop participants responded, (ca 166 attendants with no response)

The results from the poll show that “Availability of transformation products and mixture composition” was identified as the biggest gap, with 48% of respondents putting this in their top three. The “Availability of analytical methods” (number 2) and “Availability of monitoring data” (number 3) data gaps are linked to each other, as monitoring is not possible without suitable analytical methods and often these analytical methods are not developed until there is a requirement (regulatory) to monitor. The " Availability of transformation products and mixture composition" gap is also related to both of the other gaps as transformation products and mixtures can make up a large amount of unknowns both in monitoring campaigns and analytical programs. Missing information related to P, M and T properties were ranked as less important gaps (gaps 7-9). Risk governance gaps were closer to the middle of the list. “Missing water remediation infrastructure” was ranked as the smallest gap.

C.3 The size of current PMT/vPvM substance gaps

At the end of the workshop, everyone was asked to assess the size of the 10 gaps above according to whether they felt they were "huge", "closing" or "small". At the time of the online poll there were approximately 380 people in attendance and of these, 120 people responded, with approximately 240 people who didn't respond depending on the question. The results in table C2 show a summary of the distribution of the three responses (as percentages) for each gap and the text below provides a short summary for each of the gaps.

Table C2: Summary of results for poll two. How big are the PMT/vPvM substance gaps?

Gap	Percent of respondents "huge gap"	Percent of respondents "gap closing"	Percent of respondents "small gap"
Availability of Persistency data	41	50	9
Availability of Mobility data	37	47	16
Availability of Toxicity data	60	30	10
Availability of Analytical methods	33	57	10
Availability of Monitoring Data	64	32	4
Availability of transformation products and mixture composition data	91	7	2
Missing risk assessment tools/models	34	56	10
Missing water remediation infrastructure	66	20	14
Missing chemical legislation	23	63	14
Missing safe and sustainable substitutes	60	34	6

Gap: Availability of persistency data. This was divided between "huge gap" and "gap closing" and could reflect the fact that there is little or no information for the low volume/intermediate REACH registered substances. The mandatory PBT assessment of substances with registration volumes > 10 tpa means that more testing is carried out. In addition, the screening test used for ready/inherent biodegradability can be used in order to demonstrate that a substance is not persistent.

Gap: Availability of mobility data. This gap was also divided between respondents who identified it as a "huge gap" and a "closing gap". The huge gap response to this gap could be related to the fact that K_{OC} data for ionic substances is rare and scattered in addition to the fact that D_{OW} does not account for ion exchange. The closing gap and small gap responses can reflect the fact that there is much more data and applicable models for neutral substances.

Gap: Availability of toxicity data. The majority of respondents answered this was a "huge gap" which could reflect the lack of data that exists for PM/vPvM substances, despite chronic exposure data existing. In addition, there are few long-term physiologically based pharmokinetic models.

Gap: Availability of analytical methods. The majority of respondents believed this to be a "closing gap", likely indicative of the vast improvement in analytical methods that have come

about in the past 5 years related to target and non-target analysis (e.g. HILIC columns, super critical fluid chromatography) and suspect screening databases (such as the Norman Network SLE).

Gap: Availability of monitoring data. The majority of respondents identified this as a "huge gap" which may reflect the fact that this gap is actually an incentive gap. Currently, regulatory requirements are what dictate and direct monitoring programs. Without the requirement, monitoring will likely not be carried out and hence there is a monitoring data gap. The research community who publish monitoring studies are able to support closing the gap, however most likely these state of the art research groups and labs just see the tip of the iceberg.

Gap: Transformation products and mixture composition data. This was ranked as the most important gap in the first poll and here an overwhelming majority of respondents identified this as a "huge gap". Experimental databases have only identified 451 transformation products, QSARs suffer from the problem that they often give multiple predictions and approximately 30 % of REACH registered substances are complex mixtures (UVCBs).

Gap: Missing risk assessment tools/models. The majority of respondents answered that the gap was "closing" which reflects the fact that the majority of respondents feel that tools and models exist or are being developed. Currently the EUSES model under REACH can be used in this regard, however the applicability domain of many of these models is under question (is not always suitable for ionic compounds).

Gap: Missing water remediation infrastructure. The majority of the respondents thought this was a "huge gap" and many developed countries have limited drinking water production infrastructure and they rely on chemical regulation to ensure preventative protection upstream, rather than relying on down stream remediation solutions. The remediation solution that shows most promise for PMT/vPvM removable is reverse osmosis which is very expensive and resource intensive.

Gap: Missing chemical legislation. Respondents identified this as a "closing gap" and this is almost certainly due to the recent legislative steps that have been taken via the Chemicals Strategy for Sustainability towards a Toxic free environment and the follow up action points whereby PMT/vPvM will be introduced as hazard classes in the CLP regulation and will be integrated into REACH. In addition, the broad PFAS restriction will also affect PMT/vPvM substances as many PFAS are also PMT/vPvM substances. The "huge gap" respondents may have focused on the need for harmonisation between legislation.

Gap: Missing safe and sustainable substitutes. The majority of respondents identified this as a "huge gap" perhaps spurred on by the difficulty in finding suitable substitutes from a technical and economic perspective.

Based on the percentage of respondents who identified a gap as "huge", the table C3 below shows a comparison of the rank of each of the gaps according to which gap was identified as the largest at the start and end of the workshop.

Table C3: Comparison of the ranks of the gaps according to which is the largest at the start and end of the workshop

Gap	Rank at beginning of the workshop	Rank at end of workshop
Availability of transformation products and mixture composition data	1	1
Availability of analytical methods	2	9
Availability of monitoring data	3	2
Missing safe and sustainable substitutes	4	3
Missing risk assessment tools/models	5	8
Missing chemical legislation	6	10
Availability of toxicity data	7	4
Availability of mobility data	8	7
Availability of persistency data	9	6
Missing water remediation infrastructure	10	5

D Overview of project dissemination activities

D.1 Introduction to dissemination activities

Throughout the project a variety of different communication and dissemination activities were carried out. The purpose of the activities was to raise awareness about PMT/vPvM substances and the work carried out in the project. The project results have the potential to be included in future regulation and registration requirements under REACH, and as such communication and dissemination was given a special focus. Below is a summary for each of the activities that were defined at the onset of the project.

D.2 Activity 6.1: At least two presentations at European conferences

Table D1 shows the presentations that have been held by the project consortium during the project period. Results from the project have been presented at two European conferences (Society of Environmental Toxicology and Chemistry and the International conference on emerging contaminants) as well as at numerous national meetings.

Table D1: List of presentations held during the project period

Title of presentation	Names of authors	Name and year of event	Form of event
The identification of persistent, mobile, toxic (PMT) chemicals as SVHC based on their equivalent level of concern to persistent, bioaccumulative, toxic chemicals defined in Article 57(f) of REACH	Sarah E. Hale, Lena Vierke, Hans Peter H. Arp and Michael Neumann	Society for Environmental Toxicology and Chemistry (SETAC) Europe, 2018	In person
Identifying PMT substances amongst REACH registered substances	Hans Peter H. Arp Sarah E. Hale, Albrecht Striffler, Daniel Sättler, Ivo Schliebner and Michael Neumann	SETAC Europe, 2018	In person
REACH registered substances that are emerging hazardous drinking water contaminants	Sarah E. Hale, Michael Neumann, Ivo Schliebner, Daniel Sätler, Hans Peter H. Arp	International conference on emerging contaminants, 2018	In person
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	Ivo Schliebner, Hans Peter H. Arp, Hans Peter H. Arp, Daniel Sattler, Lena Vierke, Michael Neumann	International conference on emerging contaminants, 2018	In person

Title of presentation	Names of authors	Name and year of event	Form of event
Discussion leader	Hans Peter H. Arp	ChemSec Event to Launch PMT/vPvM on the SINLlist: "Ready, Set, Substitute it Now!" 14th November, 2019	In person
The identification and assessment of PMT substances under REACH. (2020)	Hans Peter H. Arp, Sarah E. Hale, Ivo Schliebner and Michael Neumann	SETAC Europe, 2020	In person
PMT: Persistente, mobile und toxische Stoffe: Herausforderungen für die Wasserversorgung und Wasseranalytik	Ulrich Borchers, Hans Peter H. Arp and Michael Neumann	Mülheimer Wasseranalytisches Seminar, 2020	Digital
Analytik persistenter und mobiler Wasserkontaminanten - Limitationen, Perspektiven und Anwendungsbeispiele	Daniel Zahn and Isabelle Neuwald	Mülheimer Wasseranalytisches Seminar, 2020	Digital
The environmental risk and remediation of persistent, mobile, toxic (PMT) and very persistent and very mobile (vPvM) substances in the aquatic environment	Sarah E Hale	ECETOC scoping meeting 2020	In person
Establishing criteria for Persistence and Mobility: State-of-the-art and research needs	Hans Peter H. Arp, Sarah E. Hale, Ivo Schliebner and Michael Neumann	Workshop on Persistent, Mobile and Toxic Substances: A challenge for Analytical Chemistry and Water Quality Control, 2020	Digital
Discussion panel member	Hans Peter H. Arp	Cefic Technical workshop ‘Screening, prioritising and assessing the impact of mobile chemicals on drinking water resources’, 2020	Digital
Persistente und mobile Stoffe – von was reden wir?" / in English: "Persistent and mobile compounds - what are we talking about?	Marco Scheurer	TZW-Kolloquium, 2020	Digital
Life cycle effects from removing hazardous substances in sludge and plastics through thermal treatment. Additional: Information on characteristics of persistent and mobile substances in sludges and wastewaters	Hans Peter H. Arp	EIONET ad-hoc working group on chemicals meeting: Emerging risks of chemical mixtures in the reuse of wastewater and	Digital

Title of presentation	Names of authors	Name and year of event	Form of event
		sludge in a circular economy, 2020	
Fluorerte og andre persistente, mobile og toksiske miljøgifter i drikkevannet / in English Fluorinated and other persistent, mobile and toxic substances in drinking water	Hans Peter H. Arp	Norwegian Academy of Science and Letters symposium, 2020	In person
Poster: PMT/vPvM substances under REACH: Monitoring in surface and raw waters	Isabelle Neuwald, Vassil Valkov, Hans Peter H Arp, Daniel. Zahn	Langenauer Wasserforum 2021	Digital
Source Tracking: Identifikation von Eintragsquellen, Identifikation neuer persistenter, mobiler und toxischer Stoffe im Rohwasser	Ulrich Borchers	Langenauer Wasserforum 2021	Digital
PMT substances: persistent, mobile and toxic	Sarah E. Hale	Nordic seminar on proritization of substances, 2021	Digital
Risk Assessment Indictors of PMT/vPvM substances	Hans Peter H. Arp, Sarah E. Hale, Ulrich Borchers, Laura Wiegand, Vassil Valkov, Isabelle Neuwald, Daniel Zahn, Karsten Nödler, March Scheurer	SETAC Copenhagen 2022	In person
Keynote: Towards Reducing Pollution of PMT/vPvM Substances to Protect Water Resources	Hans Peter H. Arp	SETAC Copenhagen 2022	In person
Prioritizing Emerging Persistent and Mobile Organic Substances in Groundwater and Drinking water through Hazard and Risk Assessment for Substitution and Remediation	Hans Peter H. Arp and Sarah E. Hale	Nordrocs 2022	In person
Ultra-short-chain PFAS in the sources of German drinking water – prevalent, overlooked, difficult to remove, and unregulated	Isabelle Neuwald, Daniel Hübner, Laura Wiegand, Vassil Valkov, Ulrich Borchers, Karsten Nödler, Marco Scheurer, Sarah Hale, Hans Peter Arp, Daniel Zahn	Annual Meeting of the German Waterchemical Society 2022	Online

Title of presentation	Names of authors	Name and year of event	Form of event
The occurrence, distribution and environmental behaviour of persistent, mobile and toxic and very persistent and very mobile substances in the sources of German drinking water	Isabelle Neuwald, Daniel Hübner, Laura Wiegand, Vassil Valkov, Ulrich Borchers, Karsten Nödler, Marco Scheurer, Sarah Hale, Hans Peter Arp, Daniel Zahn	Annual Meeting of the German Waterchemical Society 2022	Online

D.3 Activity 6.2: At least one peer reviewed publication in English

Table D2 shows the 12 peer reviewed publications that have been prepared during the project period that are directly related to the PMT/vPvM substance work carried out, all acknowledging the project for funding.

Table D2: List of peer reviewed publications resulting from the project

Title	Authors	Journal	Year	DOI
The NORMAN Suspect List Exchange (NORMAN-SLE): Facilitating European and Worldwide Collaboration on Suspect Screening in High Resolution Mass Spectrometry	Hiba Mohammed Taha, Reza Aalizadeh, Nikiforos Alygizakis et al.	Environmental Sciences Europe	2022	https://doi.org/10.1186/s12302-022-00680-6
The occurrence, distribution and potential sources of persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM) substances in the sources of German Drinking Water	Neuwald, I. J., Hübner, D., Wiegand, L., Valkov, V., Borchers, U., Nödler, K., Scheurer, M., Hale, S. E., Arp, H. P. H., Zahn, D.	Environmental Science and Technology	2022	https://doi.org/10.1021/acs.est.2c03659
On Assessing the Persistence and Mobility of Organic Substances to	Arp, H. P. H and Hale S. E.	ACS Environmental Au	2022	https://doi.org/10.1021/acsenvironau.2c00024

Title	Authors	Journal	Year	DOI
Protect Freshwater Resources				
Ultra-Short-Chain PFASs in the Sources of German Drinking Water: Prevalent, Overlooked, Difficult to Remove, and Unregulated	Neuwald, I. J., Hübner, D., Wiegand, L., Valkov, V., Borchers, U., Nödler, K., Scheurer, M., Hale, S. E., Arp, H. P. H., Zahn, D.	Environmental Science and Tecnology	2022	10.1021/acs.est.1c07949
Sorption and Mobility of Charged Organic Compounds: How to Confront and Overcome Limitations in Their Assessment	Sigmund, G, Arp, HPH, Aumeier, BM, Bucheli, TD, Chefetz, B, Chen, W, Droge, STJ, Endo, S, Escher, BI, Hale, SE, Hofmann, T, Pignatello, J, Reemtsma, T, Schmidt, TC, Schonsee, CD, Scheringer, M	Environmental Science and Technology	2022	10.1021/acs.est.2c00570
Towards improved characterization of the fate and impact of hydraulic fracturing chemicals to better secure regional water quality	Jin, B., Han, M., Huang, C., Arp, H. P. H., & Zhang, G.	Environmental Science: Processes and Impacts	2022	https://doi.org/10.1039/D2EM00034B
The distribution of persistent, mobile and toxic (PMT) pharmaceuticals and personal care products monitored across Chinese water resources	Huang, C., Jin, B., Han, M., Yu, Y., Zhang, G., & Arp, H. P. H	Journal of Hazardous Materials Letters	2021	https://doi.org/10.1016/j.hazl.2021.100026
What's in a Name: Persistent, Mobile, and Toxic (PMT) and Very Persistent and Very Mobile (vPvM) Substances	Sarah E. Hale, Hans Peter H. Arp, Ivo Schliebner and Michael Neumann	Environmental Science & Technology.	2020	https://doi.org/10.1021/acs.est.0c05257
Persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM) substances	Sarah E Hale, Hans Peter H. Arp, Ivo Schliebner and Michael Neumann	Environmental Sciences Europe	2020	https://doi.org/10.1186/s12302-020-00440-4

Title	Authors	Journal	Year	DOI
pose an equivalent level of concern to persistent, bioaccumulative and toxic (PBT) and very persistent and very bioaccumulative (vPvB) substances under REACH.				
Persistent, mobile and toxic substances in the environment: a spotlight on current research and regulatory activities.	Rüdel, H., Körner, W., Letzel, T., Neumann, M., Nödler, K., & Reemtsma, T.	Environmental Sciences Europe	2020	https://doi.org/10.1186/s12302-019-0286-x
The need to adopt an international PMT strategy to protect drinking water resources.	Jin, B., Huang, C., Yu, Y., Zhang, G., & Arp, H. P. H.	Environmental Science & Technology	2020	https://doi.org/10.1021/acs.est.0c04281
Getting in control of persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM) substances to protect water resources: - Strategies from diverse perspectives	Hale, S.E Neumann, M., Schliebner, I., Schulze, J., Averbeck, F.S., Castell-Exner, C., Collard, C., Drmač, D., Hartmann, J., Hofman-Caris, R., Hollender., J de Jonge, M., Kullick, T., Lennquist, A., Letzel, T., Nödler, K., Pawlowski, S., Reineke, N., Rorije, E., Scheurer, M., Sigmund, G., Timmer, H., Trier, X., Verbruggen, E., Arp, H.P.H	Environmental Sciences Europe	2022	https://enveurope.springeropen.com/articles/10.1186/s12302-022-00604-4

D.4 Activity 6.3: A publication in German

The article in German was published in the 12/2021-issue of “energie | wasser-praxis”, the journal of the Deutscher Verein des Gas- und Wasserfaches e. V. (DVGW) - the German association for gas and water. The article is called “Persistente, mobile und toxische Stoffe: Vorkommen in Trinkwasserressourcen und deren Risikobeherrschung”. The authors are Isabelle Neuwald, Daniel Zahn, Karsten Nödler, Ulrich Borchers, Laura Wiegand and Marco Scheurer. The article primarily addresses water suppliers in Germany and focuses on

PMT/vPvM substances in general followed by a more detailed discussion of the issues surrounding PMT/vPvM substances in water supply and the need for resource protection.

D.5 Activity 6.5: Internet pages hosted by UBA in English and German

The UBA internet page related to PMT/vPvM substances has been significantly updated in English and German. Table D3 shows a brief description of all the webpages that are available at https://www.umweltbundesamt.de/en/PMT-substances and https://www.umweltbundesamt.de/PMT-stoffe.

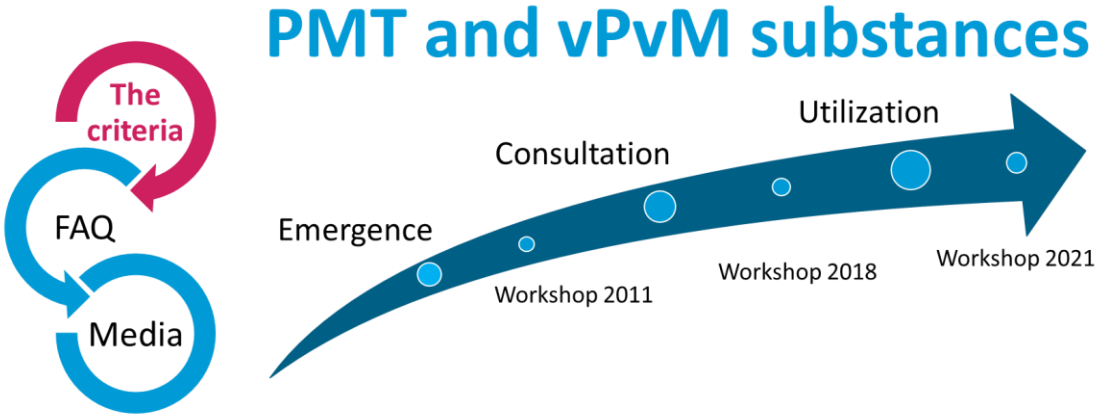
Table D3: Details about the PMT/vPvM substance web pages hosted by UBA

Web page title	Description of contents
Introduction to PMT/ vPvM substances	General information about the PMT/vPvM substance concept and why these substances are problematic. Long literature list of all outreach activities.
The criteria	A list of the PMT/vPvM criteria in their numerical form
Frequently asked questions	A list of FAQ and answers prepared during the project related to the substances, the criteria, their analysis, their occurrence etc
Media coverage	A selection of media coverage and dissemination from journalist, regulators, scientists, NGOs and legal bodies
Emergence of the PMT/vPvM criteria	Details of the scientific development of the criteria that occurred between 2009-2015 under REACH. The criteria can identify substances which have intrinsic properties that indicate a hazard to the sources of our drinking water.
First PMT workshop 2011	Information about the workshop "Evaluation of the relevance of substances to raw water in the context of the REACH regulation" where water suppliers, water research institutes, universities and authorities attended.
Public Consultation on the PMT/vPvM criteria	Details of the period between 2016 and 2019, where several public consultations were carried out to ensure a wide agreement on the PMT/vPvM criteria. The criteria were unveiled at the 30th Caracal meeting in 2019
Second PMT workshop 2018	Information about the workshop "PMT and vPvM substances under REACH. Voluntary measures and regulatory options to protect the sources of drinking water" which was attended by over 100 experts from 15 nations representing the water suppliers, chemical industry, academia and regulators.
Utilization of the criteria to identify PMT/vPvM substances	Details of the work carried out since 2019 where the PMT/vPvM criteria have been widely used under the EU´s chemicals legislation REACH to identify persistent and mobile substances.

Web page title	Description of contents
Third PMT workshop 2021	Information about the workshop "Getting control of PMT and vPvM substances under REACH" which was held as a digital meeting and where audience numbers peaked at 510.

The webpages have links to the most relevant supporting literature and a navigation function allowing people to move through the history of the PMT/vPvM substance work as shown in Figure D1.

Figure D1: Schematic used on the UBA website about PMT/vPvM substances



Source: Original Figure originally published on https://www.umweltbundesamt.de/en/PMT-substances

D.6 Activity 6.6: Wikipedia pages on PMT in English and German

A draft Wikipedia page in English and German has been developed, based on the current Wikipedia page for Persistent, bioaccumulative and toxic substances (https://en.wikipedia.org/wiki/Persistent,_bioaccumulative_and_toxic_substances). Independent from this project, German Wikipedia pages on PMT substances (https://de.wikipedia.org/wiki/PMT-Stoff) and vPvM substances (https://de.wikipedia.org/wiki/VPvM-Stoff) have appeared. The draft Wikipedia pages prepared for this project may be added to these existing pages.

D.7 Activity 6.7: PMT Youtube video

A song inspired by the PMT/vPvM substances list in Arp et al., (2023b) was published on youtube, using the ZeroPM-H2020 youtube channel, linking to the list of substances. It can be viewed on this website: https://www.youtube.com/watch?v=JAUeKIWIppk.

D.8 Activity 6.8: Communication with Chemical Safety NGOs and Journalists

During the project period, the consortium has been in contact with various chemical safety NGOs and journalists in order to present project results, provide comments for interviews and enter an active discussion. The most prominent of these are ChemSec (https://chemsec.org/about-us/), Chemical Watch (https://chemicalwatch.com/the-company/), CHEM Trust (https://chemtrust.org/) and The Green Science Policy Institute (https://greensciencepolicy.org/) all of whom support the PMT/vPvM substance criteria and their use. Table D4 summarises the various communication and outputs from discussion with these NGOs.

Table D4: Details about communication and outreach with NGOs and journalists

NGO name and date	Communication form	Description
European Commission May 2021	Narrative in the Science for Environment Policy newsletter	Article " Bioaccumulative and mobile substances: equivalent concerns in water resources"
Chemical Watch, July 2020	Interview comments from Hans Peter Arp for online article	Article "European Commission planning to make PMT, vPvM "categories" for SVHCs"
Chemical Watch, December 2020	Interview comments from Sarah Hale for online article	Article "Mobile substances are of "equivalent concern" to PBTs, say scientists"
Green Science Policy Institute	Presentation at PFAS Science and Policy monthly call by Sarah Hale	Short presentation called "Persistent, mobile and toxic (PMT) substances and their equivalent level of concern to persistent, bioaccumulative and toxic (PBT) substances"

ChemSec and CHEM Trust gave the following presentations at the Third PMT workshop

- PMT/vPvM substances on the SIN List, Anna Lennquist, ChemSec
- How to achieve better protection of the environment and human health from PMT/vPvM substances, Ninja Reineke, CHEM Trust

D.9 Activity 6.9: Spin-off Horizon 2020 Project

The research work in this project to stimulate the prevention, prioritization and technical solutions to PMT/vPvM substances formed the basis of a successfully funded research project, from the European Union Horizon 2020 research and innovation programme under grant agreement No 101036756. The project is called: ZeroPM - Zero Pollution of Persistent and Mobile substances. More information can be found on the website www.zeropm.eu.

