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Contaminants in water resources: Prioritization and recommendations for conducting a “cold” biodegradation simulation test according to OECD TG 309

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Abstract: Contaminants in water resources: Prioritization and recommendations for conducting a “cold” biodegradation simulation test according to OECD TG 309

The threat to drinking water resources from persistent and mobile substances has been recognized for decades. It is essential for water utilities and monitoring/regulatory authorities to know whether the chemicals detected in their own water resources are persistent and therefore pose a threat to drinking water production. By eliminating the need for ^{14}C-labeling of the test substance, a valid “cold” degradation test according to OECD TG 309 can be easily, cost effectively and efficiently performed by water utilities and authorities with laboratory infrastructure and established analytical methods for chemicals detected in their water resources.

The first objective of this report was to define criteria which, if met, would make a test substance suitable for a "cold" degradation test according to OECD TG 309. The second objective was to evaluate water contaminants with respect to their intrinsic suitability for conducting such a test. It must be noted that this report only assesses whether a contaminant is likely to be suitable for a "cold" degradation test according to OECD TG 309, but not whether such a test is scientifically or legally required for that contaminant.

The list of 832 contaminants prioritized for a "cold" biodegradation testing according to OECD TG 309 has been divided into two priority levels: contaminants that have already been detected in drinking water, groundwater, raw water or bank filtrate (category A, 422 contaminants) and contaminants that have only been detected in wastewater treatment plant effluent and/or surface water (category B, 410 contaminants).

The third objective of this report was to develop recommendations for a simple, cost-effective, and efficient implementation of a valid "cold" biodegradation test in accordance with OECD TG 309. The recommendations apply only to those test substances for which no pronounced and significant decrease in concentration in the aqueous phase is expected during the test. The recommendations are intended to make it easier for a wide range of users, such as water utility laboratories and government agencies with established analytical facilities, to perform a "cold" degradation test in accordance with OECD TG 309 and aim at selecting the test conditions (temperature, concentration range of the test substance, inoculum) in such a way that standardized, generally valid, comparable and environmentally relevant results are obtained for the test substance.

Kurzbeschreibung: Befundstoffe in Wasserressourcen: Priorisierung und Empfehlungen zur Durchführung eines „kalten“ Abbautests nach OECD TG 309

Hinweis: Dieser Bericht ist auch in deutscher Sprache als TEXTE 174/2024 erhältlich.

Auf die Gefährdung der Trinkwasserressourcen durch persistente und mobile Stoffe wird seit Jahrzehnten hingewiesen. Für Wasserversorgungsunternehmen (WVU), Überwachungs- und Regulierungsbehörden ist es essenziell zu wissen, ob die in den Wasserressourcen detektierten Chemikalien persistent sind und somit gegebenenfalls eine Bedrohung für die Trinkwassergewinnung darstellen. Durch den Verzicht auf eine ^{14}C-Markierung der Testsubstanz (sog. „kalter“ Abbautest) kann für Befundstoffe in den eigenen Wasserressourcen ein valider Abbautest nach OECD TG 309 auch von WVU und Behörden mit entsprechender Laborinfrastruktur und etablierter Analytik einfach, kostengünstig und effizient durchgeführt werden.

Das erste Ziel des vorliegenden Sachverständigengutachtens war es Kriterien zu definieren, bei deren Erfüllung eine Testsubstanz geeignet für einen "kalten" Abbautest nach OECD TG 309 ist. Das zweite Ziel war die Beurteilung bekannter Befundstoffe in Wasserressourcen hinsichtlich ihrer intrinsischen Eignung für einen solchen Abbautest. In diesem Sachverständigengutachten wurde also beurteilt, ob ein Befundstoff vermutlich für einen „kalten“ Abbautests nach OECD TG

309 geeignet ist, jedoch nicht, ob dieser Test wissenschaftlich oder regulatorisch für diesen Befundstoff notwendig ist.

Die Liste mit 832, für einen „kalten“ Abbautests nach OECD TG 309 priorisierten, Befundstoffen wurde in zwei Prioritätsstufen unterteilt: Befundstoffe, die bereits in Trinkwasser, Grundwasser, Rohwasser oder Uferfiltrat nachgewiesen wurden (Kategorie A, 422 Befundstoffe) und Befundstoffe, die bislang ausschließlich in Kläranlagenablauf und/oder Oberflächenwasser nachgewiesen wurden (Kategorie B, 410 Befundstoffe).