E Selected PMT/vPvM substances for fact sheets

10 substances were selected for fact sheet development, as presented in Table E1. These 10 substances were selected based on the PMT/vPvM hazard classification, the priority level in this report, presence in monitoring data, and in one case (6-PPD) because it was a precursor of a PMT/vPvM substance.

Table E1: PMT/vPvM substances selected for development of fact sheets

Substance Name	EC number	PMT/vPvM hazard and priority
Melamine	203-615-4	vPvM & PMT, Highest-Priority
Sodium 3-(allyloxy)-2-hydroxypropanesulphonate	258-004-5	vPvM, High-Priority
1,2,4-triazole	206-022-9	PMT, High-Priority
1,3-diphenylguanidine	203-002-1	vPvM & PMT, High-Priority
Benzotriazole	202-394-1	vPvM & PMT, Highest-Priority
2-acrylamido-2-methylpropanesulphonic acid	239-268-0/ 225-948-4	vPvM, Highest-Priority
Cyanuric acid	203-618-0	vPvM & PMT, Highest-Priority
Trifluoroacetic acid	200-929-3	vPvM, Highest Prioirity
Trifluoromethanesulphonic acid	216-087-5	vPvM, Highest-Priority
N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine (6PPD)	212-344-0	Hydrolysable, precursor of a vPvM & PMT

During the course of the project, the competent authority in Germany submitted an intention for the identification of melamine as a SVHC based on its equivalent level of concern having probable serious effects to the environment. Melamine is therefore not included in the factsheets below.

E.1 Sodium 3-(allyloxy)-2-hydroxypropanesulphonate

Table E2: Substance identifiers for Sodium 3-(allyloxy)-2-hydroxypropanesulphonate

EC name (public):	Sodium 3-(allyloxy)-2-hydroxypropanesulphonate
IUPAC name (public):	sodium 2-hydroxy-3-(prop-2-en-1-yloxy)propane-1-sulfonate
Index number in Annex VI of the CLP Regulation:	Not given
Molecular formula:	C6H12O5S.Na
Molecular weight or molecular weight range:	218.21 g/mol
Synonyms:	*sodium 3-(allyloxy)-2-hydroxypropanesulphonate* *1-Propanesulfonic acid, 2-hydroxy-3-(2-propen-1-yloxy)-, sodium salt (1:1)* *sodium 2-hydroxy-3-(prop-2-en-1-yloxy)propane-1-sulfonate* *sodium 3-(allyloxy)-2-hydroxypropane-1-sulfonate* *AHPS*

Type of constituent: ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

E.1.1 Hazard information

Classification

Harmonised Classification in Annex VI of the CLP

There is currently no harmonised classification in Annex VI of the CLP.

Self classification

- In the registration:

In the registration dossier the following classification is given:

  - H315: Causes skin irritation
  - H318: Causes serious eye damage
  - H361: Suspected of damaging fertility or the unborn child <state specific effect if known> <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>.

- Additional classifications in the C&L Inventory:

There are no additional classifications in the C&L inventory.

Proposal for Harmonised Classification in Annex VI of the CLP

In 2020, the French competent authority submitted a proposal for harmonized classification and labelling of sodium 3-(allyloxy)-2-hydroxypropanesulphonate as Eye Dam. 1, H318 and Repr. 1B, H360F. At the time of writing (May 2021), an opinion had not been adopted.

CLP Notification Status

There are no notifications listed.

Additional information

All additional information below is taken from the registration dossiers.

Persistence

Biodegradation in water – screening tests

Key value is based on the observations in a study on biodegradation according OECD guideline 301C showing less than ten percent degradation under test conditions. The substance has to be regarded as not readily biodegradable. Under test conditions less than ten percent of the test item has been degraded based on analysis by BOD, DOC and substance-specific analysis by HLPC. This result is supported by (Q)SAR estimations (BIOWIN v4.10) indicating non-readily biodegradability, but potential for inherent degradation (Biowin 3 and 4 calculation indicates timeframe weeks - days).

Biodegradation in water and sediment: simulation tests

A simulation study in surface water according OECD 309 was performed. Under test conditions no relevant degradation within 60 days was observed. Based on the identified uses as well as the results from the distribution modelling direct and/or indirect exposure of sediment and/or soil is not expected. Therefore no further testing is considered and the substance is assumed to be very persistent in the environment. The mineralisation rate and route of degradation of [14C] - HAPS was investigatedin Calwich Abbey natural water system. The mean mass balance for all incubation groups was 98.32 % AR, this excludes the sterile vessels were recoveries were low, suspected due to a dosing issue. For the non-sterilised, viable test systems, parent compound was found to be stable with a mean of 93.49 % AR remaining at the end of the incubation period (61 DAT). For the sterilised samples, HAPS was found to be stable with 99.69 % AR (mean) remaining at 61 DAT.

Mobility

In absence of experimental data value has been estimated by KOCWIN v.2.00 based on the experimentally determined partition coefficient n-octanol/water. Based on the estimated Koc the substance is considered to be highly mobile in soil according to the McCall scheme. LogKoc: -0.4121, Koc at 20 °C: 0.387

Toxicity

Short-term toxicity to fish

Based on the results of a preceding range-finding test a final test was performed as a limit test. Seven carp per test group were exposed to a control and a HAPS concentration of 100 mg a.i./L. The total test period was 96 hours and a static test system was applied. Samples for analytical confirmation of actual exposure concentrations were taken at the start and the end of the test period.

Analysis of the samples taken at the start and the end of the limit test showed that measured concentrations were in agreement with nominal (100 %). The study met the acceptability criteria prescribed by the protocol and was considered valid.

HAPS induced no visible or lethal effects in carp at or below 100 mg a.i./L (NOEC). The 96h-LC50 exceeded 100 mg a.i./L (corrected for purity and based on analytically confirmed nominal concentrations).

Short-term toxicity to aquatic invertebrates

The study procedures described in this report were based on the OECD guideline No. 202, 2004. In addition, the procedures were designed to meet the test methods of the EEC directive 92/69, Part C.2, 1992 and the ISO International Standard 6341, 1996.

The batch of HAPS tested was a light yellow liquid consisting of 25.0 % HAPS (active ingredient; a.i.), 72.75 % water and 2.25 % sodium hydroxide. HAPS was completely soluble in test medium at the concentration tested. All concentrations reported were corrected for the purity of the test substance (25 %).

A limit test was combined with a range-finding test. Twenty daphnia per test group (4 replicates, 5 per vessel) were exposed to a control and a HAPS concentration of 100 mg/L in the limit test. In the combined range-finding test test daphnia (2 replicates, 5 per vessel) were exposed to HAPS concentrations of 0.1, 1.0, and 10 mg a.i./L. The total test peroid was 48 hours and a static test system was applied. Samples for analytical confirmation of actual exposure concentrations were taken at the start and the end of the test period.

Analysis of the samples taken at the start and the end of the limit test showed that measured concentrations were in agreement with nominal (97 -98 %).

The study met the acceptability criteria prescribed by the protocol and was considered valid.

HAPS did not induce acute immobilisation of Daphnia magna at 100 mg a.i./L after 48 hours of exposure (NOEC). The 48h-EC50 exceeded 100 mg a.i./L (corrected for purity and based on analytically confirmed nominal concentrations).

Toxicity to aquatic algae and cyanobacteria

The study procedures described in this report were based on the OECD guideline No. 201, 2006. In addition, the procedures were designed to meet the test methods of the EEC Directive 92/69, Part C.3, 1992 and the ISO International Standard 8692, 2004. The batch of HAPS tested was a light yellow liquid consisting of 25.0% HAPS (active ingredient: a.i.), 72.75% water and 2.25% sodium hydroxide. HAPS was completely soluble in test medium at the concentrations tested. All concentrations reported were corrected for the purity of the test substance (25%).

A combined limit/range-finding test was performed. Exponentially growing algal cultures were exposed to a control and a nominal HAPS concentration of 100 mg a.i./L in the limit test. In the combined range-finding test algae were exposed to nominal HAPS concentrations of 0.1, 1.0 and 10 mg a.i./L. The total test period was 48 hours and the initial algal cell density was 10^4 cells/mL. Samples for analytical confirmation of actual exposure concentrations were taken at the start, after 24 and 48 hours of exposure. Analysis of the samples taken during the test showed that the

measured concentrations were in agreement with nominal (94 -98%). The study met the acceptability criteria predescribed by the protocol and was considered valid. No significant reduction of growth rate was recorded up to and including a HAPS concentration of 100 mg a.i./L. Both the EC50 for growth rate reduction and the EC50 for yield inhibition exceeded 100 mg a.i./L (corrected for purity and based on analytically confirmed nominal concentrations.).

Toxicity to microorganisms

In the conducted test, the test item was tested using five concentrations (ranging from 3820 to 3.82 mg/L test item resp. 1452 to 1.45 mg act. ingr./L HAPS). Duration of the test was three hours. Activated sludge was used as inoculum. It was taken from a domestic sewage treatment plant and washed before usage. The dry matter was determined as 3.18 g suspended solids/L, giving a concentration of 1.59 g suspended solids/L in the test.

3,5 -Dichlorophenol was used as positive control. Five concentrations were tested; a 3h-EC50 of 8.2 mg/L (95% c.i.: 3h-EC50 < 12 mg/L) was determined, which lies within the demanded range of 2 -25 mg/L.

As inhibition was below 10 % in the highest treatment (3820 mg/L, using five replicates) and no statistically significant difference to the control was observed, this concentration was stated as the NOEC and no second experiment was performed.

E.1.2 Information on tonnage and usage

Registrations	☒ Full registration(s) (Art. 10) ☐ Intermediate registration(s) (Art. 17 and/or 18)
Total tonnage band for substance (excluding volume registered under Art 17 or Art 18, or directly exported)	≥ 1 000 to < 10 000 tonnes per annum

Overview of uses of Sodium 3-(allyloxy)-2-hydroxypropanesulphonate

The substance is manufactured and/or imported in the European Economic Area in quantities at ≥ 1 000 to < 10 000 tonnes per annum. This volume does not take into account any exports into countries not being member of the EEA. This substance is used in formulation or re-packing, at industrial sites and in manufacturing.

Table E3: Uses according to public information at ECHA's registration data base (date of access: May 2021).

Use	Information
Uses as intermediate	Not used as an intermediate.
Formulation or re-packaging	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. Release to the environment of this substance can occur from industrial use: formulation of mixtures and formulation in materials.

Uses at industrial sites	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. This substance is used for the manufacture of: food products. Release to the environment of this substance can occur from industrial use: in processing aids at industrial sites.
Uses by professional workers	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. ECHA has no public registered data on the types of manufacture using this substance. ECHA has no public registered data on the routes by which this substance is most likely to be released to the environment.
Consumer Uses	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. ECHA has no public registered data on the routes by which this substance is most likely to be released to the environment.
Article service life	ECHA has no public registered data on the routes by which this substance is most likely to be released to the environment. ECHA has no public registered data indicating whether or into which articles the substance might have been processed.

Uses according to SPIN database [4]

For the latest reporting year (2019) the database on Substances in preparations in Nordic countries (SPIN) reports the following data:

Country	#prep	tonnes	Consumer preparations	Confidential
SE	0	0	-	Yes

Additional data for 2019 can not be obtained as the data is classified as confidential.

[4] www.spin2000.net; date of access: 24.05.2021

E.2 1,2,4- triazole

Table E4: Substance identifiers for 1,2,4- triazole

EC name (public):	1,2,4-triazole
IUPAC name (public):	1H-1,2,4-triazole
Index number in Annex VI of the CLP Regulation:	613-111-00-X
Molecular formula:	$C_2H_3N_3$
Molecular weight or molecular weight range:	69.0654 g/mol
Synonyms:	*1,2,4,-Triazole* *1H-1,2,4-Triazole* *4H-1,2,4-triazol* *4H-1,2,4-triazole* *triazole 124* *s-Triazole* *4H-1,2,4-Triazole (VAN)*

Type of constituent: ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

E.2.1 Hazard information

Classification

Harmonised Classification in Annex VI of the CLP

Table E5: Harmonised classification according to Annex VI of Regulation (EC) No 1272/2008

	Index No	International Chemical Identification	EC No	CAS No	Hazard Class and Category Code(s)	Hazard statement code(s)	Spec. Conc. Limits, M-factors
	613-111-00-X	1,2,4-triazole	206-022-9	288-88-0	Acute Tox. 4 *	H302	
					Eye Irrit. 2	H319	
					Repr. 2	H361d	
Revised harmonized classification and labelling by RAC opinion adopted at 15-Mar-2019	613-111-00-X	1,2,4-triazole	206-022-9	288-88-0	Acute Tox. 4 *	H302	oral: ATE = 1320 mg/kg bw
					Eye Irrit. 2	H319	
					Repr. 1B	H360DF	

Self classification

- In the registration:

Classifications reported in registrations (ECHA dissemination website3, assessed at 28-Oct.-2019) are in accordance with those listed in Annex VI of CLP regulation. The Registrants apply no additional classifications.

- Additional classifications in the C&L Inventory:

Self classification according to ECHA's C&L inventory

Hazard Class and Category Code(s)	Hazard Statement Code(s)
Eye Irrit. 2A	H319
Aquatic Chronic 3	H412

Proposal for Harmonised Classification in Annex VI of the CLP

Belgium proposed to add the oral ATE = 1320 mg/kg bw for the Acute Tox. 4 and to modify the Repr. 2 to Repr. 1B. RAC followed this proposal at 15-March-2019. The revised classification is included in the 17th ATP to CLP [5] and shall apply from 17 December 2022.

CLP Notification Status

CLP Notifications

	CLP Notifications [6]
Number of aggregated notifications	18
Total number of notifiers	595

Additional information

All additional information below is taken from the registration dossiers.

Persistence
The readily biodegradable potential of 1,2,4-triazole has been investigated in the frame of an OECD 301 A test (Thiebaud, 1995). Under the test conditions it is concluded that 1,2,4-triazole is not readily biodegradable.

[5] https://eur-lex.europa.eu/legal-content/DE/TXT/?uri=CELEX%3A32021R0849&qid=1626249101859

[6] http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database (accessed 21. May 2021)

In addition, an OECD Guideline 302B study (inherent biodegradability: Modified Zahn-Wellens Test) was performed. The test substance showed only a very low degree of degradation (1%) after 28 days (US EPA, 2009).

Nevertheless, a simulation biodegradation test in soil has been performed (Tarara, 2004) and it can be concluded that 1,2,4-triazole is degraded under the investigated conditions in northern and southern Europe with no observation of a significant vertical movement. The test item 1,2,4-triazole was significantly degraded at three test sites Burscheid, Albaro and Little Shelford within the course of the study and it was nearly completely degraded at site Vilobi d'Onyar. The slower degradation at this site can be explained by the temperature and rainfall to be below long-term averages at the test location for several months during the runtime of the study. Half-life were determined between 6.8 to 28.1d.

Based on the results of the study Tarara (2004) it can be concluded that 1,2,4-triazole is degraded under the investigated conditions in northern and southern Europe with no observation of a significant vertical movement. The test item 1,2,4-triazole was significantly degraded at three test sites Burscheid, Albaro and Little Shelford within the course of the study and it was nearly completely degraded at site Vilobi d'Onyar. The slower degradation at this site can be explained by the temperature and rainfall to be below long-term averages at the test location for several months during the runtime of the study. Half-lives were determined between 6.8 to 28.1d.

Mobility

An experimental log KOC of 1.6 has been reported (get reference from HP). This values places 1,2,4-triazole in the very mobile category as defined by Neumann and Schiblener (ref). The definition of very mobile is "the lowest organic carbon-water coefficient log KOC over the pH range of 4-9 is less than 3.0."

Toxicity

Short term toxicity to fish

A test with the sodium salt (sodium 1,2,4 -triazol-1-ide) has been performed according to OECD 203 guideline and GLP requirements (Thiebaud, 2001). Under environmental conditions, the sodium salt is reactive with water, and the 1,2,4-triazole can therefore be considered as its degradation product. On this basis it seems reasonable to use the available data to assess the toxicity of the 1,2,4 -triazole. The substance was not lethal to Danio Rerio exposed for 96h to the measured concentration of 97mg/L. Another study has been performed according to OECD 203 guideline on Oncorhynchus mykiss with 1,2,4-triazole (Rufi, 1983). LC50_96h has been determined to be 760 mg/L expressed in terms of nominal concentrations. But the concentration was not maintained during the test.

Long term toxicity to fish

The chronic toxicity of 1,2,4-Triazole to juvenile Rainbow Trout (Oncorhynchus mykiss) was determined in a static-renewal test over an exposure period of 28 days accoding to OECD 215 guideline and GLP requirements (Dorgerloh, 2001). In this test fish were exposed to nominal concentrations of 1.00, 3.20, 10.0, 32.0 and 100 mg test item/L. The concentrations were maintained during the test. The fish wet weights on day 28 and the 'pseudo' specific growth rates

show no significant difference compared to the pooled control groups in the period of 0 - 28 days. The the NOErC (0-28d) is reported as > 100 mg test item/L.

Short term toxicity to aquatic invertebrates

The acute toxicity of 1,2,4 Triazole to Daphnia magna has been investigated in an OECD 202 test according to GLP requirements (Thiebaud and Kae, 1996). In the test conditions, no effect was observed at the highest concentration tested. The concentrations were maintained within 80% throughout the duration of the test. Therefore, the EC50-48h was determined to be higher than 494.7 mg/L. In addition, the acute toxicity of 1,2,4 Triazole to Daphnia magna has been investigated in another OECD 202 test (Rufli, 1982) and can be used as a supporting study. The EC50-24h was determined to be higher than 900 mg/L (nominal concentrations). However, the concentrations were not completely maintained within 80% throughout the duration of the test. To conclude, 1,2,4 Triazole is considered as not harmful to aquatic invertebrates.

Toxicity to aquatic algae and cyanobacteria

The acute toxicity of 1,2,4 Triazole to Pseudokirchnerella subcapitata has been investigated in an OECD 201 test according to GLP requirements (Thiebaud & Bouraly, 1998). In the test conditions, the ErC50 -72h is 45 mg/L and the NOEC is 3.49 mg/L. The test concentrations were maintained within 80% during the test. Therefore, 1,2,4 Triazole is considered as harmful to algae. Another test similar to OECD guideline 201 has been performed and can be used as a supportive study (De Morsier, 1982). The cell concentration was determined at 120 hours instead of at least at 24, 48 and 72 hours after the start of the test. Therefore only an EC50-value after 5 days is given. in addition, concentrations were not maintained within 80% during the test. The EC50 -5d was determined to be 6.3 mg/L (nominal concentrations).

Toxicity to microorganisms

The toxicity of 1,2,4 triazole was studied according to an OECD 209 guideline and GLP requirements (Muckle, 2009). All validity criteria were met.

The inhibition which was caused by the test item1,2,4-Triazole did not rise above 45%. The graph inhibition vs. concentration shows a very gentle slope altogether. No adequate increase in inhibition was observed. In the first experiment, 27% inhibition (mean) was observed at the lowest concentration of 1 mg/L. The inoculum in the first experiment was more sensitive than in the second experiment. Therefore, the inhibition values in the second experiment (test item and positive control) were slightly lower. But the difference within the values was in a normal range of a biological system.

Due to the test item's properties (inhibitor of nitrification), the test item shows stronger inhibitory action to nitrifying micro-organisms which are present in the activated sludge, so that respiration of these micro-organisms is completely inhibited, whereas carbon oxidising micro-organisms are less inhibited. So in an additional experiment in presence of an inhibitor in all treatments (control, positive control and test vessels), calculation of the separate total, heterotrophic and nitrification oxygen uptake rate would have been possible. But in the highest concentrated treatment low total inhibition values (< 50%) were found; the calculated EC50 for total respiration is above 1000 mg/L. Therefore, the sponsor decided that no second experiment had to be performed in order to discern between inhibition of nitrificators and inhibition of total population.

The result of the test can be considered valid.

Toxicity to soil macroorganisms except arthropods

The results of this study show neither lethal nor sublethal effects of 1,2,4-triazole on earthworms E. fetida. Mortality, growth, reproduction and feeding activity of the earthworms were not affected by exposing them to 7.08 µg/kg, 35.41 µg/kg and 70.81 µg/kg soil of 1,2,4-triazole. Consequently the conclusion of this study is that 1,2,4-triazole does not cause lethal or sublethal effects on earthworms E. fetida if applied in amounts up to 70.81 µg/kg soil. The NOEC found in this study was 70.81 µg/kg soil, the highest concentration tested.

Toxicity to soil microorganisms

The influence of 1,2,4 Triazole on soil microorganisms was determined in control and treated soil samples by measuring the microbial CO2 evolved during short-term respiration experiments after glucose amendments. Furthermore, its influence on the nitrification of lucerne meal, was investigated. In this study, one fresh agricultural soil, a sandy loam, was moistened to 42% of its maximum water-holding capacity and incubated in the dark at 20 ±2°C following treatment with the test item. The two application rates are equivalent to doses of 0.033 mg and 0.333 mg 1,2,4 Triazole/kg dry soil, respectively.

On the basis of the results obtained, it can be concluded that 1,2,4 triazole will cause no adverse effect on organic matter turnover, and hence on soil fertility, even at rates up to ten times the recommended field rate.

E.2.2 Information on tonnage and usage

Registrations	☒ Full registration(s) (Art. 10) ☐ Intermediate registration(s) (Art. 17 and/or 18)
Total tonnage band for substance (excluding volume registered under Art 17 or Art 18, or directly exported)	≥ 1 to < 10 tonnes per annum

Overview of uses of 1,2,4- triazole

The substance is manufactured and/or imported in the European Economic Area in quantities at ≥ 1 to < 10 tonnes per annum. This volume does not take into account any exports into countries not being member of the EEA. This substance is used by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing.

Table E6: Uses according to public information at ECHA's registration data base (date of access: May 2021).

Use	Information
Uses as intermediate	Not used as an intermediate.

Formulation or re-packaging	This substance is used in the following products: fertilisers. This substance has an industrial use resulting in manufacture of another substance (use of intermediates). Release to the environment of this substance can occur from industrial use: formulation of mixtures and as processing aid. Other release to the environment of this substance is likely to occur from: indoor use as processing aid and outdoor use resulting in inclusion into or onto materials (e.g. binding agent in paints and coatings or adhesives).
Uses at industrial sites	This substance is used in the following products: fertilisers, laboratory chemicals and pharmaceuticals. This substance has an industrial use resulting in manufacture of another substance (use of intermediates). This substance is used in the following areas: agriculture, forestry and fishing and health services. This substance is used for the manufacture of: chemicals. Release to the environment of this substance can occur from industrial use: as an intermediate step in further manufacturing of another substance (use of intermediates), manufacturing of the substance, formulation of mixtures, as processing aid and of substances in closed systems with minimal release. Other release to the environment of this substance is likely to occur from: indoor use as processing aid and outdoor use resulting in inclusion into or onto materials (e.g. binding agent in paints and coatings or adhesives).
Uses by professional workers	This substance is used in the following products: fertilisers. This substance is used in the following areas: agriculture, forestry and fishing. Other release to the environment of this substance is likely to occur from: outdoor use as reactive substance.
Consumer Uses	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. ECHA has no public registered data on the routes by which this substance is most likely to be released to the environment.
Article service life	ECHA has no public registered data on the routes by which this substance is most likely to be released to the environment. ECHA has no public registered data indicating whether or into which articles the substance might have been processed.

Uses according to SPIN database [7]

For the latest reporting year (2019) the database on Substances in preparations in Nordic countries (SPIN) reports the following data:

Country	#prep	tonnes	Consumer preparations	Confidential
DK	5	0	-	-

[7] www.spin2000.net; date of access: 24.05.2021

Country	#prep	tonnes	Consumer preparations	Confidential
SE	6	0	-	-

From the use categories to be reported for SPIN (use category description scheme UC 62), the greatest amount of 1,2,4-triazole is used as photochemicals (total number of preparations reported 17, 0.9 tonnes over the years 2002-2004).

Data from SPIN is not fully representative for the European Economic Region because products and frequency of application may differ between the different geographical regions in the EU. In addition, the SPIN database not only refers to products where substances are intentionally added, but also deals with occurrence of substances as impurities.

Based on the data from the notifications for 2019, SPIN concludes a potential exposure for 1,2,4-triazole for surface water, air and wastewater. SPIN concludes a probable consumer and occupational exposure and SPIN concludes a very probable exposure for soil.

Table E7: Exposure potential of 1,2,4-triazole from products, according to SPIN database, with use index out of 5, unless specified

Country	Quant.	Surface water	Air	Soil	Wastewater	Consumers	Occupational	Range of Use (RoU)	Article index (max: 3)
DK	1	1	1	3	3	4	4	1	1
SE	1	3	3	5	3	4	4	2	1

On the basis of this information there is evidence that in principle, uses of 1,2,4-triazole result in relevant emissions into all environmental compartments.

Additional information

Regulatory obligations exist for 1,2,4-triazole under the following regulations:

- Active Implantable Medical Devices Directive - Hazardous Substances, Directive 90/385/EEC
- CAD - Chemical Agents Directive, Article 2(b)(i) - Hazardous Agents
- Construction Product Regulation - Annex I (3) - Hazardous Substances
- Construction Product Regulation - Article 6(5) - SDS and Declaration
- Cosmetic Products Regulation, Annex II - Prohibited Substances
- End-of-Life Vehicles Directive - Hazardous Substances
- Ecolabels - Restrictions for Hazardous Substances/Mixtures
- Active and Intelligent Materials - CMR Substances not allowed for use
- General Product Safety Directive - Hazardous Substances
- In Vitro Diagnostic Medical Devices Directive - Hazardous Substances

- Marine Environmental Policy Framework Directive - Hazardous Substances
- Medical Devices Directive - Hazardous Substances
- Protection of Pregnant and Breastfeeding Workers Directive, Annex I+II
- Safety and Health of Workers at Work Directive - Hazardous Substances
- Safety and Health of Workers at Work Directive - Workplace Signs - minimum requirements & signs on containers and pipes
- Waste Framework Directive, Annex III - Waste - Hazardous Properties

E.3 1,3-diphenylguanidine

Table E8: Substance identifiers for 1,3-diphenylguanidine

EC name (public):	1,3-diphenylguanidine
IUPAC name (public):	1,3-diphenylguanidine
Index number in Annex VI of the CLP Regulation:	612-149-00-4
Molecular formula:	C13H13N3
Molecular weight or molecular weight range:	211.2624 g/mol
Synonyms:	*1,3-Diphenylguanidine* *N,N'-Diphenylguanidine* *Guanidine, N,N'-diphenyl-*

Type of constituent: ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

E.3.1 Hazard information

Classification

Harmonised Classification in Annex VI of the CLP

Index No	International Chemical Identification	EC No	CAS No	Classification	
612-149-00-4	1,3-diphenylguanidine	203-002-1	102-06-7	Hazard Class and Category Code(s)	Hazard Statement Code(s)
				Acute Tox. 4 *	H302
				Skin Irrit. 2	H315
				Eye Irrit. 2	H319
				STOT SE 3	H335
				Aquatic Chronic 2	H411
				Repr. 2	H361f ***

Self classification

- In the registration:

The C&L Inventory contains notifications on classification and labelling according to CLP criteria from 554 notifiers[8].

The number of notifications for each Hazard Class Category Codes and Hazard statement code(s) is given in the table below.

Hazard Class Category Codes and Hazard statement code(s)	Number of Notifiaction
STOT SE 3	543
H335	428
H335 (data lacking) (Inhalation)	25
H335 (Lungs)	38
H335 (Not applicable)	1
H335 (not specified)	16
H335 (organs)	1
H335 (other:-)	11
H335 (other:respirato...) (Inhalation)	18
H335 (other:unknown)	4
H335 (Respiratory tra...) (Inhalation)	1
Skin Irrit. 2	**536**
H315	536
Aquatic Chronic 2	**536**
H411	536
Repr. 2	**535**
H361	40
H361 (f)	427
H361 (Oral)	25
H361 (Oral) (f)	3
H361 (Suspected of da...)	40

[8] Date of access and data compilation: 30-Aug-2021

Hazard Class Category Codes and Hazard statement code(s)	Number of Notifiaction
Eye Irrit. 2	**534**
H319	534
Acute Tox. 4	**376**
H302	376
Acute Tox. 3	**178**
H301	178
Eye Dam. 1	**19**
H318	19
Aquatic Chronic 3	**18**
H412	18
Repr. 1B	**18**
H360 (May damage fert...)	18
Eye Irrit. 2A	**1**
H319	1

- Additional classifications in the C&L Inventory:

Proposal for Harmonised Classification in Annex VI of the CLP

There are no further proposals at November 2021.

CLP Notification Status

There is no CLP notification status given.

Additional information

All additional information below is taken from the registration dossiers.

Persistence

Hydrolysis

The substance undergoes hydrolysis at elevated temperatures and pH (Wohlfahrt and Niebergahl 1984), but it should be noted that these temperatures are not environmentally relevant (Canada 2013, https://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=7B3B293F-1).

A number of reported data were available on 1,3-diphenylguanidine from 1960 to 1988. However, data assessment was difficult because the studies were poorly documented. In two studies (Chou

et al., 1983 ; Kondo, 1988), DPG was for example noted as rapidly degraded in non-adapted river water but no sound biodegradation follow-up was performed. In addition, the results of Saegar et al. (1988) suggested that the test item could be readily biodegradable. That is the reason why a full GLP OECD 301D study was commissioned in 2015. This study showed that DPG is readily biodegradable and that no persistent metabolite can be expected.

Chou et al. (1980) conducted a study of primary degradation of DPG (1,3-Diphenylguanidine) at a pH of 7.5 measured at the beginning of the test, and found total loss of the parent substance within 14 days of exposure to unadapted river water.

The key study (study report#1, 2015) shows that 1,3-diphenylguanidine is hydrolytically stable in water at environmental pH. No hydrolysis took place at 50°C at pH 4; 7 and 9 and neither at 37°C at pH 1.2, indicating that 1,3-diphenylguanidine is hydrolytically stable. The estimated half-life at 25°C of the substance tested is higher than one year at pH 4; 7 and 9. In this context, no degradation product has been investigated in this study.

Additional studies (Wohlfahrt, R. & Niebergall, H.1984 and 1985, Reliability Index (RI)=3), investigated the hydrolytic properties of DPG (0.3 g/L or 0.3 wt. % in water) in relation to the pH value at high temperature (80°C). These additional studies do not investiguate the potential hydrolysis of DPG under environmental conditions but allow to identify 1,3-diphenylurea and aniline as hydrolysis products under industrial process (*i.e.* during vulcanization process) at high temperature in contact with water. 1,3-diphenylurea was further hydrolyzed to aniline in both the acidic and alkaline environments.

The eMSCA concludes that the DPG is hydrolytically stable in water under environmental conditions.

Phototransformation in air

The QSAR data on phototransformation in air are summarised as the following results: Reaction with hydroxyl radicals at 25oC:, Overall OH Rate Constant: =85.3159 x 10-12cm3/molecule-sec, Half Life: =0.125 days, 1.504 hours (12-hour day; 1.5x106OH/cm3). Reference AOPWIN v1.92 model

Based on the data on photochemical degradation in the air, DPG is considered to rapidly degrade in the atmosphere *via* photo oxidation process. The eMSCA can support this conclusion.

Phototransformation in water

The registrant reports an estimated half-life of DPG in water of approximately 37.5 days (900 hours) using EPI Suite software, and based on the available information, the eMSCA can support this conclusion.

Phototransformation in soil

The registrant reports an estimated half-life of DPG in soil of approximately 75 days (1800 hours) using EPI Suite software, and based on the available information, the eMSCA can support this conclusion.

Biodegradation

Biodegradation in water

Screening tests

The study on biodegradation in water (screening tests) is summarised as:

According to OECD guideline 301D (ready biodegradability:closed bottle test) - 86 after 14 days (%degradation O2 consumption) (based on ThOD-NH3), 85 after 28 days (%degradation O2 consumption) (based on ThOD-NO3)

The study (Study Report#2, 2015; Reliability Index (RI) =1) presents the biotic degradation of 1,3-diphenylguanidine following the OECD guideline 301D. In ready biodegradability tests, microorganisms are inoculated into a chemically defined liquid medium containing the test substance as sole carbon and energy source. The 1,3-diphenylguanidine is exposed to microorganisms present in river water, under aerobic conditions for a period of at least 28 days. The biodegradation percentages calculated with ThODNH3 represents the degradation of 1,3-diphenylguanidine. Results of the test show that 85% of the substance was biodegraded at day 28 in the closed bottle, and over 60% biodegration is achieved after approximately 10 days. The test substance therefore fulfilled the 14-day time window criterion for ready biodegradable substances. Hence, it can be concluded that the 1,3-diphenylguanidine is readily biodegradable.

Mode of degradation in actual use

The study on mode of degradation in actual use is summarised in the following table:

Mode of degradation in actual use

Using a simultaneous TG/DSCFTIR techniques under nonisothermal conditions, results showed Thermal decomposition of N,N0-diphenylguanidine (DPG) was investigated by simultaneous TG/DSCFTIR techniques under nonisothermal conditions. Online FTIR measurements illustrate that aniline is a major product of DPG decomposition (Hu Q. et al., 2012)

Guanidine derivatives have been widely used as vulcanization accelerators in rubber industry. 1,3-diphenylguanidine (DPG) has been used as a primary and secondary accelerator in the vulcanization of rubber. Although it is well known that DPG could be broken down at high temperature, leading to the formation of carcinogenic aniline, little is known about the thermal decomposition kinetics of DPG.Thermal decomposition of N,N0-diphenylguanidine (DPG) was investigated by simultaneous TG/DSCFTIR techniques under nonisothermal conditions. Online FTIR measurements illustrate that aniline is a major product of DPG decomposition. The observation that the activation energy depends on the extent of conversion indicates that the DPG decomposition kinetics features multiple processes. The initial elimination of aniline from DPG involves two pathways because of the isomerization of DPG. Mass spectrometry and thin film chromatography suggest that there are two major intermediate products with the major one of C21N3H17. The most probable kinetic model deduced through multivariate nonlinear regression method agrees well with the experimental data with a correlation coefficient of 0.9998. The temperature-independent function of conversion f(a), activation energy E and the pre-exponential factor A of DPG decomposition was also established through model-fitting method in this research.

Based on the available data, the eMSCA concludes that aniline is a major product of thermal decomposition of DPG.

Mobility

The following results are shown according to OECD guideline 106 (Adsorption-Desorption using a batch equilibrium method) - Adsorption coefficient: Soil I: log Koc=2.5 at 20.3°C (org.C=1.74%), Soil II: log Koc=2.81 at 20.3°C (org.C=0.67%), Soil III: log Koc=2.95 at 20.3°C (org.C=1.98%), Soil IV: log Koc=3.14 at 20.3°C (org.C=1.66%), Soil V: log Koc=2.91 at 20.3°C (org.C=1.54%). The mean value of the organic carbon-water partition coefficient (Koc) is 807mL/g corresponding to LogKoc = 2.9.

For QSAR model KOWIN - KOCWIN v.2.00 QSAR estimation. Adsorption coefficient: log Koc: ca. 3.21 (estimated data (from MCI)), Koc: ca. 1652 (estimated data (from MCI)), log Koc: ca. 2.43 (estimated data (from log Kow)), Koc: ca. 273.4 (estimated data (from log Kow)).

With a pKa > 10, 1,3-diphenylguanidine is in cationic form at environmentally relevant pH, and thus has a very high affinity for organic matter and other matrix having a high cation exchange capacity. According to ECHA guidances, the behavior of a substance is based partly on its adsorption / desorption properties. Thus, substances with a Koc below 500 to 1.000 L/kg are generally unlikely adsorbed to sediment. To avoid extensive testing of chemicals, a log Koc (or log Kow) ≥ 3 can be used as a trigger value for sediment effects assessment. In practice a cut-off value for log Kow of 3 can be applied for adsorption potential. We acknowledge that for "classic" organic substances (i.e. non polar, non surface active, soluble in water, low adsorptive properties, etc), the Koc should be estimated using read-across or QSPR methods as a first step. In the information provided by the applicant, the adsorption potential of 1,3-diphenylguanidine is estimated by QSAR on the basis of log Kow. The organic carbon-water partition coefficient (Koc) was calculated using KOCWIN v. 2.0. Based on the first-order molecular connectivity index (MCI) and the logKow = 2.89. Koc (estimated from MCI) = 1652 L/kg, logKoc = 3.22, and the Koc (estimated from logKow) =273.4 L/kg; log Koc=2.44. However for ionized substance at environmentally relevant pH like 1,3-diphenylguanidine, substance adsorption is not triggered by the lipophilicity (i.e. log Kow of the substance), but by other mechanisms (i.e. ionic interaction). Applying QSPR methods for estimating the adsorption potential of 1,3-diphenylguanidine would lead to a probable underestimation of Koc.

A recent study (Study Report#3, 2015; RI=1) has assessed the adsorption/desorption capacity of the 1,3-diphenylguanidine using the OECD 106 guideline (using a batch equilibrium method). Five different types of soils are investigated: soil 1 (Speyer 2.2, loamy sand), soil 2 (Speyer 2.3, sandy loam), soil 3 (Speyer 2.4, loam), soil 4 (Speyer 6S, clay) and soil 5 (Am Fischteich, silt loam). A tested concentration of 1.077mg/l and a soil-to aqueous phase ratio of 1:5 is used for all five soils. After 24h of agitation, aliquots of the aqueous phase were measured with HPLC (LC-MS). Results show that adsorption equilibrium has reached 52.3%, 46.4%, 77,9%, 82% and 71.3% of the applied amount absorbed to soils 1 to 5, respectively. The amount of test item desorbed reached an equilibrium after about two hours of desorption. The mean values for the adsorption and desorption coefficients related to the organic carbon content of the soils, Koc and Kdes,oc were 807 mL/g and 1077 mL/g, respectively. So, Log Koc ranged from 2.5 to 3.13 with five soils displaying arithmetic mean log Koc = 2.9. These results indicate that 1,3 diphenylguanidine does not bind strongly on soil.

Based on the available experimental data and QSAR predictions provided by the registrant, the eMSCA concludes that DPG does not bind strongly on soil.

Volatilisation

In the registration dossier, the vapour pressure of 1,3 -diphenylguanidine was evaluated in a study performed in accordance with OECD testing guideline 104 and GLP requirements. The method used is the Knudsen cell effusion method coupled to a microbalance. As the logarithm of the vapour pressure of a pure substance is a linear function of the inverse of the temperature, the vapour pressure is determinated in a limited temperature range (80 -100°C). Three vapour pressure are determinated: at 81°C, P = 6.524Pa; at 90°C P=5.548 Pa and at 100°C P= 5.896 Pa. The vapour pressure of 1,3 -diphenylguanidine extrapolated at 20°C is 7.4e-11 Pa. The hydrosulbility of DPG was found equal to 325mg/L at 20°C (i.e. 1.54 mol/m3) So as a consequence the Henry's law value equals 4.82e-8 Pa.m3.mol-1 at 20°C.

However, not enough information is available to confirm the reliability of this data.

Therefore, the MSCA of France has proposed a calculation of Henry's law constant using the validated values of water solubility 325 mg/L, the validated vapour pressure of 3.7x 10-10 Pa and molecular mass of 211.2, which gives a value of 2.4 x 10-10 Pa.m3.mol-1.

Value used for risk assessment: Henry's law constant calculated from solubility in water and vapour pressure values is 2.4 x 10-10 Pa.m3.mol-1. Substance Evaluation Conclusion document EC No 203-002-1. FR-MSCA 21 December 2020

Toxicity

Short-term toxicity to fish

In a study performed by Bayer AG in 1970 the determination of the acute toxicity of DPG to golden orfes (Leuciscus idus) gave LC0 -72h = 1mg/l and a LC100 -48h = 10 mg/l. Nevertheless, this study is considered as not reliable due to the tested period (48h) which was shorter than the recommended exposure time period.

The acute toxicity of DPG (1,3-diphenylguanidine) toOryzias latipes was investigated using the Japanese Industrial Standard test (JIS K 0102 -1986 -71) (static or semi-static; 25°C +/- 2°C; solubilizer not specified). A LC50 of 10 mg/l was determined after a 48-h exposure. This study is considered as invalid due to significant methodological deficiencies.

A data sheet of the Monsanto Company (1986) contains the following information:

Pimephales promelas LC50 -96h = 4.2 mg/l

Lepomis macrochirus LC50 -96h = 9.6 mg/l

Salmo sp. LC50 -96h = 11 mg/l

Lastly, in an insufficiently documented study on Cyprinus carpio (single oral administration in gelatine capsule; flow-through system; 18°C), the following effects were observed by Loeb & Kelly (1963):

Dose in mg/kg bw Effect / Test Duration

3.2; 6.0 and 8.7 mg/kg bw no effects within 114 h

9.5 and 17 mg/kg bw not specified symptoms after < 120 h, recovery after < 312 h

5.6 mg/kg bw mortality after 71 h

9.5 and 70 mg/kg bw not specified symptoms after >= 22 h, mortality after 125 h

Nevertheless, gavage of fish cannot be considered as relevant for aquatic ecotoxicological hazard assessment.

Long-term toxicity to fish

DPG (1,3-Diphenylguanidine) has been shown to be toxic to fish and algae and harmful to daphnia in several acute studies (fish: 96 h LC50 = 4.2-11 mg/l; algae: 72 h EC50 = 7.5 mg/l; 96 h EC50 = 1.7 mg/l; daphnid : 24 h EC50 = 73.6 mg/l; 48 h EC50 = 17mg/l). The PNEC can be determined using the NOECs from the algae (0.3 mg/l) and daphnid chronic 21 d (0.6 mg/l) studies (excluding the EbC50 results), by applying an uncertainty factor of 50. The resulting PNEC would be 6 µg/l. In order to refine this PNEC value for the aquatic compartment we performed a long-term test on fish (following OECD 210 guidelines).

In brief, Pimephales promelas eggs were exposed to graded concentrations of DPG for 34 days (0.041, 0.13, 0.41, 1.3 and 4.2 mg/L) under semi-static conditions. After 8 days, all larvae had hatched. Both hatching and larval survival rates were recorded daily. At the end of the test, all surviving larvae were weighted and measured. No significant effect was observed on fish length and weight. The NOEC for both hatching and larval survival was 1.3 mg/L. EC50 for larval survival was 1.8 mg/L.

From this result, the retained NOEC will be 0.3 mg/L (algae results).

Short-term toxicity to aquatic invertebrates

In a study performed by Monsanto on the acute toxicity of 1,3 -diphenylguanidine to Daphnia a 48h-LC50 was estimated at 17 mg/l.

The acute toxicity of DPG to Daphnia magna was assessed using the methods outlined by the Commitee on Methods for Toxicity Tests with Aquatic Organisms. Water quality parameters of temperature, dissolved oxygen and pH were measured at the termination of the test and were within acceptable limits. The results of the 48 hour static Daphnia magna toxicity study are summarized as follows. 1,3-diphenylguanidine 48-hour LC50 = 17 (14-21) mg/1. The no effect level observed for 1,3-diphenylguanidine was 5.6 mg/1 after 48 hours.

In a more recent study performed according to the proposed procedures of the German federal environment agency (Umweltbundesamt) to determine the swimming ability of water fleas (Daphnia magna) in a static, non aerated system (21°C; pH=8, 9mg/o2/l), the 24 -hour EC50 was found to be 62.4 mg/l (geometrical mean; EC0 = 22 mg/l and EC100 = 177 mg/l). The daphnia population tested in the control was not sensitive enough to the reference substance potassium dichromate, according to the guideline.

Long-term toxicity to aquatic invertebrates

In a chronic toxicity study performed with Daphnia magna (life-cycle test following OECD 202; pH 7.7 - 8.8; 21.8°C; semi-static, non aerated system; analysis by HPLC) a 21d EC50 of >1.9 and < 6.0 mg/l was estimated for both immobilization / mortality and reproduction. At a concentration of 0.6 mg/l and 1.9 mg/l the reproduction rate dropped by 4.1 and 19.8% respectively and at concentration of 6.0 - 60 mg/l live animals were no longer seen after five days.

Toxicity to aquatic algae and cyanobacteria

A phytotoxicity test was performed at Bionomics Marine Research Laboratory (BMRL), Pensacola, Florida, to determine the effect of DPG (BN-79-1384358-le) on the freshwater alga Selenastrum capricornutum. Results of the test are reported as 24-, 48-, 72-, and 96-hour EC50. Cell numbers in exposed and control cultures were also determined after 96 hours of exposure and another 96-hour EC50 was calculated.

This study on the toxicity of 1,3 -diphenylguanidine to algae permitted to estimate an EC50 -96h = 1.4 - 1.7 mg/l concerning the cell division rate (determined by cell counter). The results obtained during this test are summarized hereafter:

EC50s based on chlorophyll a determination:

24h >5.6 mg/l

48h 3.5 mg/l (0.2-56)

72h 2.0 mg/l (0.2-17)

96h 1.4 mg/l (0.2-7.4)

96h EC50 based on cell number = 1.7 mg/l (0.4-7.4)

NOEC not calculated but based on available data can be taken as 0.3 mg/l at both 72 and 96h (for chlorophyll a and growth rate data at 96h).

In another test relative to the cell division inhibition (DIN 38412 part 9) the following values were determined for the green algae Scenedesmus subspicatus after 72 hours at a pH of 7.6 - 8.9 and 23°C+/-2°C: EC10 = 0.013 mg/l and EC50 = 2.6 mg/l (based on the biomass); EC10 = 2.1 mg/l and EC50 = 7.5 mg/l (based on the growth rate).

Toxicity to microorganisms

Tomlinson et al. (1966) investigated the effect of 1,3-diphenylguanidine on the nitrification process in municipal waste waters. They incubated purified activated sludge (dw = 1350 - 1700 mg/l) for 2 - 4 hours in residential waste water that was free of suspended particles in a shake culture (25°C; pH= 7.6 - 7.8) at various test compound concentrations. The nitrification rate was determined quantitatively by colorimetric measurement of the NO2- and NO3- concentrations. The effective concentration for decreasing the nitrification rate by 75% in the first stage (NH4 + =>NO2 -) compared to the control was estimated at 50 mg/l (highest tested ineffective concentration).

In vitro studies on cell homogenates of Escherichia coli B showed an inhibitive effect of 1,3 -diphenyl guanidine on specific steps of protein biosynthesis, due to non competitive inhibition of the phenylalanyl-tRNA synthetase. 50% inhibition occured at a molar inhibitor/amino acid ratio of 3.2. At an L-phenylalanine concentration of 0.3 mmol/l (49.5 mg/l) this corresponds to an EC50 of 202.8 mg/l 1,3 -diphenylguanidine/l.

Lastly, in the oxygen consumption test following OECD guideline 209, with unadapted activated sludge from a laboratory plant as inoculums, an EC50 -3 hours of 147 mg/l was estimated (79 -208 mg/l).

Toxicity to terrestrial plants

Studies on the influence of urea derivatives on the germination rate of higher plants were carried out on lettuce seeds (Lactuca sativa) by Kefford et al. (1965). The seedlings were first preincubated for 24 hours in the absence of light on pre-treated filter paper at 25°C (negative control 1 ml water; positive control 1 ml germination-inducing kinetin solution, 5E-05 mol/l) and then illuminated with red light. The lighting intensity was selected to achieve a 20% germination rate in the negative controls; in the positive controls the germination rate was 85 -95%. The germination rate was determined after a further 48 -hour incubation in the absence of light.

At 0.21 mg/l 1,3 -diphenylguanidine did not affect the germination rate compared to the negative controls. At a concentration of 2.1 mg/l it induced a germination rate of 57 % and at 21.1 mg/l of 104% compared to the positive controls. A parallel investigation showed no influence on the cell division activity to tobacco cells.