Das dritte Ziel dieses Sachverständigengutachtens war es, Empfehlungen für eine einfache, kostengünstige und effiziente Durchführung eines testrichtlinienkonformen und validen „kalten“ Abbautests nach OECD TG 309 zu erarbeiten. Die Empfehlungen gelten ausschließlich für solche Testsubstanzen, für die im Testverlauf keine ausgeprägte und signifikante Konzentrationsabnahme in der Wasserphase erwartet wird. Die Empfehlungen sollen einem breiten Anwenderkreis, z. B. den Laboratorien von WVU und Behörden mit etablierter Analytik, die Durchführung eines „kalten“ Abbautests nach OECD TG 309 erleichtern und zielen darauf ab, die Testbedingungen (Temperatur, Konzentrationsbereich der Testsubstanz, Inokulum) so zu wählen, dass für die Testsubstanz standardisierte, allgemeingültige, vergleichbare und umweltrelevante Ergebnisse erzielt werden.

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List of abbreviations

Abbreviation	Explanation
BF	Bank filtrate
CLP	Classification, Labelling and Packaging of substances
CSS	Chemicals Strategy for Sustainability
DW	Drinking water
ECHA	European Chemicals Agency
GC	Gas chromatography
GW	Ground water
HILIC	Hydrophilic interaction liquid chromatography
IC	Ion exchange chromatography
InChI	IUPAC International Chemical Identifier
IUPAC	International Union of Pure and Applied Chemistry
NaNa	Not adsorbable and not degradable
NER	Non-extractable residues
OECD	Organisation for Economic Co-operation and Development
PFAS	Per- and polyfluoroalkyl substances
PMOC	Persistent and mobile organic compounds
PMT/vPvM	Persistent mobile and toxic / very persistent and very mobile
PPOP	Polar persistent organic compounds
PPP, P3	Persistent polar pollutants
QSAR	Quantitative structure–activity relationship
RIVM	National Institute for Public Health and the Environment
RPLC	Reverse phase liquid chromatography
RW	Raw water
SFC	Supercritical fluid chromatography
SMILES	Simplified Molecular Input Line Entry System
SW	Surface water
TG	Technical guideline
UBA	German Federal Environment Agency
WTPE	Wastewater treatment plant effluent

Summary

The threat posed to drinking water resources by persistent and mobile substances has been recognized for decades. Lack of or insufficient intrinsic degradability (persistence) is scientifically considered to be the most problematic property of a chemical. Water utilities warn that the production of drinking water requires increasing efforts. However, for many substances, some of which have been detected in drinking water resources for decades, there is still no conclusive assessment of their intrinsic biodegradability in the aquatic environment by the responsible companies. However, it is essential for water utilities and monitoring and regulatory authorities to know whether the chemicals detected in their water resources are persistent and therefore pose a threat to drinking water production.

If a chemical of no exclusive relevance to soils or sediments has not been cleared of the suspicion of lacking or insufficient intrinsic degradability (persistence) in the screening assessment, ECHA recommends as a standard that the OECD TG 309 degradation test should always be performed first. By eliminating the need to label the test substance with ^{14}C, a valid OECD TG 309 degradation test can be easily, cost effectively and efficiently performed by water suppliers and authorities with laboratory infrastructure and established analytical methods for substances found in their water resources.

The first objective of this report was to define criteria which, if fulfilled, would make a test substance suitable for a "cold" degradation test according to OECD TG 309. The criteria should indicate whether a test substance does not exhibit pronounced intrinsic aerobic biodegradability in the aqueous phase and, at the same time, due to its physicochemical properties, neither adsorbs to suspended matter, sediment or glass surfaces nor passes into the gas phase, i. e. remains in the aqueous phase during the test period.

The second objective was to assess the intrinsic suitability of 1250 water contaminants for a "cold" degradation test according to OECD TG 309. In this report, the defined criteria were used to assess whether a contaminant is likely to be suitable for a "cold" degradation test according to OECD TG 309, but not whether such a test is scientifically or legally required for that contaminant.

Distribution coefficients such as log K_{OC} and log D were used to estimate the sorption tendency, and the Henry coefficient (calculated at 12 °C, the recommended temperature for the biodegradation test) was used to estimate the volatility of the test substances. Both existing assessments and various QSAR (quantitative structure-activity relationship) methods were used to assess whether a test substance can be assumed to have sufficient intrinsic biodegradability.