Bempong & McCoy (1972) studied the effect of 1,3 -diphenylguanidine on the mitotis cycle of root cells of fiels beans (Vicia faba). The cells were pre-treated for three hours with 0.02% colchicine, transferred for 5, 10 or 16 hours to aerated water, exposed to the tested substance (1 -10 mg/l 1,3 -diphenylguanidine) under intensive aeration for 30 -minutes and finally, after thorough washing, transferred to aerated water for 5 -29 hours. A concentration-related reduction in the mitotis index was observed (0.43 - 9.48; control 13.94) and the appearance of chromosome aberrations in 5 -55% of the cells tested.

These two studies have been considered as not relevant for the hazard assessment due to their unsuitable test systems and their methodological deficiences. In a more recent terrestrial plant study conducted on monocotyledons and dicotyledons did not show a high level of concern for 1,3 -diphenylguanidine in these species (Brassica rapa:EC50 = 358 mg/kg;Avena sativa: EC50 = 1169 mg/kg).

Toxicity to soil microorganisms

Williams (1984) studied the effect of 1,3 -diphenylguanidine on the growth of soil micro-organisms. The compound was spread on a polycarbonate membrane or imbedded on aluminiun foil in an epoxy resin (Araldit), and was thus in indirect (via membrane pores) or direct contact with a not further specified soil (moistened John Innes N°.1 soil). No colonies formed during the 3 -month experiment.

The compound was also placed in nutrient agar, inoculated with an aquaeous soil extract (3.0E07 individuals/ml) and incubated for 4 and 14 days at 25°C. The LD50 for both incubation times was

given as > or = 0.1%, based on the growth rate of control experiments. This concentration was characterized by the author as highly toxic, although when converted it corresponds to an amount of < or = 1 g/l. The author pointed out that experiments of this type are not suitable for evaluating the microbial degradation of rubber (and thus the microbial toxicity of the rubber chemicals added) as they do not consider the chemical change of the test compound during vulcanization.

According to claimed uses of 1,3 -diphenylguanidine soil exposure is likely. At the moment no relevant data is available for characterizing its effects on micro-organisms inhabiting soils. As the risk assessment demonstrates that there is no risk for those organisms using the PNEC derived through equilibrium partitioning method, no test is needed for covering this question.

Toxicity to birds

In accordance with column 2 of REACH Annex X, testing on long-term or reproductive toxicity to birds (required in section 9.6.1.) should be carefully considered taking into account the large mammalian dataset that is usually available at this tonnage level.

The study on birds does not need to be conducted as sufficient reliable data is available from the mammalian data set. So, any need for testing should be carefully considered taking into account the large mammalian dataset that is usually available at this tonnage level. Nevertheless, this endpoint allows considering potential secondary poisoning issues to birds following chronic exposure to 1,3-diphenylguanidine via the fish and earthworm food chains. 1,3-diphenylguanidine and its salts are not expected to bioaccumulate in fish/earthworm tissues. Moreover, 1,3-diphenylguanidine is not expected to be persistent in aquatic and terrestrial media. Considering all those elements one can safely conclude that secondary poisoning is not expected as birds will not be exposed to 1,3-diphenylguanidine via food consumption.

On the top of that, a study on 1,3 -diphenylguanidine showed no acute toxicity to 3 song bird species: Agelaius phoeniceus, Sturnus vulgaris and Passer domesticus. After a 2 -6 weeks adaptation phase, wild-caught birds received a single oral administration of the compound dissolved in propylene glycol. The LD50 for all three species was above the highest administrated dose of 100 mg/kg bw.

E.3.2 Information on tonnage and usage

Registrations	☒ Full registration(s) (Art. 10) ☐ Intermediate registration(s) (Art. 17 and/or 18)
Total tonnage band for substance (excluding volume registered under Art 17 or Art 18, or directly exported)	≥ 1 000 to < 10 000 tonnes per annum.

Overview of uses of 1,3 -diphenylguanidine

The substance is manufactured and/or imported in the European Economic Area in quantities at ≥ 1 000 to < 10 000 tonnes per annum. This volume does not take into account any exports into countries not being member of the EEA. This substance is used by consumers, in articles, by

professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing.

Table E9: Uses according to public information at ECHA's registration data base (date of access: May 2021).

Use	Information
Uses as intermediate	Not used as an intermediate
Formulation or re-packaging	This substance is used in the following products: polymers. Release to the environment of this substance can occur from industrial use: formulation in materials and formulation of mixtures.
Uses at industrial sites	This substance is used in the following products: polymers. This substance is used for the manufacture of: rubber products and chemicals. Release to the environment of this substance can occur from industrial use: as processing aid.
Uses by professional workers	This substance is used in the following products: polymers. This substance is used for the manufacture of: rubber products. Other release to the environment of this substance is likely to occur from: indoor use (e.g. machine wash liquids/detergents, automotive care products, paints and coating or adhesives, fragrances and air fresheners), outdoor use, outdoor use in long-life materials with low release rate (e.g. metal, wooden and plastic construction and building materials), outdoor use in long-life materials with high release rate (e.g. tyres, treated wooden products, treated textile and fabric, brake pads in trucks or cars, sanding of buildings (bridges, facades) or vehicles (ships)), indoor use in long-life materials with low release rate (e.g. flooring, furniture, toys, construction materials, curtains, foot-wear, leather products, paper and cardboard products, electronic equipment) and indoor use in long-life materials with high release rate (e.g. release from fabrics, textiles during washing, removal of indoor paints).
Consumer Uses	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. Other release to the environment of this substance is likely to occur from: outdoor use in long-life materials with low release rate (e.g. metal, wooden and plastic construction and building materials), outdoor use in long-life materials with high release rate (e.g. tyres, treated wooden products, treated textile and fabric, brake pads in trucks or cars, sanding of buildings (bridges, facades) or vehicles (ships)) and indoor use in long-life materials with low release rate (e.g. flooring, furniture, toys, construction materials, curtains, foot-wear, leather products, paper and cardboard products, electronic equipment).
Article service life	Other release to the environment of this substance is likely to occur from: outdoor use in long-life materials with low release rate (e.g. metal, wooden and plastic construction and building materials) and indoor use in long-life materials with low release rate (e.g. flooring, furniture, toys, construction materials, curtains, foot-wear, leather products, paper and cardboard products, electronic equipment). This substance can be found in complex articles, with no release intended: vehicles, machinery, mechanical appliances and

	electrical/electronic products (e.g. computers, cameras, lamps, refrigerators, washing machines) and electrical batteries and accumulators. This substance can be found in products with material based on: rubber (e.g. tyres, shoes, toys), rubber used for large surface area articles (e.g. construction and building materials for flooring) and rubber used for toys and other articles intended for children's use (e.g. baby bottle nipples, soothers).

Uses according to SPIN database [9]

For the latest reporting year (2019) the database on Substances in preparations in Nordic countries (SPIN) reports the following data:

Country	#prep	tonnes	Consumer preparations	Confidential
SE	92	4.9	-	-
DK	0	0	-	yes

From the use categories to be reported for SPIN (use category description scheme UC 62), all 1,3-diphenylguanidine is used in the "others" use category from the preparations from 2019.

Data from SPIN is not fully representative for the European Economic Region because products and frequency of application may differ between the different geographical regions in the EU. In addition, the SPIN database not only refers to products where substances are intentionally added, but also deals with occurrence of substances as impurities.

Based on the data from the notifications for 2019, SPIN concludes a potential exposure for 1,3-diphenylguanidine for surface water. SPIN concludes a probable occupational exposure.

Table E10: Exposure potential of 1,3-diphenylguanidine from products, according to SPIN database, with index out of 5 unless specified

Country	Quant.	Surface water	Air	Soil	Wastewater	Consumers	Occupational	Range of Use (RoU)	Article index (max: 3)
DK	1	1	1	1	3	3	3	1	2
SE	3	3	2	2	2	2	4	2	3

[9] www.spin2000.net; date of access: 24.05.2021

On the basis of this information there is evidence that in principle, uses of 1,3-diphenylguanidine result in relevant emissions into certain environmental compartments.

Additional information

Regulatory obligations exist for 1,3-diphenylguanidine under the following regulations:

- Active Implantable Medical Devices Directive - Hazardous Substances
- CAD - Chemical Agents Directive, Article 2(b)(i) - Hazardous Agents
- Construction Product Regulation - Annex I (3) - Hazardous Substances
- Construction Product Regulation - Article 6(5) - SDS and Declaration
- Cosmetic Products Regulation, Annex II - Prohibited Substances
- End-of-Life Vehicles Directive - Hazardous Substances
- Ecolabels - Restrictions for Hazardous Substances/Mixtures
- Active and Intelligent Materials - CMR Substances not allowed for use
- General Product Safety Directive - Hazardous Substances
- In Vitro Diagnostic Medical Devices Directive - Hazardous Substances
- Marine Environmental Policy Framework Directive - Hazardous Substances
- Medical Devices Directive - Hazardous Substances
- Protection of Pregnant and Breastfeeding Workers Directive, Annex I+II
- Safety and Health of Workers at Work Directive - Hazardous Substances
- Safety and Health of Workers at Work Directive - Workplace Signs - minimum requirements & signs on containers and pipes
- Waste Framework Directive, Annex III - Waste - Hazardous Properties

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E.4 Benzotriazole

Table E11: Substance identifiers for benzotriazole

EC name (public):	Benzotriazole
IUPAC name (public):	1H-1,2,3-benzotriazole
Index number in Annex VI of the CLP Regulation:	Not given
Molecular formula:	C6H5N3
Molecular weight or molecular weight range:	119.12 g/mol
Synonyms:	*Benzotriazole* *1H-Benzotriazole*

Type of constituent: ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

E.4.1 Hazard information

Classification

Harmonised Classification in Annex VI of the CLP

There is currently no harmonised classification in Annex VI of the CLP.

Self classification

- In the registration:

Classifications reported in registrations list the following

  - H302: Harmful if swallowed.
  - H319: Causes serious eye irritation.
  - H411: Toxic to aquatic life with long lasting effects.

- Additional classifications in the C&L Inventory:

Table E12: Self classification according to ECHA's C&L inventory

	CLP Notifications[10]
Number of aggregated notifications	40
Total number of notifiers	1766

[10] C&L Inventory database, http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database (accessed 19 October 2021)

Proposal for Harmonised Classification in Annex VI of the CLP

There are no further proposals at November 2021.

CLP Notification Status

There is no CLP notification status given.

Additional information

Studies are listed that are available in the registration dossier

Persistence

Based on all available information it has to be assumed that Benzotriazole is not readily biodegradable in freshwater and marine environment at least. Due to the incomplete report and the unclear status of the adaptation of the sludge in the OECD 302B test from Kanne no final conclusion on the biodegradability has been possible. The results of the study have indicated a relevant potential on inherent biodegradation.

The substance was tested in a OECD309 revealing a half-live of larger than 10.000 days (Hofman-Caris and Claßen, 2020). Therefore the substances fulfils the criterium for a very persistent substance according o annex XIII of REACH.

With respect to all available information indicating no or minimal biodegradabilty 1H-Benzotriazole has been considered as non-biodegradable in aquatic compartment until the results of the proposed testing are available.

Breedveld et al. examined the aerobic and anaerobic degradation of Benzotriazole in the terrestrial compartment. Therefore, series of batch reactors were inoculated with microorganisms from the area of the abandoned airport Gardermoen, Norway and airport Fornebu, Norway. Benzotriazole (1 mg/L) as substrate as well as other substances for achieving necessary oxygen consumption (benzoate or glycol) were added. As control (aerobic conditions) CuSO4 was used. After five month period no degradation of the test substance was observed under anaerobic conditions. In parallel series under aerobic conditions degradation of Benzotriazole in liquid phase was observed. Since similar loss has been observed in the control evaporation is assumed to be the major process responsible.

Gruden et al. reported findings from 18-month study with activated sludge from the STP in Boulder, Colorado exposed to different concentrations of Methylbenzotriazoles showing no breakdown products in all microcosms and bench-scale digesters used for the study. Due to the high similarity of used Methylbenzotriazoles and Benzotriazole results have been considered relevant for the degradation of both substances.

In addition, available information on inhibition of nitrification in topsoil samples indicate the strong inhibitory potential of Benzotriazole and Tolyltriazole. In observations with 45 heterocyclic N compounds in three different soils significant inhibition of nitrification (35, 55, and 81 %) at 12 µg Benzotriazole /g soil was found (McCarty et al.).

In summary, based on the existing information it can be concluded that Benzotriazole and Tolyltriazole as well as their conjugated sodium salts are stable with regard to biodegradation in soils under environmental conditions. Available information are considered to be adequate for regulatory purposes. Biodegradation in soil is expected to show a lower rate of degradation in general. As Benzotriazole and Tolyltriazole are not readily biodegradable in the aquatic environment the same result is expected for test in soil at least indicating a non-rapidly degradation of the substances. Hence, the substances are classified for long-term hazards in the environment. For the PBT assessment the default half-life for non-readily biodegradable substances is used (DT50 > 180 days) while for the chemical safety assessment the substances are considered as non-biodegradable in soil under environmental conditions.

Mobility

Sorption behaviour of 1H-Benzotriazole and Tolyltriazole have been investigated in several studies during the last decades showing a high mobility in soil. Motivated by findings at an abandoned airport in Norway Breedveld et al. performed a sorption study in six different soils according to OECD 106 (Breedveld et al., 2003). The study has given indications showing very little sorption in different soil matrices increasing with gradient organic carbon content. The maximum adsorption was found in peat at pH 3.0 and an organic carbon content of 47.4 % (estimated log Koc 1.4). Experimental observations were supported by field studies detecting Benzotriazole in various soil samples from the surroundings of the airport at 1.2 m depth.

Hart et al. have examined the sorption behaviour of 1H-Benzotriazole and 5-Methyl-benzotrizole in short-term batch method according to an ASTM standard method in four different soil matrices with low organic carbon content (Hart et al., 2004). Results from the experiment were fitted by Langmuir, Freundlich and linear isotherms giving indications on different factors affecting the sorption behaviour of both substances. As all members of Benzotriazoles have shown a strong dipole moment (polar character) binding to soil is a complex combination of molecular driving forces with different binding sites for adsorption, absorption and hydrogen bonding. From the experimental results, a maximum log Koc of 1.89 for 1H-Benzotriazole, and 2.04 for 5-Methylbenzotriazole was calculated.

In addition, Jia et al. also have observed non-linear sorption of 1H-Benzotriazole and Tolyltriazole in mineral soils (Jia et al., 2007). A significant increase of sorption of Benzotriazoles was detected when in situ pH of soil equals range of pKa value indicating ionic interactions between triazole molecules and binding sites in soil matter. In general, the observed sorption coefficient of Tolyltriazole has been higher than of Benzotriazole. Furthermore increased sorption has been found when zerovalent Fe(0) has been present indicating multi-layer coverage.

Experimental findings for Benzotriazole and Tolyltriazole was supported by QSAR calculations using KOCWIN v.2.00 (log Koc 1.72 (BT) and 1.94(TT)). In a second estimation according to Schüürmann (Schüürmann et al., 2006) a log Koc of 1.69 for BT has been achieved.

All available information have been adequate to assess the behaviour of Triazoles in soil. Therefore, no need for further testing was assumed. In summary, all results show a log Koc < 2 indicating a high mobility in soil.

A worst case log KOC is given as 1.4.

Toxicity

Short term toxicity to fish

The acute toxicity of the test substance to the fresh-water fish species Brachydanio rerio was determined in an OECD guideline study according to GLP. The test was carried out under semi-static conditions with daily replacement of the test solutions and with 10 fish for the control medium and each concentration. The exposure duration was 96 hours. The nominal concentrations tested were 32, 56, 100, 180, and 320 mg/L. All test solutions were completely clear (visually assessed) throughout the test.

Short-term toxicity to aquatic invertebrates

Four freshwater studies with invertebrates (3 studies with D. magna, 1 study with D. galeata) are available. While the three studies with D. magna show an EC50 (48h) of about 100 mg/L, an EC50 (48h) of 15.8 mg/L with D. galeata has been observed. The difference in the sensitivity of the species is mostly likely due to the smaller size of D. galeata.

Although the publication has shown some deficiencies in reporting the publication has been selected for the chemical safety assessment as it also has been performed according to the OECD 202 test guideline and the parallel test with D. magna has shown an analogue effect value like the studies from the GLP laboratories indicating a comparable quality standard of the laboratories.

Effects in marine invertebrates has been examined in a study according to ISO/CD 14669 with Tolyltriazole using Acartia Tonsa showing an effect concentration EC50 (48h) = 55 mg/L.

Long-term toxicity to aquatic invertebrates

Three long-term freshwater studies according to OECD guideline 211 with two different daphnid species has been available showing an analogue tendency like the short-term studies. The study using D. galeata present a clearly lower effect concentration compared to the much larger D. magna. Although keeping in mind that this is a non-standard organism the EC10 has been selected as a point of departure for the further assessment. In just one study with D. magna an effect concentration has been determined (Caspers, 1991). Most likely the absence of observable effects in the second study by Seeland et al. is caused by the selection of a too low concentration range.

In addition to the freshwater studies also observations with marine species have been available. Developmental toxicity of benzotriazole to Ciona intestinalis has been examined by Kadar et al. (Kadar, 2010). Due to absence of relevant guidelines a "guideline-like" approach has been used for the experimental observations. Adult organisms have been collected from Millbay Marina, Plymouth and cultured. Subsequent the gamete have been collected and in vitro fertilized. After 48 h, the NOEC and LOEC have been determined to be 10 and 32 mg/L, respectively, based on morphological development of the embryos.

Kadar E, Dashfield S, and Hutchinson TH, Developmental toxicity of benzotriazole in the protochordate Ciona intestinalis (Chordata, Ascidiae), Anal Bioanal Chem (2010) 396:641 -647.

Toxicity to aquatic algae and cyanobacteria

Three freshwater tests with two different green algae species have been available. Key values for the chemical safety assessment have been selected from both OECD 201 guideline studies as the acute effect value has been calculated in the Blom study only while the publication of Seeland has shown the lower EC10 effect concentration.

The third study has been disregarded for the safety assessment as the reliability could not be evaluated due to deficiencies in the available reporting.

Toxicity to aquatic plants other than algae

EC10 or NOEC for freshwater plants of 3.94 mg/L based on OECD 221.

Toxicity to microorganisms

EC50 for microorganisms: 940 mg/L

EC10 or NOEC for microorganisms: 1 mg/L

Besides both included studies several further studies with Benzotriazole, Tolyltriazole as well as different commercially available aircraft deicing fluids (ADF) using Microtox test system (Vibrio fischeri) are available (Cancilla, 1997; Cancilla, 2003; Cornell, 2000; Pillard, 2001) were reviewed. The results are summarized below.

Compound: Microtox EC50 (15 min) [mg/L]: Study

5-methylbenzotriazole: 4.25 (95% CI 4.18-4.35): Cancilla, 2003

4-methylbenzotriazole: 21 (95% CI 9.0-47): Pillard, 2001

5-methylbenzotriazole: 8.7 (95% CI 8.2-9.2)

1:1 mixture of 4-MBT and 5-MBT: 7.3 (95% CI 6.9-7.7)

1H-Benzotriazole: 41.65 ± 11.01: Cancilla, 1997

5-methylbenzotriazole: 5.91 ± 1.11: different ADFs with tolyltriazole: 6-9: Cornell, 2000

E.4.2 Information on tonnage and usage

Registrations	☒ Full registration(s) (Art. 10) ☒ Intermediate registration(s) (Art. 17 and/or 18)
Total tonnage band for substance (excluding volume registered under Art 17 or Art 18, or directly exported)	≥ 1 000 to < 10 000 tonnes

Overview of uses of benzotriazole

The substance is manufactured and/or imported in the European Economic Area in quantities at ≥ 1 000 to < 10 000 tonnes per annum. This volume does not take into account any exports into countries not being member of the EEA. The substance is also registered as an intermediate. This substance is used by consumers, in articles, by professional workers (widespread uses), in formulation or re-packing and at industrial sites.

Table E13: Uses according to public information at ECHA's registration data base (date of access: May 2021).

Use	Information
Uses as intermediate	This substance is used as an intermediate. PROC 1: Chemical production or refinery in closed process without likelihood of exposure or processes with equivalent containment conditions Sector of end use: SU 8: Manufacture of bulk, large scale chemicals (including petroleum products) SU 9: Manufacture of fine chemicals
Formulation or re-packaging	This substance is used in the following products: heat transfer fluids, lubricants and greases, anti-freeze products, washing & cleaning products, pH regulators and water treatment products and polymers. Release to the environment of this substance can occur from industrial use: formulation of mixtures and formulation in materials.
Uses at industrial sites	This substance is used in the following products: lubricants and greases, heat transfer fluids, anti-freeze products, washing & cleaning products and pH regulators and water treatment products. This substance is used for the manufacture of: machinery and vehicles, fabricated metal products and plastic products. Release to the environment of this substance can occur from industrial use: in processing aids at industrial sites, of substances in closed systems with minimal release and in the production of articles.
Uses by professional workers	This substance is used in the following products: anti-freeze products, heat transfer fluids, lubricants and greases and washing & cleaning products. This substance is used for the manufacture of: machinery and vehicles. Other release to the environment of this substance is likely to occur from: indoor use as processing aid, indoor use in close systems with minimal release (e.g. cooling liquids in refrigerators, oil-based electric heaters), outdoor use in close systems with minimal release (e.g. hydraulic liquids in automotive suspension, lubricants in motor oil and break fluids) and outdoor use as processing aid.
Consumer Uses	This substance is used in the following products: lubricants and greases, washing & cleaning products, heat transfer fluids, anti-freeze products and coating products. Other release to the environment of this substance is likely to occur from: indoor use as processing aid, indoor use in close systems with minimal release (e.g. cooling liquids in refrigerators, oil-based electric heaters), outdoor use in close systems with minimal release (e.g. hydraulic liquids in automotive suspension, lubricants in motor oil and break fluids) and outdoor use as processing aid.

Article service life	Other release to the environment of this substance is likely to occur from: indoor use in long-life materials with high release rate (e.g. release from fabrics, textiles during washing, removal of indoor paints), outdoor use in long-life materials with high release rate (e.g. tyres, treated wooden products, treated textile and fabric, brake pads in trucks or cars, sanding of buildings (bridges, facades) or vehicles (ships)) and indoor use in long-life materials with low release rate (e.g. flooring, furniture, toys, construction materials, curtains, foot-wear, leather products, paper and cardboard products, electronic equipment). This substance can be found in products with material based on: metal used for packaging (excluding food packaging) and plastic used for packaging (excluding food packaging). This substance is intended to be released from: packaging material for metal parts (releasing grease/corrosion inhibitors).

Information on uses and occurrence of benzotriazole according to Wikipedia [11] is as follows:

Benzotriazole is used as a restrainer (or anti-fogging agent) in photographic emulsions or developing solutions, and as a reagent for the analytical determination of silver. It has been used extensively as a corrosion inhibitor in the atmosphere and underwater. Benzotriazole can be used as an antifreeze, in heating and cooling systems, in hydraulic fluids and as a vapor phase inhibitor.

Benzotriazole is an effective corrosion inhibitor for copper and its alloys by preventing undesirable surface reactions. Benzotriazole derivatives have chemical and biological properties that are versatile in the pharmaceutical industry. Benzotriazole derivatives act as agonists for many proteins.

Uses according to SPIN database [12]

For the latest reporting year (2019) the database on Substances in preparations in Nordic countries (SPIN) reports the following data:

Country	#prep	tonnes	Consumer preparations	Confidential
SE	374	26.7	Yes	-
DK	311	8.7	-	-

From the use categories to be reported for SPIN in 2019 (use category description scheme UC 62), the greatest amount of benzotriazole is used as cleaning/washing agents (123 preparations, 10.9 tonnes), followed by cutting fluids (226 preparations, 7.4 tonnes) and lubricants and additives (30 preparations, 4 tonnes).

[11] https://en.wikipedia.org/wiki/Benzotriazole#Applications
[12] www.spin2000.net; date of access: 24.05.2021

Data from SPIN is not fully representative for the European Economic Region because products and frequency of application may differ between the different geographical regions in the EU. In addition, the SPIN database not only refers to products where substances are intentionally added, but also deals with occurrence of substances as impurities.

Based on the data from the notifications for 2019, SPIN concludes a very probable exposure for surface water, air, soil, wastewater, consumers and occupational.

Table E14: Exposure potential of benzotriazole from products, according to SPIN database, with use index out of 5 unless specified

Country	Quant.	Surface water	Air	Soil	Wastewater	Consumers	Occupational	Range of Use (RoU)	Article index (max: 3)
DK	4	5	5	5	5	5	5	5	3
SE	3	4	4	4	5	5	5	5	3

On the basis of this information there is evidence that in principle, uses of benzotriazole result in relevant emissions into all environmental compartments.

E.5 2-acrylamido-2-methylpropanesulphonic acid

Table E15: Substance identifiers for 2-acrylamido-2-methylpropanesulphonic acid

EC name (public):	2-acrylamido-2-methylpropanesulphonic acid
IUPAC name (public):	2-(acryloylamino)-2-methylpropane-1-sulfonic acid
Index number in Annex VI of the CLP Regulation:	-
Molecular formula:	$C_7H_{13}NO_4S$
Molecular weight or molecular weight range:	207.24 g/mol
Synonyms:	*1-Propanesulfonic acid, 2-methyl-2-((1-oxo-2-propen-1-yl)amino)-* *2-Acrylamido-2-methylpropanesulfonate* *2-Acrylamido-2-methylpropanesulphonic acid* *1-Propanesulfonic acid, 2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-* *2-ACRYLAMIDO-2-METHYL-1-PROPANESULFONIC ACID*

Type of constituent: ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

E.5.1 Hazard information

Classification

Harmonised Classification in Annex VI of the CLP

There is currently no harmonised classification in Annex VI of the CLP.

Self classification

- In the registration:

Table E16: Self classification according to ECHA's C&L inventory

Hazard Class and Category Code(s)	Hazard Statement Code(s)
Acute Tox. 3	H302+H332
Eye Dam. 1	H318
STOT SE 3	H335
Acute Tox. 4	H302+H332
Skin Irrit. 2	H315
Eye Irrit. 2	H319
Aquatic Chronic 4	H413
Met. Corr. 1	H290

Hazard Class and Category Code(s)	Hazard Statement Code(s)
Skin Corr. 1C	H314

Proposal for Harmonised Classification in Annex VI of the CLP

There are no proposals for harmonized classification as of 21.0112021.

CLP Notification Status

Table E17: CLP Notifications

	CLP Notifications
Number of aggregated notifications	21
Total number of notifiers	490

Additional information

Persistence

Based on screening tests in water, results from a study from 1986 using method 40 CFR 795.3340 found that the test substance showed a low biodegradation rate of less than 10% after 44 days and was not considered to be readily biodegradable.

Mobility

No data are provided in the registration dossier at November 2021.

Toxicity

Short-term toxicity to fish

According to EPA-66013-75-009, the LC0 at 96 hours for fish for this substance was 130 mg/L and the LC50 at both 72 and 96 hours was calculated as 170 mg/L.

Short-term toxicity to aquatic invertebrates

According to EPA-660/3-75-009, the EC50 for acute toxicty at 48 hours on Daphnia magna of ATBS was shown to be 340 mg/mL (CI95% 280 - 430 mg/L). The No Observed Effect Concentration (NOEC) was 78 mg/l at 48 hours.

Toxicity to aquatic algae and cyanobacteria

According to a 1996 study using OECD Guideline 201, there was no inhibition of algal growth or biomass were seen at the single test concentration of 2000 mg/L.

Toxicity to microorganisms

In a study from 2007 using OECD Guideline 209, this substance was considered to have had no biologically significant inhibitory effect on the respiration rate of activated sludge at any of the concentrations employed in the test. Therefore, the No Observed Effect Concentration was concluded to be 1000 mg/l, the highest level tested.

In summary, no environmental effects were seen for 2-acrylamido-2-methylpropanesulphonic acid.

E.5.2 Information on tonnage and usage

Registrations	☒ Full registration(s) (Art. 10) ☐ Intermediate registration(s) (Art. 17 and/or 18)
Total tonnage band for substance (excluding volume registered under Art 17 or Art 18, or directly exported)	≥ 1 000 to < 10 000 tonnes per annum

Overview of uses of 2-acrylamido-2-methylpropanesulphonic acid

The substance is manufactured and/or imported in the European Economic Area in quantities at ≥ 1 000 to < 10 000 tonnes per annum. This volume does not take into account any exports into countries not being member of the EEA. This substance is used by professional workers (widespread uses), in formulation or re-packing and at industrial sites.

Table E18: Uses according to public information at ECHA's registration data base (date of access: May 2021).

Use	Information
Uses as intermediate	Not used as an intermediate
Formulation or re-packaging	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. Release to the environment of this substance can occur from industrial use: formulation of mixtures.
Uses at industrial sites	This substance is used in the following products: polymers. This substance has an industrial use resulting in manufacture of another substance (use of intermediates). This substance is used for the manufacture of: chemicals. Release to the environment of this substance can occur from industrial use: as an intermediate step in further manufacturing of another substance (use of intermediates).
Uses by professional workers	This substance is used in the following products: pH regulators and water treatment products and laboratory chemicals. This substance is used in the following areas: health services and scientific research and development. Other release to the environment of this substance is likely to occur from: indoor use (e.g. machine wash liquids/detergents, automotive care products, paints and coating or adhesives, fragrances and air fresheners).
Consumer Uses	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. ECHA has no

	public registered data on the routes by which this substance is most likely to be released to the environment.
Article service life	ECHA has no public registered data on the routes by which this substance is most likely to be released to the environment. ECHA has no public registered data indicating whether or into which articles the substance might have been processed.

Information on uses and occurrence of 2-acrylamido-2-methylpropanesulphonic acid according to Wikipedia [13]

Acrylic fiber: A number of enhanced performance characteristics are imparted to acrylic, modified-acrylic, polypropylene and polyvinylidene fluoride fibers: dye receptivity, moisture absorbency, and static resistance.

Coating and adhesive: The sulfonic acid group gives the monomers ionic character over a wide range of pH. Anionic charges from AMPS fixed on polymer particles enhance the chemical and shear stabilities of polymer emulsion and also reduce the amount of surfactants leaching out of paint film. It improves the thermal and mechanical properties of adhesives, and increases the adhesive strength of pressure-sensitive adhesive formulations.

Detergents: Enhances the washing performance of surfactants by binding multivalent cations and reducing dirt attachment.

Personal care products: Strong polar and hydrophilic properties introduced to a high molecular weight AMPS homopolymer are exploited as a very efficient lubricant characteristic for skin care.

Medical hydrogel: High water-absorbing and swelling capacity when AMPS is introduced to a hydrogel are keys to medical applications. Hydrogel with AMPS showed uniform conductivity, low electrical impedance, cohesive strength, appropriate skin adhesion, and biocompatible and capable of repeated use and have been used to electrocardiograph electrodes, defibrillation electrode, electrosurgical grounding pads, and iontophoretic drug delivery electrodes. In addition, polymers derived from AMPS are used as the absorbing hydrogel and the tackifier component of wound dressings. Is used due to its high water absorption and retention capability as a monomer in superabsorbents e. g. for baby diapers.

Oil field applications: Polymers in oil field applications have to stand hostile environments and require thermal and hydrolytic stability and the resistance to hard water containing metal ions. For example, in drilling operations where conditions of high salinity, high temperature and high pressure are present, AMPS copolymers can inhibit fluid loss and be used in oil field environments as scale inhibitors, friction reducers and water-control polymers, and in polymer flooding applications.

Water treatment applications: The cation stability of the AMPS-containing polymers are very useful for water treatment processes. Such polymers with low molecular weights cannot only

[13] https://en.wikipedia.org/wiki/2-Acrylamido-2-methylpropane_sulfonic_acid

inhibit calcium, magnesium, and silica scale in cooling towers and boilers, but also help corrosion control by dispersing iron oxide. When high molecular weight polymers are used, they can be used to precipitate solids in the treatment of industrial effluent stream.

Crop protection: increases in dissolved and nanoparticulate polymer formulations bioavailability of pesticides in aqueous-organic formulations.

Membranes: It increases water flow, retention and fouling resistance of asymmetric ultrafiltration and microfiltration membranes and is being studied as an anionic component in polymer fuel cell membranes.

Construction applications: Superplasticizers with AMPS are used to reduce water in concrete formulations. Benefits of these additives include improved strength, improved workability, improved durability of cement mixtures. Redispersible polymer powder, when AMPS is introduced, in cement mixtures control air pore content and prevent agglomeration of powders during the spray-drying process from the powder manufacturing and storage. Coating formulations with AMPS-containing polymers prevent calcium ions from being formed as lime on concrete surface and improve the appearance and durability of coating.

Uses according to SPIN database [14]

For the latest reporting year (2019) the database on Substances in preparations in Nordic countries (SPIN) reports the following data:

Country	#prep	tonnes	Consumer preparations	Confidential
SE	8	8.9	Yes	-
DK	0	0	-	Yes

From the use categories to be reported for SPIN (use category description scheme UC 62), all preparations of 2-acrylamido-2-methylpropanesulphonic acid for 2019 were for cleaning/washing agents.

Data from SPIN is not fully representative for the European Economic Region because products and frequency of application may differ between the different geographical regions in the EU. In addition, the SPIN database not only refers to products where substances are intentionally added, but also deals with occurrence of substances as impurities.

Based on the data from the notifications for 2019, SPIN concludes a potential exposure for 2-acrylamido-2-methylpropanesulphonic acid for air and soil. SPIN concludes a very probable consumer, occupational and wastewater exposure.

[14] www.spin2000.net; date of access: 24.05.2021

Table E19: Exposure potential of 2-acrylamido-2-methylpropanesulphonic acid from products, according to SPIN database (with use index out of 5 unless specified)

Country	Quant.	Surface water	Air	Soil	Wastewater	Consumers	Occupational	Range of Use (RoU)	Article index (max: 3)
DK	1	1	1	2	5	5	3	1	1
SE	3	2	3	3	4	4	5	2	3

On the basis of this information there is evidence that in principle, uses of 2-acrylamido-2-methylpropanesulphonic acid result in relevant emissions into all environmental compartments.

Additional information

Regulatory obligations exist for 2-acrylamido-2-methylpropanesulphonic acid under the following regulations:

- FCMs Recycled Plastic & Articles Regulation - Annex I - Authorised Use
- FCM and Articles Regulation, Annex I - Authorised Substances

E.6 Cyanuric acid

Table E20: Substance identifiers for Cyanuric acid

EC name (public):	Cyanuric acid
IUPAC name (public):	1,3,5-triazine-2,4,6-triol
Index number in Annex VI of the CLP Regulation:	Not given
Molecular formula:	C3H3N3O3
Molecular weight or molecular weight range:	129.07 g/mol
Synonyms:	*cyanuric acid* *1,3,5-Triazine-2,4,6-trione (1,3,5-Triazine-2,4,6-triol; Cyanuric acid), inhalable fraction* *1,3,5-Triazine-2,4,6(1H,3H,5H)-trione* *1,3,5-triazine-2,4,6-triol* *Isocyanuric acid* *4-amino-1,2,5-oxadiazole-3-carboxylic acid*

Type of constituent: ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

E.6.1 Hazard information

Classification

Harmonised Classification in Annex VI of the CLP

There is currently no harmonised classification in Annex VI of the CLP.

Self classification

There are no self classifications in the C&L inventory.

Proposal for Harmonised Classification in Annex VI of the CLP

There are no further proposals at the time of writing (November 2021).

CLP Notification Status

There is no CLP notification status given.

Additional information

Information is shown from the dossiers.

Persistence
Biodegradation in water and sediment: simulation tests

An experiment was carried out according to OECD 306 and showed that 4% biodegradation of the monosodium salt of cyanuric acid was attained in 60 days in seawater. The parameter that was followed for the biodegradation estimate was DOC removal.

Biodegradation in water: screening tests

The biodegradation of cyanuric acid in representative anaerobic systems was described. Primary settled domestic sewage to which cyanuric acid was added was allowed to become, or was made, anaerobic to examine cyanuric acid levels. Anaerobic mixed liquor containing 14C-cyanuric acid tracer solution; anaerobic nutrient broth with mixed inocula from sewage plant effluent and muds and soils, which also contained added cyanuric acid, were studied. 14CO2 evolved was carried by N2 through a bubble trap containing NaOH solution. This solution plus rinsings were analysed for 14C activity by liquid scintillation counting. Approximately 2 × 106 dpm were used per experiment.

Anaerobic sewage: If primary settled domestic sewage to which cyanuric acid was added was made anaerobic the cyanuric acid concentration was reduced by 25 – 50% in 48 h, and complete disappearance of the cyanuric acid was observed within 72 – 96 h. The total Kjeldahl nitrogen after the three week incubation rose from 65 µg/mL to 209 µg/ml, and the ammonia nitrogen rose from 52 µg/ml to 191 µg/mL. As the nitrogen equivalent of 430 µg of cyanuric acid per ml is 140 µg/mL, all of the ammonia and Kjeldahl nitrogen increase was accounted for by conversion of cyanuric acid.

Anaerobic mixed liquor: The 14C was evolved as 14CO2 at 4% within 7 h, 11% (total) within the next 17 h and 82% (total) in 17 days. Essentially, no 14C from cyanuric acid was synthesized into biomass. However, in one repeat of the experiment, the 14CO2 evolution was 50% in 8 days, 71% in 13 days and in a third repeat of the experiment, the 14CO2 evolution was 93% in 6 h. Therefore mixed liquor activity was very variable.

Anaerobic nutrient broth: The 14CO2 in the effluent gasses contained 80% of the radioactivity initially added.

The study concludes the following: Cyanuric acid biodegrades readily under a wide variety of natural conditions, and particularly well in systems of either low or zero dissolved oxygen level, such as anaerobic activated sludge and sewage soils, muds and muddy streams and river waters as well as ordinary activated sludge systems with typically low (1 – 3 ppm) dissolved oxygen levels. CO2 and ammonia are initial hydrolytic breakdown products References: Saldick, J. (1974) Biodegradation of cyanuric acid. Applied Microbiology 28 (6) 1004 – 1008.

In an additional study, the biodegradation of cyanuric acid in an aerobic system is described. Primary settled domestic sewage to which radiolabelled cyanuric acid was added, was used. 14CO2 evolved was carried by air through a bubble trap containing NaOH solution. The results showed that Cyanuric acid exerts no biological oxygen demand in aerobic media. In highly aerobic media cyanuric acid resists biodegradation. The ability to degrade cyanuric acid was rapidly gained and lost by bacteria grown in aerated medium when the dissolved oxygen was lowered and raised. Organisms which degrade cyanuric acid multiply in both aerobic and anaerobic conditions and do not require any acclimatisation to be active for cyanuric acid decomposition. The degradation activity is turned on and off, with a time lag of a few minutes, when the environment is made anaerobic or aerobic. With 1 to 3 µg of dissolved oxygen per ml, good removal of cyanuric acid occurs in continuous flow laboratory-aerated sewage units if the residence time is at least 6 h. At

uncharacteristically high dissolved oxygen, the removal is poorer but considerable if the residence time is longer. The overall conclusion from the study was that in highly aerobic media cyanuric acid resists biodegradation. Anaerobic growth in sewage degrades cyanuric acid. The ability to degrade cyanuric acid is rapidly gained and lost by bacteria in aerated medium when dissolved oxygen was lowered and raised.

Biodegradation in soil

Cyanuric acid was concluded to biodegrade readily in anaerobic soils based on experiments considering the evolution of CO2.

In a series of studies performed in different anaerobic soils (Saldick J 1974) it was observed that cyanuric acid biodegrades readily in anaerobic soils. Over a 23 day period degradation was highest when there is a large water to solid ratio and a potentially large anaerobic microorganism population, for example 100% degradation in farm soil in 23 days.

In a further study (Wolf & Martin 1975) the relative degradation rate of cyanuric acid was studied in Greenfield sandy loam soil. After 16 days 87% of the labelled cyanuric acid had evolved as 14CO2 and after 32 days the percentage had increased to 96% indicating that after ring cleavage the cyanuric acid C is not used for cell synthesis by the soil organisms. Evolution of 14CO2 was retarded under saturated soil conditions. Losses were 83% for cyanuric acid in 66 days. Pure culture studies with two soil fungi, Stachybotrys chartarum and Hendersonula toruloidea could degrade cyanuric acid to CO2.

In an additional study where the evolution of CO2 was also followed, results showed that after 16 days 87% of the labeled cyanuric acid had evolved as 14CO2 and after 32 days the percentage had increased to 96% indicating that after ring cleavage the cyanuric acid C is not used for cell synthesis by the soil organisms. Evolution of 14CO2 was retarded under saturated soil conditions. Losses were 83% for cyanuric acid in 66 days. Pure culture studies with two soil fungi, Stachybotrys chartarum and Hendersonula toruloidea could degrade cyanuric acid to CO2.

Mobility

The adsorption of cyanuric acid in 4 different soil types was studied (Michael and Cummings 1982) The soil / water coefficient, K was determined to be <1 for all soils, therefore, cyanuric acid is weakly adsorbed and highly mobile in all soils. Cyanuric acid also has a Log Kow = - 1.31 and therefore, has a low potential for adsorption.

Toxicity

Short-term toxicity to fish

96 h LC50 > 8000 mg/L which was the highest concentration tested.

96 h LC50 > 1000 mg/L. Cyanuric acid is not harmful to bluegill sunfish.

Based on the 96 h LC50 value of >2100 mg/L, cyanuric acid is not harmful to rainbow trout.

Acute fish studies were performed with the freshwater species bluegill sunfish, rainbow trout and fathead minnow. Bluegill sunfish were exposed to a nominal concentration of 1000 mg/L cyanuric

acid for 96 h. The LC50 was > 1000 mg/L. No mortalities or adverse effects were observed. Rainbow trout and fathead minnow were exposed to nominal concentrations of 210, 370, 650, 1200 and 2100 mg/L cyanuric acid for 96 h. No mortalities were observed and the LC50 was determined to be > 2100 mg/L for both species.

The lowest LC50 derived from the three aquatic studies on freshwater fish was > 1000 mg/L based on nominal concentrations.

An acute fish study was performed with one saltwater species, inland silver sides. Fish were exposed to nominal concentrations of 500, 1000, 2000, 4000 and 8000 mg/L cyanuric acid. No mortalities occurred at the highest concentration tested. The LC50 was determined to be > 8000 mg/L.

Long-term toxicity to fish

A fish juvenile growth test with rainbow trout was performed with the monosodium salt of cyanuric acid (equivalent to 75.6% cyanuric acid) according to OECD guideline 215. Fish were exposed for 21 days to nominal concentrations of 100, 180, 320, 560 and 1000 mg/L (equivalent to 76, 136, 242, 423 and 756 mg cyanuric acid/L).

Zero mortalities, no inhibition of tank average specific growth rate, no sublethal effects of exposure and no significant reduction in terms of the “pseudo” specific growth rate were observed when compared to the control group. The NOEC for cyanuric acid was determined to be 756 mg/L.

Short-term toxicity to aquatic invertebrates

48 h LC50 > 1000 mg/L. Cyanuric acid is not harmful to Daphnia magna.

96 h LC50 = 4438 mg/L. Cyanuric acid is not harmful to mysid shrimp.

48 h LC50 = 6000 mg/L. Cyanuric acid is not harmful to Daphnia magna.

In a 48 h static acute toxicity test (LeBlanc 1978) Daphnia magna were exposed to nominal concentrations of 1,000, 600, 360, 220, 130 and 100 mg/L cyanuric acid. No mortalities occurred at the highest concentration test (48 h LC50 = > 1000 mg/L). In another 48 h static acute toxicity study (McAllister 1978) Daphnia magna were exposed to nominal test concentrations of 0, 560, 1000, 1800, 3200 and 5600 mg/L. The 48 h LC50 was determined to be 6000 mg/L. A white precipitation was observed in all concentrations greater than 1000 mg/L. The 48 h LC50 value quoted in the report was 6000 mg/L. However this value is considered above the reported solubility of cyanuric acid. A precise LC50 value can therefore not be given. The 48 h LC50 is therefore considered to be >1000 mg/L. No mortalities were observed at this concentration. In an acute toxicity study with marine aquatic invertebrates (Anderson 2002) mysid shrimp were exposed to nominal concentrations of 0, 500, 1000, 2000, 4000 and 8000 mg/L cyanuric acid for 96 h. The 96 h LC50 was calculated to be 4438 mg/L.

Long-term toxicity to aquatic invertebrates

Raw cynauric acid revealed to be less toxic (LC50 1000 and 2000 mg/L > 1 month) than pure cyanuric acid (LT50 1000 and 2000 mg/L ≤ 17 days). The cyanuric acid seemed to act on 2 levels: 1)

by valve decalcification and 2) by deterioration of kidney function with accumulation of the product.

Exposure of Daphnia magna to monosodium salt of cyanuric acid resulted in signifciant mortalities at the test concentrations of 500,1600 and 5000 mg/l resulting in 30%, 50% and 70% mortalities by day 21 respectively, compared to an observed mortality of 20% in the control by day 21. The 21 day EC50 (immobilisation) values, based on nominal test concentrations, for the parental Daphnia (P1) was calculated to be 2600 mg/l. 95% confidence limits could not be calculated due to the unsuitable nature of the data resulting from a flat dose response. The 21-day EC50 (reproduction) based on nominal test concentrations was 2800 mg/l with 95% confidence limits of 1800 - 4400 mg/l.

A Daphnia magna reproduction study (Sewell 2007) was performed with the monosodium salt of cyanuric acid (equivalent to 75.6% cyanuric acid). Daphnia were exposed to nominal concentrations of 50, 160, 500, 1600 and 5000 mg/L (equivalent to 37.8, 121, 378, 1210 and 3780 mg cyanuric acid/L) for a period of 21 days. The numbers of live and dead adult Daphnia and young daphnids (live and dead) were determined daily. Exposure of Daphnia magna to monosodium salt of cyanuric acid resulted in significant mortalities at the test concentrations of 500,1600 and 5000 mg/L resulting in 30%, 50% and 70% mortalities by day 21 respectively, compared to an observed mortality of 20% in the control by day 21. The NOEC was considered to be 160 mg/L (equivalent to 121 mg/L cyanuric acid) on the basis that at this concentration there were no significant mortalities (immobilisation) observed in the parental generation (P1) and that there were no significant differences between the control and the 160 mg/L test group in terms of numbers of live young per adult by day 21.

Toxicity to aquatic algae and cyanobacteria

Exposure to cyanuric acid did not appear to adveresely affect Selenastrum capricornutum until 72 hours of exposure. The estimated 24 hour and 48 hour EC50s based on decrease of in vivo chlorophyll alpha were >1000 ppm while the calculated 72- and 96-hour EC50s were 872 and 712 ppm respectively. Based on decrease of cell numbers the 96 hour calcualted EC50 was 655 ppm with 95% confidence limits of 439-977 ppm.

The 72 h EbC50 value = 2700 mg/L and the 72 h ErC50 value > 5000 mg/L. The NOEC based on area under the curve was 625 mg/L; in terms of the 0-72 hour growth rate the NOEC was 1250 mg/L. After 96 hours exposure EC50 values of greater than 5000 mg/L were obtained. The NOEC based on area under the curve was 1250 mg/L; in terms of the 0-96 hour growth rate the NOEC was 5000 mg/L.

Exposure of Skeletonema costatum to cyanuric acid gave EC50 values of greater than 100 mg/L (equivalent to 76 mg/L cyanuric acid) and correspondingly the NOEC was 100 mg/L (equivalent to 76 mg/L cyanuric acid). Analysis of the test preparations at 0 and 72 hours showed measured test concentrations to be near nominal and so the results are based on nominal test concentrations only.

Freshwater algae Navicula pelliculosa were exposed to 313, 625, 1250, 2500 and 5000 mg/L (equivalent to 237, 473, 945, 1890 and 3780 mg/L cyanuric acid). The test concentration of 5000 mg/L was the highest attainable test concentration that could be prepared due to the solubility of

the test material. After 96 h exposure EC50 values of > 5000 mg/L (equivalent to 3780 mg/L cyanuric acid) were obtained. The NOEC was 1250 mg/L (equivalent to 945 mg/L cyanuric acid)

In another study the freshwater algae Selenastrum capricornutum were exposed to 56, 100, 320, 560 and 1000 mg/L nominal concentrations of cyanuric acid. Exposure to cyanuric acid did not appear to adversely affect Selenastrum capricornutum until 72 hours of exposure. The estimated 24 hour and 48 hour EC50s based on decrease of in vivo chlorophyll alpha were >1000 ppm while the calculated 72- and 96-hour EC50s were 872 and 712 ppm respectively. Based on decrease of cell numbers the 96 hour calculated EC50 was 655 ppm with 95% confidence limits of 439-977 ppm.

In a limit test marine algae Skeletonema costatum were exposed to a nominal concentration of 100 mg/L to the monosodium salt of cyanuric acid. The EC50 value was >100 mg/L (equivalent to 76 mg/L cyanuric acid) and correspondingly the NOEC was 100 mg/L (equivalent to 76 mg/L cyanuric acid). Analysis of the test preparations at 0 and 72 hours showed measured test concentrations to be near nominal and so the results are based on nominal test concentrations only.

Toxicity to microorganisms

The effect of the test material on the respiration of activated sewage sludge micro-organisms gave a 3-hour EC50 of greater than 4500 mg/l equiavlent to 3402 mg cyanuric acid/l). The No Observed Effect Concentration (NOEC) after 3 hours exposure was 2700 mg/l (equivalent to 2041 mg cyanuric acid).

A study was performed to assess the effect of the monosodium salt of cyanuric acid on the respiration of activated sewage sludge. (Clarke 2007). Activated sewage sludge was exposed to an aqueous solution of the test material at concentrations of 480, 850, 1500, 2700 and 4500 mg/L (equivalent to 363, 643, 1134, 2041 and 3402 mg cyanuric acid/L) for a period of 3 hours at a temperature of 21°C with the addition of a synthetic sewage as a respiratory substrate. The rate of respiration was determined after 30 minutes and 3 hours contact time and compared to data for the control and a reference material 3,5 -dichlorophenol. The effect of the test material on the respiration of activated sewage sludge gave a 3 hour EC50 of >4500 mg/L (equivalent to 3402 mg cyanuric acid/L). The NOEC after 3 hours exposure was 2700 mg/L (equivalent to 2041 mg cyanuric acid/L).

Sediment toxicity

The toxicity of Monosodium salt of cyanuric acid to the sediment dwelling larvae of Chironomus riparius has been investigated and gave a 28-Day EC50 (emergence) of greater than 1000 mg test material/kg dry weight of sediment (equivalent to 756 mg cyanuric acid/kg dry weight of sediment). The No Observed Effect Concentration was 1000 mg test material/kg dry weight of sediment (equivalent to 756 mg cyanuric acid/kg dry weight of sediment). The EC50 (development rate) based on nominal test concentrations was greater than 1000 mg test material/kg dry weight of sediment (equivalent to 756 mg cyanuric acid).

Toxicity to soil macroorganisms except arthropods

A study was performed to assess the acute toxicity of the monosodium salt of cyanuric acid to earthworms (Eisenia foetida) in an artificial soil (Goodband 2007). 60 earthworms (six replicates of 10 worms) were exposed to a single concentration of 1000 mg test material/kg of dry soil for a period of 14 days. The number of mortalities was determined after 7 and 14 days exposure. The 14 day LC50 for the test material based on nominal test concentrations was > 1000mg test material/kg dry soil (equivalent to 756 mg cyanuric acid/kg dry soil). The NOEC was 1000 mg test material/kg dry soil (equivalent to 756 mg cyanuric acid/kg dry soil).

E.6.2 Information on tonnage and usage

Registrations	☒ Full registration(s) (Art. 10) ☐ Intermediate registration(s) (Art. 17 and/or 18)
Total tonnage band for substance (excluding volume registered under Art 17 or Art 18, or directly exported)	≥ 10 000 to < 100 000 tonnes per annum

Overview of uses of cyanuric acid

The substance is manufactured and/or imported in the European Economic Area in quantities at ≥ 10 000 to < 100 000 tonnes per annum. This volume does not take into account any exports into countries not being member of the EEA. This substance is used by consumers, in articles, by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing.

Table E21: Uses according to public information at ECHA's registration data base (date of access: May 2021).

Use	Information
Uses as intermediate	The substance is not used as an intermediate
Formulation or re-packaging	This substance is used in the following products: polymers and water treatment chemicals. This substance has an industrial use resulting in manufacture of another substance (use of intermediates). Release to the environment of this substance can occur from industrial use: formulation of mixtures and manufacturing of the substance.
Uses at industrial sites	This substance is used in the following products: biocides (e.g. disinfectants, pest control products), laboratory chemicals, polymers and water treatment chemicals. This substance has an industrial use resulting in manufacture of another substance (use of intermediates). This substance is used for the manufacture of: chemicals, rubber products and plastic products. Release to the environment of this substance can occur from industrial use: as an intermediate step in further manufacturing of another substance (use of intermediates) and in the production of articles.
Uses by professional workers	This substance is used in the following products: water treatment chemicals and polymers.

	This substance is used in the following areas: health services and municipal supply (e.g. electricity, steam, gas, water) and sewage treatment. This substance is used for the manufacture of: plastic products. Release to the environment of this substance can occur from industrial use: formulation of mixtures and manufacturing of the substance. Other release to the environment of this substance is likely to occur from: indoor use (e.g. machine wash liquids/detergents, automotive care products, paints and coating or adhesives, fragrances and air fresheners) and outdoor use.
Consumer Uses	This substance is used in the following products: water treatment chemicals. Release to the environment of this substance can occur from industrial use: manufacturing of the substance and formulation of mixtures. Other release to the environment of this substance is likely to occur from: indoor use (e.g. machine wash liquids/detergents, automotive care products, paints and coating or adhesives, fragrances and air fresheners) and outdoor use.
Article service life	Other release to the environment of this substance is likely to occur from: outdoor use in long-life materials with low release rate (e.g. metal, wooden and plastic construction and building materials) and indoor use in long-life materials with low release rate (e.g. flooring, furniture, toys, construction materials, curtains, foot-wear, leather products, paper and cardboard products, electronic equipment). This substance can be found in products with material based on: rubber (e.g. tyres, shoes, toys) and plastic (e.g. food packaging and storage, toys, mobile phones).

Manufacture: Release to the environment of this substance can occur from industrial use: manufacturing of the substance and formulation of mixtures.

Information on uses and occurrence of cyanuric acid according Wikipedia [15]

Cyanuric acid is used as a chlorine stabilizer / buffer in swimming pools. It is also used in the antineoplastic drug teroxirone. Cyanuric acid is also used as a precursor to N-chlorinated cyanurates, which are used to disinfect water. In addition, based on its trifunctionality, cyanuric acid is a precursor to crosslinking agents, especially for polyurethane resins and polyisocyanurate thermoset plastics.

Uses according to SPIN database [16]

For the latest reporting year (2019) the database on Substances in preparations in Nordic countries (SPIN) reports the following data:

[15] https://en.wikipedia.org/wiki/Cyanuric_acid#Applications
[16] www.spin2000.net; date of access: 24.05.2021

Country	#prep	tonnes	Consumer preparations	Confidential
DK	9	1.4	Yes	-
SE	0	0	-	Yes

From the use categories to be reported for SPIN in 2019 (use category description scheme UC 62), all of the cyanuric acid is used as non-agricultural pesticides and preservatives.

Data from SPIN is not fully representative for the European Economic Region because products and frequency of application may differ between the different geographical regions in the EU. In addition, the SPIN database not only refers to products where substances are intentionally added, but also deals with occurrence of substances as impurities.

Based on the data from the notifications for 2019, SPIN concludes a potential exposure for cyanuric acid for soil. SPIN concludes a probable exposure for surface water, wastewater and consumers and SPIN concludes a very probable occupational exposure.

Table E22: Exposure potential of cyanuric acid from products, according to SPIN database (with use index out of 5 unless specified)

Country	Quant.	Surface water	Air	Soil	Wastewater	Consumers	Occupational	Range of Use (RoU)	Article index (max: 3)
SE	3	4	2	3	4	4	5	2	1

On the basis of this information there is evidence that in principle, uses of cyanuric acid result in relevant emissions to some environmental compartments.

E.7 Trifluoroacetic acid

Table E23: Substance identifiers for Trifluoroacetic acid

EC name (public):	Trifluoracetic acid
IUPAC name (public):	trifluoroacetic acid
Index number in Annex VI of the CLP Regulation:	607-091-00-1
Molecular formula:	C2HF3O2
Molecular weight or molecular weight range:	114.02 g/mol
Synonyms:	*Acetic acid, 2,2,2-trifluoro-* *Acetic acid, trifluoro-* *Perfluoroacetic acid* *trifluoroacetic acid . . . %*

Type of constituent: ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

E.7.1 Hazard information

Classification

Harmonised Classification in Annex VI of the CLP

The substance is harmonized classified. CLP classification is given in table 4.

Table E24: Harmonised classification according to Annex VI of Regulation (EC) No 1272/2008

Index No	International Chemical Identification	EC No	CAS No	Classification	
607-091-00-1	Trifluoroacetic acid	200-929-3	76-05-1	Hazard Class and Category Code(s)	Hazard Statement Code(s)
				Skin Corr. 1A	H314
				Acute Tox. 4 *	H332
				Aquatic Chronic 3	H412

On ECHAs registered substances factsheets for TFA (accessed at 22. Sep. 21), the following information is given: Please note also that the harmonised classification indicates Skin Corr.1A H314 but not Eye Dam.1 H318. A skin corrosive substance is considered to also cause serious eye damage which is indicated in the hazard statement for skin corrosion (H314: Causes severe skin burns and eye damage). Thus, in this case both classifications (Skin Corr. 1 H314 and Eye Dam. 1 H318) are required, and therefore Eye Dam.1 H318 is added although not reported in the

harmonised classification. But the hazard statement H318 'Causes serious eye damage' is not indicated on the label because of redundancy (CLP Article 27).

Self classification

Table E25: Self classification according to ECHA's C&L inventory

Hazard Class and Category Code(s)	Hazard Statement Code(s)
Met. Corr. 1	H290
Acute Tox. 4	H302+H332
Skin Corr. 1A	H314
Eye Dam. 1	H332
Aquatic Chronic 3	H412
Flam. Liq. 2	H225

Proposal for Harmonised Classification in Annex VI of the CLP

There are no proposals for harmonized classification as of 19.06.2021.

CLP Notification Status

Table E26: CLP Notifications[17]

	CLP Notifications
Number of aggregated notifications	16
Total number of notifiers	521

Additional information

Information is taken from the dossiers.

Persistence

In aqueous solution, the pH of the substance is naturally low and for testing under realistic environmentally conditions either the sodium salt (NaTFA) or pH adjustment were required.

The ready biodegradability was determined in the closed bottle test performed according to slightly modified OECD 301D, EEC 1984 Part C., and ISO Test Guidelines. Secondary activated sludge was inoculated into 10 bottles per serie containing Trifluoroacetic acid, sodium salt, sodium acetate (reference substance) or only the medium (as a control) under aerobic conditions for a prolonged period of 77 days because the pass level was not reached at day 28. The percentages

[17] http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database (accessed 19th June 2021).

biodegradation of Trifluoroacetic acid, sodium salt in the closed bottle test were 0% for 0, 7, 21, 28 and 77 days and 8% for 14 and 42 days. The result of 8% degradation at day 42 is probably an artefact due to the 40 % coefficient of variation between duplicate values of the control. The percentages biodegradation of sodium acetate in the closed bottle test was 83% at 28 days. The test substance caused no reduction in the endogenous respiration and therefore is considered to be non-inhibitory to the inoculum. Trifluoroacetic acid, sodium salt was not biodegraded in the closed bottle test and should therefore not be classified as readily biodegradable. Based on these results, an inherent biodegradability test was conducted in compliance with the methods described in OECD test Guideline 302 A and EEC Directive 87/302 with some minor deviations. Because of the great potential for promoting biodegradation under aerobic conditions, the semi-continuous activated sludge (SCAS) test was chosen and Trifluoroacetic acid, sodium salt was exposed to relatively high concentrations of microorganisms maintained by daily addition of primary settled sewage. The test was conducted for a period of 127 days and the non-purgeable organic carbon (NPOC) was determined in the effluent. The test compound caused no reduction of the biodegradation of the NPOC present in primary settled waste water, therefore Trifluoroacetic acid, sodium salt is considered to be non-inhibitory to the activated sludge. Trifluoroacetic acid, sodium salt was removed approximately 20% from the wastewater in the SCAS test. Biodegradation of Trifluoroacetic acid has to lead to the formation of fluoride that was not detected in the effluent of SCAS units. This result also demonstrates that Trifluoroacetic acid, sodium salt is not biodegraded.

Another test, not performed according to standardised guideline but with an acceptable scientific method, was conducted in order to assess the cometabolic transformation of Trifluoroacetic acid, sodium salt, by microorganisms present in various inocula for a period of 84 days. The biodegradation of this compound in the presence of various co-substrates (acetic acid, peptone, yeast extract and vitamin B12) was determined by measuring the formation of fluoride. The addition of various co-substrates did not initiate a cometabolic transformation of Trifluoroacetic acid, sodium salt. which was not biodegraded in the batch cultures.

Two other non standardized tests investigated further the biodegradability of TFA. Even if the methodology was scientifically acceptable, the report was not sufficiently documented to assess the reliability of the results. The first study evaluated the ability of aerobic bacteria, previously shown to have a broad range of degradative capabilities, to degrade trifluoroacetic acid (TFA). Nine different bacterial strains were tested in bottle assays for their dehalogenation analysis, using 14C TFA to test for production of 14CO2. This study failed to show degradation of TFA by all strains. The second test was conducted to assess its biodegradability in an engineered anaerobic reactor in a long-term (90 weeks) study. Trifluoroacetic acid was found to be cometabolically degradable in an anaerobic environment.

In conclusion, trifluoroacetic acid is not readily biodegradated in water and no biodegradation and cometabolic transformation by any of the microorganisms tested was observed under aerobic conditions. A not assignable study show that cometabolic degradation in anaerobic conditions can happen.

Biodegradation testing in soil and sediment was not conducted for TFA (according to column 2 of Annex IX of REACH), because direct and indirect exposure of soil and sediment is unlikely based on its low adsorption potential (log Kow = 0.79 and 6.8 < log Koc< 15 L/kg at 25°C).

Mobility

Two tests using the batch equilibrium methodology, one according to OECD guideline 106 and one not according to the guidelines but of of good quality were performed on 54 different soil samples. The results show that TFA is poorly absorbed to the soil and is considered as a mobile organic compound in the majority of soils investigated. The Kd ranged between 0.19 to 20 L/kg for organic and mineral soils (the organic horizon exhibiting greater retention) giving a geometric mean of 0.94 L/kg (SD=4.86, n= 20) at 25°C. Based on these results no further information on adsorption/desortion is required according to column 2 of REACH Annex IX.

An adsorption screening test carried out according to OECD guideline 106 with three soil types (humous acid sandy soil, sandy loam with a low organic matter content, slightly alkaline loamy soil). The soil/water-system consisted of about 2 g soil and about 10 mL 0.01 M Ca(CH3COO)2 solution spiked with NaTFA (sodium trifluoroacetate) on a level of about 5 mg/L. Six blanks (without NaTFA), three controls (without soil) and six test soil (two replicates per soil) were performed during the test. The conclusion drawn from these results is that the TFA-anion poorly adsorbs to the different soil components because after 16 hours of agitating in a soil/water system less than 3% of the initial amount of TFA had disappeared from the water phase. Due to the fact that less than 25% is adsorbed, no further testing is required by the OECD guidelines.

Another batch equilibrium study not performed according to standard guideline but scientifically acceptable and well documented is reported. TFA was retained by 34 of 54 soils collected from diverse locations and a subset of 12 soils were chosen as representative of the TFA retention characteristics found in this study. Organic soils that exhibited higher retention of TFA sorbed between 20 and 60% of added TFA. In contrast, mineral soils retained 0 -15% of added TFA. Classifying mobility of TFA on the basis of Kd values suggests that TFA would be considered immobile (Kd> 10) in only 3 of 54 soils studied characterized by elevated organic matter content (> 70%). Eight soils exhibited low TFA mobility (Kd=2 -10), 15 soils intermediate mobillity (Kd=0.5 -2) and TFA should be considered as mobile in eight of soils (Kd=0.1 -0.5). No significant TFA retention was found in 20 of the soils studied. The retention of TFA increased with decreasing pH and decreased with increasing concentrations of F-, Cl-, and SO42 -. It is expected that rates of TFA leaching from soils will depend on soil types, organic content, soil pH, inputs of competing anions and atmospheric deposition rates of TFA. TFA was considered as a mobile organic compound in soils at the majority of sites investigated and measured Kd value ranged between 0.17 to 20 L/kg for all soil locations. An average Kd of 0.94 L/kg at 25°C (SD= 4.86, n= 20) based on the geometric mean of reported values for representitive soils retaining TFA was calculated.

A Koc is needed for the exposure assessment of the sediment.

By default, EUSES and CHESAR use QSAR calculation according to equation from Sabljic and Güsten (1995), as reported in the EU TGD (2003), using the class of non hydrophobic chemicals. In the case of trifluoacetic acid, the class "organic acid" is more relevant. Therefore the Koc is calculated as follows: logKoc = 0.6 * logKow + 0.32, with LogKow = 0.79

[LogKoc: 0.794]

Toxicity

Environmental official classification according to Annex VI of Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008: Trifluoroacetic acid is reported under the Index No 607-091-00-1 and is classified as Aquatic Chronic 3, H412.

This official classification is conservative because, based on the key studies available, the substance should not be classified for the environment as explained below:

Short-term E/LC50 values are available for algae (key study growth rate 72hEC50 = 237 mg/L), daphnia (48hEC50 > 100 mg/L) and fish (96hLC50 > 100 mg/L). All of the key studies demonstrate E/LC50 above 100 mg/L, showing that the substance does not need to be classified for acute toxicity to aquatic organisms according to the CLP and the UN-GHS criteria.

Additionally, trifluoroacetic acid is not readily biodegradable and due to the log Kow < 4 there is no tendency to bioaccumulate. Chronic toxicity data are available for algae showing a 72hErC10 of 5.6 mg/L and for daphnia showing a 21dNOEC above 25 mg/L. Therefore, the substance does not need to be classified for chronic toxicity to aquatic organisms according to the CLP and UN-GHS criteria.

Short-term toxicity to fish

The key study for short term toxicity to fish was performed with Trifluoroacetate sodium on the freshwater fish, Danio rerio under static conditions for 96h according to OECD Guideline 203 and GLP (Groeneveld, 1992). All validity criteria were fulfilled, this study was reliable without restriction. The study is a limit test at 1200 mg/l of Trifluoroacetate sodium in duplicates (i.e. 999 mg/l of Trifluoroacetic acid, TFA) with control. No mortality was observed so the LC50 (96h) was determined as greater than 999 mg/l and the NOEC is equal to 999 mg/l of TFA.

Another 96h-acute toxicity study was performed, according to NF ISO 7346 -1, with Trifluoroacetic acid on the same species under static conditions (Barthel, 2008). A limit test was realized at 8000 mg/L of TFA with control. No mortality was observed after 96 hours therefore a NOEC (96h) greater than 8000 mg/L was derived. However, some critical information on the substance purity, the test conditions and results is missing in the report to consider this study as reliable. Therefore these results are used as supportive information.

The key value used for chemical safety assessment is an LC50 greater than 999 mg/L of Trifluoroacetic acid for short term toxicity on freshwater fish.

Short-term toxicity to aquatic invertebrates

This endpoint is covered by four studies including one with no flag thus not further taken into consideration under REACH. A key study, performed according to standard guideline and GLP, which evaluated the acute toxicity of Sodium trifluoroacetate on the water fleas Daphnia magna and two supporting studies, performed according to standard guidelines (ISO and EU C.2) but without GLP statement, which evaluated the acute toxicity of Trifluoroacetic acid and Potassium trifluoroacetate on the same species.

The key study for short term toxicity to aquatic invertebrates was performed with Sodium trifluoroacetate on Daphnia magna under defined conditions for 48h according to OECD Guideline 202 and GLP (Groeneveld, 1992). All validity criteria were fulfilled, this study was reliable without

restriction. The study is a limit test at 1200 mg/l of Trifluoroacetate sodium in triplicates (i.e. 999 mg/l of Trifluoroacetic acid, TFA) with control. The selection of the limit test was based on the results of a range finding test. No mortality was observed so the EC50 (48h) was determined as greater than 999 mg/l and the NOEC is equal to 999 mg/l of TFA.

Two other 48h-acute toxicity studies were performed. The first, according to ISO guideline without GLP statement was realized on the same species Daphnia magna (Barthel, 2008). A series of 8 concentrations up to 27 g TFA/l was tested with control. The EC50 (48h) was determined to be 9.0 g TFA/l and the NOEC (48h) was evaluated at 5.6 g TFA/l. However, the results can only be used as supportive information as no details on preliminary test and definitive test conditions are given, some critical information is missing in the report to consider this study as reliable without restrictyion. The second study was realized according to EU C.2 guideline without GLP statement, on the same species Daphnia magna (Cerbelaud, 2000). Seven concentrations were tested with a control but only the highest concentration: 100 mg Potassium trifluoroacetate/L (i.e. 111 mg/l of TFA) was performed in duplicate.

No mortality was observed after 48 hours, therefore a EC50 (48h) greater than 111 mg/l of TFA was derived. However, no information was provided on the test substance and some test conditions, this result is used as supportive information.

The key value used for chemical safety assessment is an EC50 greater than 999 mg/L of Trifluoroacetic acid for short term toxicity on aquatic invertebrates

Long-term toxicity to aquatic invertebrates

One key study (reliable without restrictions) according to the OECD guideline 211/ EU Method C.20 under GLP is available on the freshwater invertebrate Daphnia magna.

This reproduction test was performed with a test material containing 30% Sodium trifluoroacetate at five concentrations and one control during 21 days. All validity criteria were fulfilled and the biological results shows no toxicity on the survival of adults and the reproduction rate after 21-days. The NOEC and EC50 (21d) were derived as equal/greater and greater than 25 mg TFA/L (corresponding to 100 mg 30% w/w NaTFA/L), respectively.

Toxicity to aquatic algae and cyanobacteria

In a GLP-compliant study conducted according to the procedure described in the OECD Guideline 201 “Freshwater Alga and Cyanobacteria, Growth Inhibition Test", the effects of the test item trifluoroacetic acid on the growth of the unicellular green algal species Pseudokirchneriella subcapitata was investigated.

Green algae were exposed during 72h to the test item in static conditions. The initial nominal concentrations were 0.9 – 2.5 – 7.0 – 19.5 – 54.7 – 153.1 – 428.6 – 1200.0 mg/L (corresponding to the following geometric mean of measured concentration at T0h and at T72h: 0.9 – 2.7 – 7.2 – 20.2 – 55.6 – 157.6 – 438.0 – 1207.0 mg/L). The test concentrations were analytically monitored by ion-exchange chromatography with gradient elution and conductimetric detection. The test item has been satisfactorily maintained within ± 20 % of the nominal concentration in all test conditions. The endpoint was inhibition of growth, expressed as logarithmic increase of biomass (average specific growth rate) during the exposure period.

All validity criteria were fulfilled. In conclusion, the following toxicity values have been determined for the test item trifluoroacetic acid based on nominal concentrations:

- NOEC (72h): 2.5 mg/L

- ErC10 (72h): 5.59 mg/L

- ErC50 (72h): 237.07 mg/L

Data of various reliability are available for seven freshwater species and three marine water species. Selenastrum capricornutum was the only species showing adverse effects.

For marine algae no ErC50 can be derived and the lowest NOEC value of 97 mg/l was defined for Phaedactylum tricornutum.

Key value for chemical safety assessment

EC50 for freshwater algae: 237 mg/L

EC10 or NOEC for freshwater algae: 5.6 mg/L

EC10 or NOEC for marine water algae: 97 mg/L

Toxicity to aquatic plants other than algae

The duckweed, Lemna gibba G3, was cultured in a range concentrations of sodium trifluoroacetate under static test conditions at 25°C for 7 days. The following nominal concentrations tested were 19, 38, 75, 150, 300, 600, 1200 and 2400 mg/L. A control was performed with culture inoculum only. Triplicate cultures of the control and of each concentration of the test substance were employed. Each replicate test vessel was inoculated with 3 plants, each consisting of 4 fronds (total of 12 fronds). The pH values determined at the start and finish of the test ranged from 4.6 to 4.7 at the start, and from 5.0 to 5.6 at the end of the study. The daily temperature measurements in the incubator ranged from 24.7 to 25.1°C. The light intensity was 9220 Lux. The test substance was mixed with 14C-labelled trifluoroacetic acid to enable radiochemical analysis of the test solutions at the start and finish, and analysis of the plant tissue at the end of the exposure. Moreover, the bioconcentration factor was determined for each measured concentrations. The measured concentrations at start of the test ranged from 102 to 113% of the nominal values. At each nominal concentration the mean measured values at the finish were the same as those at the start of the test. The number of fronds and the dry weights of tissue were determined during the test. Furthermore, other symptoms of toxicity were determined : from day 5 onwards, plants in the nominal 600,1200 and 2400 mg/L exhibited pale, misshapen fronds with decreased root growth, compared with the control. There were no observed symptoms at or below a nominal concentration of 300 mg/L compared with the control.

The EC50 for increase in frond number and increase in frond dry weight were as follows:

EC50 (frond increase) = 915 mg/L of TFA

EC50 (weight increase) = 999 mg/L of TFA

These values were based on nominal concentrations which were confirmed by radiochemical analysis. There were no significant (p=0.05) inhibitory effects on frond or weight increase, at a nominal concentration of 300 mg NaTFA/L (250 mg TFA/L). The tissues showed only slight bioconcentration of the test substance after 7 days, with bioconcentration factors ranging from 1.0 to 1.6, based on radiochemical analysis.

Toxicity to microorganisms

This endpoint is covered by four studies. A key study, performed according to standard guidelines and GLP, which evaluated the influence of Sodium trifluoroacetate on the activated sludge respiration rate under defined conditions and three supporting studies, not performed according to international guidelines and without GLP statement, which evaluated the effects of trifluoroacetic acid on freshwater microbial communities, on microbial methanogenesis, and on acetate metabolism by stream microbial communities.

In the key study, the 3 hours EC10, EC20 and EC50 could not be quantified because up to the highest nominal test concentration (1000 mg NaTFA/L, corresponding to 832 mg TFA/L) less than 10% inhibition was noted. Nevertheless, the 3-hour EC20 and EC50 are clearly higher than 832 mg TFA/L under the present test conditions. The NOEC/EC10 may be established above 832 mg TFA/L.

Moreover, three supporting studies indicated no acute/chronic effects of TFA on acetate metabolism (TFA did not reduce methane formation from acetate) and no effect of TFA on tested methanogenic systems (TFA is inert in these methanogenic systems and there is no evident toxicity to either the methanogenic or fermentative population). However, a potential to be actively incorporated by microorganisms have been found.

Sediment toxicity

Based on the log Kow of 0.79 at 25°C below the trigger value of log Kow ≥3, a justification for non submission of data was presented. indicating that the substance is unlikely to adsorb to sediment and that the assessment conducted for the aquatic compartment will also cover the sediment compartment.

Toxicity to terrestrial plants

Two key studies were performed according to the testing OECD 208 guideline to measure the effect of sodium trifluoroacetate (NaTFA) in soil on seed germination and early plant growth of Sunflower (Helianthus annuus), Mung Bean (Phaseolus aureus) and Wheat (Triticum aestivum). Nine seeds per pot, in four replicates were sown in soil containing nominal concentrations of 1, 10, 100 and 1000 mg sodium trifluoroacetate / kg (dry soil) plus control.

There were statistically significant decreases in the proportion of seeds which had germinated and emerged after 14 days and the EC50s for germination were as follows:

Sunflower : EC50 germination = 250 mg NaTFA/kg (208 mg TFA/kg)

Mung Bean : EC50 germination = 770 mg NaTFA/kg (640.8 mg TFA/kg).

Wheat: EC50 germination= 1000 mg/kg NaTFA/kg

At the end of the test, 28 days after the seeds were sown, the mean fresh weight of the seedling shoots (cropped at soil level) were significantly reduced and the calculated EC50 for growth, based on nominal concentrations were as follows:

Sunflower : EC50, Shoot growth (28d) = 12 mg NaTFA/kg (10 mg TFA/kg).

Mung Bean : EC50, Shoot growth (28d) = 5.7 mg NaTFA/kg dry soil (4.7 mg TFA/kg).

Wheat: EC50 Shoot growth (28d) = 12 mg NaTFA/kg dry soil (10 mg TFA/kg dry soil).

There was no significant effect on shoot weight at 1 mg sodium trifluoroacetate / kg and therefore

Sunflower : NOEC shoot weight (28d) < 1 mg NaTFA/kg (< 0.83 mg TFA/kg).

Mung Bean : NOEC shoot weight (28d) = 1 mg NaTFA/kg dry soil (0.83 mg TFA/kg).

Wheat: NOEC shoot weight (28d) = 1 mg NaTFA/kg dry soil (= 0.83 mg TFA/kg dry soil).

The toxicity of TFA is mainly observed when the seeds are sown and resulted in a reduced shoot growth. The germination is also impacted but at a lowest level. A NOEC of 1 mg/ kg dry soil NaTFA corresponding to 0.83 mg/kg dry soil TFA is safe for both stage.

The other studies reported were not been performed according to standard guidelines but they support the key studies results.

Four studies were performed under hydroponic conditions on different plant species. One study investigated the Soybean and show that the plants were developmentally stunted and had shoot weights that were significantly reduced above the NOEC shoot fresh weight (36d) = 0.674 µL TFA/kg soil ww (corresponding to 1mg TFA/kg soil ww). Further, the effect of seven halogenated aliphatic acids including TFA on the initial growth of wheat and tomato roots and shoots was studied.The results showed different sensitivity between the Monocotyledonae and the Dicotyledonae species. Wheat shoot was more inhibited than tomato shoot. Wheat root was not inhibited and Tomato root was more inhibited than tomato shoot. Also, the effect of TFA on seed germination of ten species by aqueous exposure were investigated. No effect on germination was found up to 832 mg TFA/L for all species. Finally, the toxicity to plantago major by aqueous exposure and a NOEC (14d), based on leaf or root weight, of 26.6 mg TFA/L was reported.

Three studies assessed as not assignable based on insufficiently documented reports investigated the TFA effects by atmospheric pathways. One study on several plants testing mist and rain deposition of TFA demonstrated a NOEC (25d) > 83,2 mg TFA/L for height and fresh weight on sunflower, soya, wheat, maize, oilseed rape, rice and plantain and LOEC (44d) = 83,2 mg TFA/L for visible injury on soya. Another study on the effect of TFA on wheat after pulverization shows 45% destruction on pre-emerging phase with 1.8 mg TFA/kg and 50% destruction on post-emerging phase with 7.4 mg TFA/kg. Finally one study performed on Pinus ponderosa exposed to TFA applied as mist to foliar surfaces demonstrated an accumulation in needles as a function of concentration applied and no visual morphological or photosynthetic effects at 0,01 µg TFA/l. Further the results indicate that atmospheric uptake may not be the dominant pathway of uptake in environmental conditions but rather root uptake.

Finally, four other studies investigated the mode of action of TFA to plants. One study described the uptake of Trifluoroacetic acid in Lycopersicon esculentum using 19F and 1H nuclear magnetic resonance imaging and spectroscopy. The spectroscopy results show that the TFA is transported through the stem and accumulates in the leaves. Another study investigated the toxicity to wheat in relation to bioaccumulation by aqueous exposure of the roots to 14C-radiolabelled sodium trifluoroacetate for 35 days. The inhibition of the growth of plants including tissue chlorosis and necrosis was associated with an increasing 14C-residues levels in the leaf tissues over the period of exposure and a bioconcentration factor (BCF) of 43 after 35 days. In an other report, Sunflower seedlings were exposed to a single concentration of 14C-radiolabelled trifluoroacetic acid in the aqueous (hydroponic) medium. 14C-residues in the leaf tissues increased continuously over the period of exposure, with a bioconcentration factor (BCF) of approximately 22 after 12 days. The stem tissue behaved similarly but with a lower rate of accumulation (12 -day BCF approximately 5). Root tissue reached apparent equilibrium after 5 days exposure with a BCF of approximately 3. All tissues showed a decline in 14C-residue concentrations on transfer to clean medium with some evidence of depuration. In another study, growth and development of nitrogen-fixing soybean seedlings was assessed in the presence of trifluoroacetic acid in soil cultures. Overall the results show that TFA, at 1 mg/kg does not interfere with the ability of nitrogen-fixing bacteria to infect and colonize the plant, nor does it interfere with the normal development and nitrogen-fixation by the growing plant.

According to column 2 of REACH Annex X, long term toxicity study on plants does not need to be conducted for trifluoroacetic acid because direct and indirect exposure of soil is unlikely based on its low potential for adsorption to soil (log Kow = 0.79 and Kd= 0.94 L/kg at 25°C) and no risk have been characterised by the Chemical Safety Assessment according to Annex I. Moreover, the two terrestrial plant tests performed according to OECD 208 are assumed to cover a sensitive stage in the life-cycle of a plant and therefore data obtained from these studies have been used as estimates of chronic toxicty as mentionned in the Chapter R.7C of the Guidance on Information requirements and CSA of ECHA.

E.7.2 Information on tonnage and usage

Registrations	Full registration(s) (Art. 10) Intermediate registration(s) (Art. 17 and/or 18)
Total tonnage band for substance (excluding volume registered under Art 17 or Art 18, or directly exported)	≥ 100 to < 1 000 tonnes per annum

Overview of uses of trifluoroacetic acid

The substance is manufactured and/or imported in the European Economic Area in quantities at ≥ 100 to < 1 000 tonnes per annum. This volume does not take into account any exports into countries not being member of the EEA. This substance is used by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing. This substance is also used as an intermediate.

Table E27: Uses according to public information at ECHA's registration data base (date of access: May 2021).

Use	Information
Uses as intermediate	This substance is used as an intermediate. It is used as an intermediate in chemical manufacture. The process categories listed are: PROC 1: Chemical production or refinery in closed process without likelihood of exposure or processes with equivalent containment conditions. PROC 3: Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment conditions. PROC 2: Chemical production or refinery in closed continuous process with occasional controlled exposure or processes with equivalent containment conditions. PROC 8b: Transfer of substance or mixture (charging and discharging) at dedicated facilities PROC 9: Transfer of substance or mixture into small containers (dedicated filling line, including weighing) PROC 15: Use as laboratory reagent The sector end use is in the manufacture of fine chemicals.
Formulation or re-packaging	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. Release to the environment of this substance can occur from industrial use: formulation of mixtures.
Uses at industrial sites	This substance is used in the following products: laboratory chemicals. This substance is used for the manufacture of: chemicals. Release to the environment of this substance can occur from industrial use: as an intermediate step in further manufacturing of another substance (use of intermediates), in processing aids at industrial sites and in the production of articles.
Uses by professional workers	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. ECHA has no public registered data on the types of manufacture using this substance. Other release to the environment of this substance is likely to occur from: indoor use as reactive substance.
Consumer Uses	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. ECHA has no public registered data on the routes by which this substance is most likely to be released to the environment.
Article service life	ECHA has no public registered data on the routes by which this substance is most likely to be released to the environment. ECHA has no public registered data indicating whether or into which articles the substance might have been processed.

Information on uses and occurrence of trifluoroacetic acid according to Wikipedia [18]:

TFA is the precursor to many other fluorinated compounds such as trifluoroacetic anhydride, trifluoroperacetic acid, and 2,2,2-trifluoroethanol. It is a reagent used in organic synthesis because of a combination of convenient properties: volatility, solubility in organic solvents, and its strength as an acid. TFA is also less oxidizing than sulfuric acid but more readily available in

[18] https://en.wikipedia.org/wiki/Trifluoroacetic_acid#Uses

anhydrous form than many other acids. One complication to its use is that TFA forms an azeotrope with water (b. p. 105 °C). TFA is popularly used as a strong acid to remove t-butyl derived side-chain protecting groups in Fmoc peptide synthesis, and in other organic syntheses to remove the t-butoxycarbonyl protecting group. At a low concentration, TFA is used as an ion pairing agent in liquid chromatography (HPLC) of organic compounds, particularly peptides and small proteins. TFA is a versatile solvent for NMR spectroscopy (for materials stable in acid). It is also used as a calibrant in mass spectrometry. TFA is used to produce trifluoroacetate salts.

Uses according to SPIN database [19]

For the latest reporting year (2019) the database on Substances in preparations in Nordic countries (SPIN) reports the following data:

Country	#prep	tonnes	Consumer preparations	Confidential
DK	44	0.2	-	-
SE	0	0	-	Yes

When looking at the use categories reported for SPIN (use category description scheme UC 62), the number of preparations and tonnes is zero for all years, but the uses listed are laboratory chemicals and pharmaceuticals.

Data from SPIN is not fully representative for the European Economic Region because products and frequency of application may differ between the different geographical regions in the EU. In addition, the SPIN database not only refers to products where substances are intentionally added, but also deals with occurrence of substances as impurities.

Based on the data from the notifications for 2019, SPIN concludes a potential exposure for trifluoroacetic acid for air, soil and wastewater. SPIN concludes a very probable consumer and occupational exposure.

Table E28: Exposure potential of trifluoroacetic acid from products, according to SPIN database

Country	Quant.	Surface water	Air	Soil	Wastewater	Consumers	Occupational	Range of Use (RoU)	Article index (max: 3)
DK	1	2	3	2	3	5	5	1	1
SE	3	2	3	3	3	4	4	1	1

[19] www.spin2000.net; date of access: 24.05.2021

On the basis of this information there is evidence that in principle, uses of trifluoracetic acid result in relevant emissions into several environmental compartments.

Additional information

Regulatory obligations exist for trifluoroacetic acid under the following regulations:

- Active Implantable Medical Devices Directive - Hazardous Substances
- CAD - Chemical Agents Directive, Article 2(b)(i) - Hazardous Agents
- Construction Product Regulation - Annex I (3) - Hazardous Substances
- Construction Product Regulation - Article 6(5) - SDS and Declaration
- End-of-Life Vehicles Directive - Hazardous Substances
- Ecolabels - Restrictions for Hazardous Substances/Mixtures
- General Product Safety Directive - Hazardous Substances
- In Vitro Diagnostic Medical Devices Directive - Hazardous Substances
- Inland Transport of Dangerous Goods Directive, Annex I – ADR
- Inland Transport of Dangerous Goods Directive, Annex II – RID
- Inland Transport of Dangerous Goods Directive, Annex III – AND
- Medical Devices Directive - Hazardous Substances
- Physical, Biological and Chemical Agents & Processes and Work
- Safety and Health of Workers at Work Directive - Hazardous Substances
- Workplace Signs - minimum requirements & signs on containers and pipes

Waste Framework Directive, Annex III - Waste - Hazardous Properties.

E.8 Trifluoromethanesulphonic acid

Table E29: Substance identifiers for Trifluoromethanesulphonic acid

EC name (public):	Trifluoromethanesulphonic acid
IUPAC name (public):	trifluoromethanesulfonic acid
Index number in Annex VI of the CLP Regulation:	Not given
Molecular formula:	CHF3O3S
Molecular weight or molecular weight range:	150.07121 g/mol
Synonyms:	*Methanesulfonic acid, 1,1,1-trifluoro-* *PERFLUOROMETHANESULFONIC ACID* *Triflic acid*

Type of constituent: ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

E.8.1 Hazard information

Classification

Harmonised Classification in Annex VI of the CLP

There is currently no harmonised classification in Annex VI of the CLP [20].

Self classification

- In the registration:

Classifications reported in the registration [21] are:

  - H290: May be corrosive to metals.
  - H302: Harmful if swallowed.
  - H314: Causes severe skin burns and eye damage.
  - H335: May cause respiratory irritation.

- Additional classifications in the C&L Inventory:

Table E30: Self classification according to ECHA's C&L inventory

Hazard Class and Category Code(s)	Hazard Statement Code(s)
Met. Corr. 1	H290
Acute Tox. 4	H302, H312

[20] https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/75011
[21] https://echa.europa.eu/registration-dossier/-/registered-dossier/5311/2/1

Hazard Class and Category Code(s)	Hazard Statement Code(s)
Skin Corr. 1B	H314
Eye Dam. 1	H318
STOTE SE 3	H335
Skin Corr. 1A	H314
Skin Corr. 1C	H314
Aquatic Chronic 4	H413

Proposal for Harmonised Classification in Annex VI of the CLP

There are no proposals for harmonized classification as of 22.06.2021.

CLP Notification Status

Table E31: CLP Notifications [22]

	CLP Notifications
Number of aggregated notifications	30
Total number of notifiers	2332

Additional information

Information is taken from the dossiers.

Persistence
One experimental study (2013) was performed in order to evaluate the aerobic ultimate biodegradation potential of Trifluoromethanesulfonic acid in a test for ready biodegradability, according to the OECD 301D guideline and under GLP conditions and was selected as key study. This study used a test item concentration of 21.97 mg/L (corresponding to a theoretical oxygen consumption of 5.86 mg/L). The solution of the test item in mineral medium was inoculated with a relatively small number of micro-organisms from a mixed population and kept in completely full, closed bottles in the dark at constant temperature. Degradation was followed by analysis of dissolved oxygen over a 28-day period. The amount of oxygen taken up by the microbial population during biodegradation of the test item, corrected for uptake by the blank inoculum run in parallel, is expressed as a percentage of COD. There was 0% of degradation of test item after 28 days. The positive control reached the pass level already on day 3. As degradation in the toxicity flask was more than 25 % at the end of the test, the test item can be stated as not toxic towards

[22] http://echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database (accessed 19th June 2021).

the inoculum in a concentration of 11.72 mg/L. In these test conditions, Trifluoromethanesulfonic acid was not readily biodegradable.

Mobility

The logKoc value has been calculated from the logKow using the equation of the TGD. Based on the low logKow of trifluoromethanesulfonic acid, it is expected to have a low potential for adsorption onto soil and sediment (i.e. the substance has a logKow below 3). For the calculation in the CSA, the equation of the TGD (Sabljic and Günsten, 1995) is applied to derive the logKoc value of the substance from its log Kow value. As no specific class is available for Trifluoromethanesulfonic acid in the proposed equations (e.g. no sulfonic acid class), the equation for "nonhydrophics" is selected as follows:

LogKoc = 0.52 * logKow + 1.02 = 0.52 * 0.3 + 1.02 = 1.176

[LogKoc: 1.176]

Toxicity

Short-term toxicity to fish

The purpose of the study was to estimate the acute toxicity (LC50) of trifluoromethanesulfonic acid to rainbow trout,Oncorhynchus mykiss, under static test conditions. The study followed the OECD Guideline for Testing of Chemicals #203, the EU Method C.1 and was performed under GLP conditions. After a preliminary test, nominal trifluoromethanesulfonic acid test concentrations of 6.3, 13, 25, 50 and 100 mg/L were chosen for the definitive exposure. No mortality was observed during the study, therefore, the 96-hour LC50 value was >100 mg/L and the No Observed-Effect Concentration (NOEC) was determined to be 100 mg/L. In these test conditions, Trifluoromethanesulfonic acid is not harmful to fish.

Short-term toxicity to aquatic invertebrates

The purpose of the study was to estimate the acute toxicity (EC50) of trifluoromethanesulfonic acid to daphnids (Daphnia magna) under static test conditions. This study was conducted according to OECD Guideline for Testing of Chemicals 202, the EU Method C.2 and the GLP. The nominal concentrations tested were 6.3, 13, 25, 50, and 100 mg/L. No immobilised daphnids were observed during the study, therefore the 48-hour EC50 value was > 100 mg/L and the No-Observed-Effect Concentration (NOEC) was determined to be 100 mg/L. In these test conditions, Trifluoromethanesulfonic acid is not harmful to daphnids.

Long-term toxicity to aquatic invertebrates

In an OECD TG211 study, the 21-day NOEC value was determined to be >= 100 mg/L. One reliable study is available for this endpoint (Urann K., 2014). The purpose of this study was to estimate the effect of the test item Trifluoromethanesulfonic acid on the reproductive output of Daphnia magna according to the OECD 211 guideline and performed under GLP conditions.

Daphnia magna were exposed in a semi-static test to aqueous test media containing the test item for 21 days. Ten replicates of 10 daphnids each were tested for each treatment and control group. The Daphnids were exposed to the test item at the following nominal exposure concentrations:

6.3, 13, 25, 50 and 100 mg/L. Mean measured concentrations ranged from 100 to 110% of nominal concentrations therefore the results are based on nominal values. The chronic effect of trifluoromethanesulfonic acid was evaluated based on the survival, reproduction and growth (mean total body length) of the daphnids. No mortality has been observed during the study. Therefore, the NOEC for survival was determined to be 100 mg/L and the LOEC was determined to be > 100 mg/L.

Following 21 days of exposure, the organisms exposed to the 6.3, 13, 25, 50 and 100 mg/L treatment levels had released a mean cumulative offspring per female of 193, 197, 201, 206 and 187, respectively. Statistical analysis (Dunnett's Multiple Comparison Test) determined no significant difference in offspring per female among daphnids exposed to any of the treatment levels compared to the control (184 offspring per female). Control daphnids released their first brood of offspring on test day 7. First brood release by daphnids occurred on day 7 for all treatment levels, with the exception of the 100 mg/L treatment level where first brood release occurred on day 8. Throughout the exposure, no aborted eggs, dead offspring or epiphia were observed. Therefore, the NOEC for reproduction was determined to be 100 mg/L and the LOEC was determined to be > 100 mg/L. Total body length at exposure termination among control daphnids averaged 4.89 mm. Total body length among daphnids exposed to the 6.3, 13, 25, 50 and 100 mg/L treatment levels averaged 4.94, 4.98, 4.92, 4.90 and 4.98 mm, respectively. Statistical analysis (Dunnett's Multiple Comparison Test) determined no significant difference in total length among daphnids exposed to any of the treatment levels compared to the control (4.89 mm). Therefore, the NOEC for total body length was determined to be 100 mg/L and the LOEC was determined to be > 100 mg/L.

Toxicity to aquatic algae and cyanobacteria

The objective of the study was to determine the effect of trifluoromethanesulfonic acid on the growth of the freshwater green alga, Pseudokirchneriella subcapitata. Procedures used in this study followed the OECD Guideline for Testing of Chemicals #201 and the GLP. Although the test item concentration was found to be stable during the study, the results are based on mean measured concentrations of trifluoromethanesulfonic acid. The 72-hour NOEC for growth rate was determined to be 5.7 mg/L. The 72-hour ErC50value was determined to be 48 mg/L with lower and upper 95% confidence limits of 31 and 67 mg/L, respectively. The OECD validation criteria were fulfilled. In these test conditions, trifluoromethanesulfonic acid is harmful to algae.

Toxicity to microorganisms

The objective of the study was to assess the effect of the test item trifluoromethanesulfonic acid on the respiration of activated sewage sludge, over a period of 3 hours. The criterion measured was the inhibition of the respiration rate of the activated sludge, exposed to different concentrations of the test item, and expressed as a percentage of the control. From these values, the EC50 (concentration at which respiration rate is 50% of that in the control) was calculated. The 3h EC50 of the reference item was 11.7 mg/L in this study. Therefore, the criterion for validation of the inoculum is fulfilled. The highest tested concentration of the test item, i.e. 1000 mg/L, did not inhibited the respiration rate of the inoculum. This concentration can therefore be considered as a NOEC. The 3h EC50 of the test item, with test item as is or neutralized, was > 1000 mg/L. In these conditions, trifluoromethanesulfonic acid is not harmful to microorganisms.

E.8.2 Information on tonnage and usage

Registrations	☒ Full registration(s) (Art. 10) ☒ Intermediate registration(s) (Art. 17 and/or 18)
Total tonnage band for substance (excluding volume registered under Art 17 or Art 18, or directly exported)	≥ 100 to < 1 000 tonnes per annum

Overview of uses of trifluoromethanesulfonic acid

The substance is manufactured and/or imported in the European Economic Area in quantities at ≥ 100 to < 1 000 tonnes per annum. This volume does not take into account any exports into countries not being member of the EEA. This substance is used by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing. This substance is used as an intermediate.

Table E32: Uses according to public information at ECHA's registration data base (date of access: May 2021).

Use	Information
Uses as intermediate	This substance is used as an intermediate. Process category PROC 3: Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment conditions Sector of end use SU 9: Manufacture of fine chemicals
Formulation or re-packaging	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. Release to the environment of this substance can occur from industrial use: formulation of mixtures.
Uses at industrial sites	This substance is used in the following products: laboratory chemicals and polymers. This substance is used in the following areas: scientific research and development. This substance is used for the manufacture of: chemicals and electrical, electronic and optical equipment. Release to the environment of this substance can occur from industrial use: as processing aid, as an intermediate step in further manufacturing of another substance (use of intermediates), in processing aids at industrial sites and in the production of articles.
Uses by professional workers	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. This substance is used in the following areas: scientific research and development. Other release to the environment of this substance is likely to occur from: indoor use (e.g. machine wash liquids/detergents, automotive care products, paints and coating or adhesives, fragrances and air fresheners).
Consumer Uses	ECHA has no public registered data indicating whether or in which chemical products the substance might be used. ECHA has no public registered data on the routes by which this substance is most likely to be released to the environment.

Article service life	ECHA has no public registered data on the routes by which this substance is most likely to be released to the environment. ECHA has no public registered data indicating whether or into which articles the substance might have been processed.

Uses according to SPIN database [23]

For the latest reporting year (2019) the database on Substances in preparations in Nordic countries (SPIN) reports the following data:

Country	#prep	Tonnes	Consumer preparations	Confidential
DK	0	0	-	Yes
SE	0	0	-	Yes

All of the data from 2019 is confidential and use categories are not detailed.

Data from SPIN is not fully representative for the European Economic Region because products and frequency of application may differ between the different geographical regions in the EU. In addition, the SPIN database not only refers to products where substances are intentionally added, but also deals with occurrence of substances as impurities.

Based on the data from the notifications for 2019, SPIN concludes a potential exposure for trifluoromethanesulphonic acid for air, soil, wastewater and consumers. SPIN concludes a very probable occupational exposure.

Table E33: Exposure potential of trifluoromethanesulphonic acid from products, according to SPIN database

Country	Quant.	Surface water	Air	Soil	Wastewater	Consumers	Occupational	Range of Use (RoU)	Article index (max: 3)
DK	1	1	3	3	3	3	5	1	2
SE	2	2	3	2	3	3	5	1	3

On the basis of this information there is evidence that in principle, uses of trifluoromethanesulphonic acid result in relevant emissions into certain environmental compartments.

[23] www.spin2000.net; date of access: 24.05.2021

E.9 N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine

Table E34: Substance identifiers for N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine

EC name (public):	N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine
IUPAC name (public):	N-(1,3-dimethylbutyl)-N'-phenylbenzene-1,4-diamine
Index number in Annex VI of the CLP Regulation:	Not given
Molecular formula:	C18H24N2
Molecular weight or molecular weight range:	268.404 g·/ mol
Synonyms:	*1,4-Benzenediamine, N1-(1,3-dimethylbutyl)-N4-phenyl-* *6PPD*

Type of constituent: ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

E.9.1 Hazard information

Classification

Harmonised Classification in Annex VI of the CLP

There is currently no harmonised classification in Annex VI of the CLP.

Self classification

- In the registration:

Classifications reported in registrations list the following

- H302: Harmful if swallowed.
- H317: May cause an allergic skin reaction.
- H360: May damage fertility or the unborn child <state specific effect if known > <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>.
- H410: Very toxic to aquatic life with long lasting effects

- Additional classifications in the C&L Inventory:

There are no additional classifications in the C&L inventory.

Proposal for Harmonised Classification in Annex VI of the CLP

There are no proposals for harmonized classification in Annex VI of the CLP as of November 2021.

CLP Notification Status

There are no notifications listed.

Additional information

Information from the dossiers is provided.

Persistence

Biodegradation in water: screening test

A test was conducted according to the OECD Guideline 301 C (Ready Biodegradability: Modified MITI Test). Based on BOD analysis, approximately 2 % of N-(1,3-dimethylbutyl)-N'-phenylbenzene-1,4-diamine was biodegraded after 4 weeks. (MITI, 1995). Based on HPLC analysis, approximately 92 % of N-(1,3-dimethylbutyl)-N'-phenylbenzene-1,4-diamine was degraded and the following degradation products were determined: Phenylbenzoquinone imine, p-benzoquinone, 1,3-dimethylbutylamine, 4-anilinophenol, aniline.

Biodegradation in water and sediment: simulation tests

The primary biodegradation for biological and chemical transformations of 6PPD was studied using Mississippi river water under aerobic conditions. Controls of this biodegradation study were made with sterile and with deionized water. After 22 h, when the experiment was finished, 97 % of 6PPD had disappeared from the active river water, 96 % from the sterile river water, and 88 % from the deionized water. The estimated half-lives due to primary transformation ranged from 2.9 to 6.8 hours.

No transformation products were identified. The study is not comparable to a full test according to OECD guidelines. The test duration was only 22h. Thus, only abiotic degradation can be observed. Taking information from ready biodegradation tests into account, biodegradation is not expected under the test conditions. (Monsanto 1981) These results only reflect the primary degradation of the substance.

Biodegradation in soil

Information is given related to the similar substance 7PPD as well as a justification for read across.

Aerobic conditions:

DT50 values derived from First Order Multi Compartment kinetics (FOMC) kinetics were 1.4 – 1.9 days for Soils II-IV and < 1 day for soil I. The faster decline in acid soil I (pH 3.8) was explained by the instability of 7PPD under acidic conditions.

The metabolism of 14C-7PPD in aerobic soils is proposed to proceed via formation of minor transient metabolites and mineralization. The main portion of the residue is binding to the soil matrix and appears to become unavailable for further degradation/mineralization.

Anaerobic conditions:

The short DT50 of the parent (1.5 days) in the flooded test system was attributed to aerobic degradation. Following that rapid initial decline, 7PPD dissipated slowly. A DT90 of >1000 days was

calculated. The metabolite 1-N-(5-methyl-hexan-2-yl)-4-N-phenylcyclohexa-2,5-dione-4,4-diimine also known as 7QDI, (cis/trans isomers) was observed.

7QDI Isomer 1: DT50 = 57.9 d; DT90 = 192 d

7QDI Isomer 2: DT50 = 79.7 d; DT90 = 265 d

7QDI Isomer 1+2: DT50 = 66.9 d; DT90 = 222 d

Degradation was described by SFO (Single First Order) model.

Justification for the read-across: 1,4-Benzenediamine, N-(1,4 -dimethylpentyl)-N'-phenyl- (7PPD) has a similar structure as 6PPD. It is a member of the paraphenylene diamine family. The difference is that 7PPD has an C7 branched aliphatic chain, whereas 6PPD has C6 branched aliphatic chain. Additional information on the read-across is given in the read-across-justification document attached to IUCLID chapter 13.

The outcome of recent scientific developments considering bound residues are reflected in the following guidance documents:

European Commission (2012), Health and Consumers Directorate, “DG SANCO working document on “evidence needed to identify POP, PBT and vBvP properties for pesticides”.:

“Unextractable residues should be excluded from further assessment. They can be considered degradation loss, not bioavailable and therefore unable to exert toxicity. This approach is consistent with the SCHER opinion on aclonifen EQS (30 march 2011). Future Guidance might foresee taking into account “adsorbed unextractable residues”, which could be mobilised in the long-term and become relevant for further assessment.”

US Environmental Protection Agency (2014) “Guidance for Addressing Unextracted Residues in Laboratory Studies,http://www.epa.gov/pesticides/science/efed/policy_guidance/team_authors/environmental_fate_tech_team/Unextracted_Residues_in_Lab_Studies.htm:

“Extraction solvent systems should include solvents in which the parent compound and/or its transformation products are highly soluble. Systems for the extraction of neutral organic compounds should include non-polar solvents. Combinations of solvents, including a weak acid or weak base, may enhance the extraction efficiency. Some example polar solvents with dielectric constants ranging from 18 to 80 at environmental temperatures include water, formic acid, methanol, ethanol, isopropanol, acetone, acetonitrile, and dimethyl sulfoxide. Some example polar solvents with lower dielectric constants ranging from 6.0 to 9.1 include acetic acid, ethyl acetate, tetrahydrofuran, and dichloromethane. Example nonpolar solvents include hexane, benzene, toluene, 1,4-dioxane, chloroform, and diethyl ether (dielectric constants range from 1.9 to 4.8). Judgment should be used in the choice of solvents since factors other than dielectric constant may be important. Generally, unless there is a reason for a different approach, at least one solvent from each of the three groups identified above by range of dielectric constant should be used when there are a high proportion of unextracted residues (i.e., greater than 10% of the applied). Also, the solvent system pH should be adjusted to maximize recovery of compounds known to exhibit acid-base behavior.”

In order to cover the groups of solvents proposed by EPA, the 7PPD soil simulation used a solvent with high dielectric constant (acetone) and one solvent in the lower dielectric constant group (dichlormethane). A very unipolar solvent was considered but not used as the nature of the chemical was not thought to result in very unpolar residues. However, as the substance has amino groups and was expected to perhaps form ionic structures, an alkalic solvent system including ammonium hydroxide was additionally used.

The following extraction procedures had been used in the study in order to cover the requirements of EPA (2014 (Supercritical fluid extraction: tested in pretest and found not useful):

Ambient extraction with acetone / dichloromethane (3x)

Soxhlet-extraction with acetone / dichloromethane

Ammonium hydroxide / acetone / dichloromethane

ECHA (2014) REACH Guidance document R11 “Endpoint specific guidance”, November 2014

“With regard to persistence it is insufficient to consider removal alone where this may simply represent the transfer of a substance from one environmental compartment to another (e.g. from the water phase to sediment). Degradation may be biotic (e.g. hydrolysis) or abiotic and result in complete mineralization, or simply in the transformation of the parent substance (primary degradation). Where only primary degradation is observed, it is necessary to identify the degradation products and to assess whether they possess PBT/vPvB properties.”

If binding to the matrix is understood as primary degradation, the bound residue should be assessed for PBT.

ECHA (2012) REACH Guidance document R7b “PBT/vPvB assessment”, November 2012:

“Knowledge of bound residues and incorporation into biomass also needs to be considered and should be seen as a potential removal pathway. The OECD 308 (2002) guideline advises as follows: Bound residues represent compounds in soil, plant or animal that persists in the matrix in the form of the parent substance or its metabolites after extractions. The extraction method must not substantially change the compounds themselves or the structure of the matrix….. In general, the formation of bound residues reduces the bioaccessibility and the bioavailability significantly. Extraction of the sample, often with a suitable organic solvent is generally repeated 3 or 4 times until no further yield is achieved. Typically a range of solvents are used of increasing polarity…..Finally the use of strong acids, bases or refluxing could alter both the compounds of interest and the matrices…

When a substance is not fully mineralized but degraded to more persistent degradation products, the PBT/vPvB properties of these should be evaluated before a final judgement of whether the substance fulfils the P criteria.”

The last paragraph is understood that also bound residues (which are indeed more persistent than the parent substance) should be taken into consideration. In order to characterise the bound residues the following investigations were performed:

Binding of non-extractables to different soil components

7.8 - 16.4 % AR was bound to fulvic acids,

9.8 - 30.5 % AR to the humic acids and

23.3 - 57.3% AR to insoluble humins

Harsh acidic reflux extraction, following ambient and Soxhlet-extraction had an altering effect. 9.7 to 14.9 % radioactivity could be extracted. No parent substance was found.

Taking the different non-destroying extraction methods and the characterization of the bound residue into account, it can be concluded that all efforts have been undertaken in order to bring the residues into solution. Further characterization of the bound residues indicate that they are strongly (chemically) bound and only a small portion can be released even with exhaustive, altering extraction methods.

2. Anaerobic soil study with analogous substance 7PPD(N-(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine, CAS No. 3081-01-4)

Within the aerobic phase (0 to 4h), extractables (mainly parent) diminish with a DT50 of 1.5 days. In the anaerobic phase parent decreases slowly from 23.2% AR on day 1 to 13 -17 % until day 120. One metabolite ("7QDI", the oxidised form of 7PPD) is formed only during the anaerobic phase with a maximum of 38% (day 3) and reduction to 7.5% (day 120) with a DT50 of 66.9 days.

Considering the exposure pathway of the rubber additives mainly via TRWP and TWP, the main process in soil for degradation loss is aerobic. Those particles are expected to remain on soil surfaces for a rather long period. During this period, strong adsorption or binding to soil occurs. Transport to anaerobic parts of soil is unlikely.

According to European Commission (2012), Health and Consumers Directorate, “DG SANCO working document on “evidence needed to identify POP, PBT and vBvP properties for pesticides”, “anaerobic data should be used, but only as additional information. As regards the initial establishment of a list of CFS, anaerobic data should not be considered.”

Mobility

Experimental testing is stated not to be applicable as the substance is hydrolytically unstable (half-life is 8 h at 26°C). However, using the logKOW MCI method, logKOC 3.45 was used in order to yield the PNEC sediment (Currenta, 2014a). 4-Hydroxydiphenylamine (CAS 122-37-2)and 1,3-dimethylbutylamine (CAS 108-09-8) were identified as the primary hydrolysis product.

Toxicity

Short-term toxicity to fish

Fish is the most sensitive organism for the family of PPDs and their degradation products. The lowest effect values were found for 6PPD (0.028 mg/L). However the recovery was only about 30%. Primary hydrolysis products (4 -HDPA and

N-phenylbenzoquinone-imine have not been analysed but they are expected to have been formed during the test. Thus, the effect measured covers not only 6PPD but also the hydrolysis products. It

is therefore anticipated that the effect value based only on 6PPD is higher. The effect value for p-hydroquinone (0.044 mg/L) is rather close to the value for 6PPD.

For 4-HDPA and N-phenylbenzoquinone-imine only calculated values are available. The calculated values should be used only for a rough estimation due to the high uncertainty of the method. However they show a trend: The effect values of these three intermediate compounds to fish are at a higher level and there is no indication for a higher toxicity exceeding those for 6PPD or p-hydroquinone.

Long-term toxicity to fish

The chronic toxicity of N-(1,3-dimethylbutyl)-N'-phenylbenzene-1,4-diamine to fish was tested with Oryzias latipes in an Early-Life Stage Toxicity Test according to OECD Guideline 210. The 30d NOEC is 0.0037 mg/L. (National Institute of Technology and Evaluation, Japan, 2002).

Short-term toxicity to aquatic invertebrates

Short-term tests have been performed with 6PPD as well as with other similar PPDs yielding EC50-values in the range of 0.2 to 1.7 mg/L. The result of the study performed with 4-HDPA (0.69 mg/L) is within this range.

N-(1,3-dimethylbutyl)-N'-phenylbenzene-1,4-diamine (6PPD) is hydrolytically unstable at pH 7 and 4-hydroxydiphenylamine (CAS 122-37-2) was identified as the most sensitive (secondary) hydrolysis product.

The lowest effect value in acute tests was found for p-Hydroquinone (0.13 mg/L) which is close to the values for the PPDs (0.2 to 1.9 mg/L) and 4-HDPA (0.69 mg/L).Although p-Hydroquinone is a secondary hydrolysis product of 6PPD, it was chosen as a source of key value as it shows the lowest effect concentrations of all PPDs and their degradation products and therefore represents the worst case.

For 4-HDPA and, N-Phenylbenzoquinone-imine calculated values are available. These calculated values should only be used only for a rough estimation due to the high uncertainty of the method. However they show a trend: The effect values of these three intermediate compounds to daphnids are at a higher level and there is no sign for a higher toxicity than found for the PPDs or any of their degradation products.

Long-term toxicity to aquatic invertebrates

4-Hydroxydiphenylamine (4 -HPDA) is the hydrolysis product from N-(1,3-dimethylbutyl)-N'-phenylbenzene-1,4-diamine (6PPD). A secondary hydrolysis product is p-hydroquinone.

The lowest effect value in long-term tests was found for p-hydroquinone (0.007 mg/L, expressed in 6PPD equivalents) which is lower than the value for 4-HDPA (0.028 mg/L).Although p-hydroquinone is a secondary hydrolysis product of 6PPD, it was chosen as a source of key value as it shows the lowest effect concentrations of the degradation products and is therefore the worst case.

Toxicity to aquatic algae and cyanobacteria

The lowest effect values for 6PPD and the degradation products was found for p-Hydroquinone (EC50 0.335 mg/L) and for 4HDPA (NOEC 0.23 mg/L.). p-Hydroquinone is the (secondary) hydrolysis product of 6PPD. The effect concentration of this substance was used as a key value as it represents the worst case. The lowest NOEC for algae was found in a study for 4 -HDPA. Supporting information from experimental and from calculated data is given for the degradation products of 6PPD, 4 -hydroxydiphenylamine and N-phenyl-p-benzoquinone-imine. The results of these studies are effect levels higher than those stated for the key studies. The read-across justification is attached in a separate document in chapter 13 IUCLID.

Toxicity to microorganisms

A test with activated sludge with a duration of 3 hours was performed according to ISO 8192 (Test for Inhibition of Oxygen Consumption by Activated Sludge). An EC50 of 420 mg/L related to the concentration of N-(1,3-dimethylbutyl)-N'-phenylbenzene-1,4-diamine was observed (Currenta 2012). Two studies performed with p-hydroquinone, a secondary hydrolysis product of 6PPD, show that this substance is relatively toxic to organisms (NOEC 1 mg/L, IC50 71 mg/L).

Toxicity to soil macroorganisms except arthropods

Long-term EC10, LC10 or NOEC for soil macroorganisms: 100 mg/kg soil dw. No toxicity to soil macroorganisms for 6PPD is available. 7PPD is an analogue substance. Due to the analogous structure of 7PPD, this study is used in a read-across approach for 6PPD. A detailed justification for the read-across is given in a separate document attached to IUCLID chapter 13.

Toxicity to terrestrial arthropods

Long-term EC10, LC10 or NOEC for terrestrial plants: 7.8 mg/kg soil dw. No toxicity to terrestrial plants for 6PPD is available. 7PPD is an analogue substance. Due to the analogous structure of 7PPD, this study is used in a read-across approach for 6PPD. A detailed justification for the read-across is given in a separate document attached to IUCLID chapter 13.

Toxicity to soil microorganisms

According to the OECD Guideline 216 (Soil Microorganisms: Nitrogen Transformation Test), he study was conducted in order to determine possible effects of 7PPD on soil microorganisms through measuring microbial nitrate formation in treated versus untreated soils after 28 days of incubation. A NOEC of 100 mg/L and a LOEC of 333 mg/L within 28 days related to nitrate formation. 7PPD is considered to have no adverse long-term effects on nitrate formation in soil at concentrations up to and including 100 mg test item/kg soil dry weight.

E.9.2 Information on tonnage and usage

Registrations	☒ Full registration(s) (Art. 10) ☐ Intermediate registration(s) (Art. 17 and/or 18)
Total tonnage band for substance (excluding volume registered under Art 17 or Art 18, or directly exported)	≥ 10 000 to < 100 000 tonnes per annum

Overview of uses of N-(1,3-dimethylbutyl)-N'-phenylbenzene-1,4-diamine

The substance is manufactured and/or imported in the European Economic Area in quantities at ≥ 10 000 to < 100 000 tonnes per annum. This volume does not take into account any exports into countries not being member of the EEA. This substance is used by consumers, in articles, by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing.

Table E35: Uses according to public information at ECHA's registration data base (date of access: May 2021).

Use	Information
Uses as intermediate	Not used as an intermediate
Formulation or re-packaging	This substance is used in the following products: polymers and fuels. Release to the environment of this substance can occur from industrial use: formulation in materials, in the production of articles, as processing aid and formulation of mixtures.
Uses at industrial sites	This substance is used in the following products: polymers and fuels. This substance is used in the following areas: formulation of mixtures and/or re-packaging. This substance is used for the manufacture of: rubber products and plastic products. Release to the environment of this substance can occur from industrial use: as processing aid, in the production of articles, formulation in materials and of substances in closed systems with minimal release.
Uses by professional workers	This substance is used in the following products: polymers and fuels. This substance is used for the manufacture of: rubber products. Other release to the environment of this substance is likely to occur from: indoor use in long-life materials with low release rate (e.g. flooring, furniture, toys, construction materials, curtains, foot-wear, leather products, paper and cardboard products, electronic equipment) and indoor use in long-life materials with high release rate (e.g. release from fabrics, textiles during washing, removal of indoor paints).
Consumer Uses	This substance is used in the following products: fuels. Other release to the environment of this substance is likely to occur from: outdoor use in long-life materials with low release rate (e.g. metal, wooden and plastic construction and building materials), outdoor use in long-life materials with high release rate (e.g. tyres, treated wooden products, treated textile and fabric, brake pads in trucks or cars, sanding of buildings (bridges, facades) or vehicles (ships)), indoor use in long-life materials with low release rate (e.g. flooring, furniture, toys, construction materials, curtains, foot-wear, leather products, paper and cardboard products, electronic equipment) and outdoor use in close systems with minimal release (e.g. hydraulic liquids in automotive suspension, lubricants in motor oil and break fluids).
Article service life	Other release to the environment of this substance is likely to occur from: indoor use in long-life materials with low release rate (e.g. flooring, furniture, toys, construction materials, curtains, foot-wear, leather products, paper and cardboard products, electronic equipment), outdoor use in long-life materials with high release rate (e.g. tyres, treated wooden products, treated textile and fabric, brake pads in trucks or cars, sanding of buildings (bridges, facades) or vehicles (ships)) and outdoor use in long-life materials with low release rate (e.g. metal, wooden and plastic construction and building materials).

	This substance can be found in complex articles, with no release intended: machinery, mechanical appliances and electrical/electronic products (e.g. computers, cameras, lamps, refrigerators, washing machines), electrical batteries and accumulators and vehicles. This substance can be found in products with material based on: rubber (e.g. tyres, shoes, toys).

Uses according to SPIN database[24]

For the latest reporting year (2019) the database on Substances in preparations in Nordic countries (SPIN) reports the following data:

Country	#prep	tonnes	Consumer preparations	Confidential
SE	251	32.5	-	
DK	0	0	-	Yes

From the use categories to be reported for SPIN in 2019 (use category description scheme UC 62), the greatest amount of N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine is used in the "others" category (243 preparations, 20 tonnes) and as stabilizers (3 preparations, 11 tonnes). Data from SPIN is not fully representative for the European Economic Region because products and frequency of application may differ between the different geographical regions in the EU. In addition, the SPIN database not only refers to products where substances are intentionally added, but also deals with occurrence of substances as impurities. Based on the data from the notifications for 2019, SPIN concludes a potential exposure for N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine for wastewater and air and a probable consumer and occupational exposure.

Table E36: Exposure potential of N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine from products, according to SPIN database

Country	Quant.	Surface water	Air	Soil	Wastewater	Consumers	Occupational	Range of Use (RoU)	Article index (max: 3)
DK	1	2	2	2	3	4	4	1	3
SE	3	2	3	2	3	2	4	2	3

On the basis of this information there is evidence that in principle, uses of N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine result in relevant emissions into several environmental compartments.

[24] www.spin2000.net; date of access: 24.05.2021