The list of 832 contaminants prioritized for a "cold" degradation testing according to OECD TG 309 has been divided into two priority levels: contaminants that have already been detected in drinking water, groundwater, raw water or bank filtrate (category A, 422 contaminants) and contaminants that have only been detected in wastewater treatment plant effluent and/or surface water (category B, 410 contaminants).

The third objective of this report was to develop recommendations for a simple, cost-effective and efficient implementation of a valid "cold" degradation test according to OECD TG 309. The recommendations apply only to those test substances for which no pronounced and significant decrease in concentration in the aqueous phase is expected during the test:

- No ^{14}C-labelling of the test substance and perform the ‘*pelagic test*’ variant.
- Test the test substances in a mixture and align the mixture of test substances and analysis.

- Two test concentrations per test substance; sum of the test concentrations in a mixture maximum 10 µg/L and 50 µg/L.
- Add the reference substance directly to the test vessels containing the test substances and select according to analytical compatibility.
- The spiked concentration of the reference substance corresponds to one hundred times the analytical limit of quantification.
- Prepare stock and spiking solutions in deionized water and use the water-soluble salts of the test substances.
- The sampling location of water and sediment for the test is relevant for the institution performing the test.
- Perform the degradation test at 12 °C and in the dark, test duration of 60 days.
- Shake test vessels, do not stir.
- Adapt the dimensions of the test vessels and the sampling strategy to the variant of the degradation test and the analytical requirements.
- Four technical replicates for a single test substance and six for mixtures.
- Do not perform a sterile control.
- Sampling for analysis of the test/reference substance(s) after 0, 3, 7, 14, 28, 42 and 60 days.
- Freeze samples and analyze in a common sequence.

The recommendations are intended to make it easier for a wide range of users, such as water utility laboratories and government agencies with established analytical facilities, to perform a "cold" degradation test in accordance with OECD TG 309 for substances found in their own water resources. To be able to test as many chemicals as possible in the shortest possible time, it is essential to minimize the effort required to perform the test and to ensure that it is simple, cost-effective and efficient. The recommendations aim at selecting the test conditions (temperature, concentration range of the test substance, inoculum) in such a way that standardized, generally valid, comparable and environmentally relevant results are obtained for the test substance.

Zusammenfassung

Hinweis: Dieser Bericht ist auch in deutscher Sprache als TEXTE 174/2024 erhältlich.

Auf die Gefährdung der Trinkwasserressourcen durch persistente und mobile Stoffe wird seit Jahrzehnten hingewiesen. Eine fehlende bzw. unzureichende intrinsische Abbaubarkeit (Persistenz) wird wissenschaftlich als die problematischste Stoffeigenschaft einer Chemikalie bewertet. Wasserversorgungsunternehmen (WVU) warnen, dass die Trinkwassergewinnung steigenden Aufwand erfordert. Für zahlreiche Befundstoffe in den Trinkwasserressourcen fehlt allerdings nach wie vor eine abschließende Bewertung ihrer intrinsischen Abbaubarkeit in der aquatischen Umwelt durch die verantwortlichen Unternehmen. Für WVU, Überwachungs- und Regulierungsbehörden ist es aber essenziell zu wissen, ob die in den eigenen Wasserressourcen detektierten Chemikalien persistent sind und somit gegebenenfalls eine Bedrohung für die Trinkwassergewinnung darstellen.

Wenn eine Chemikalie, die keine besondere Relevanz für Böden oder Sedimente hat, im Screening nicht vom Verdacht einer fehlenden oder unzureichenden intrinsischen Abbaubarkeit (Persistenz) entlastet wurde, empfiehlt die ECHA, standardmäßig immer zuerst den Abbautest nach OECD TG 309 durchzuführen. Durch den Verzicht auf eine ^{14}C-Markierung der Testsubstanz (sog. „kalter“ Abbautest) kann für Befundstoffe in den eigenen Wasserressourcen ein valider Abbautest nach OECD TG 309 auch von WVU und Behörden mit Laborinfrastruktur und etablierter Analytik einfach, kostengünstig und effizient durchgeführt werden.

Das erste Ziel des vorliegenden Sachverständigengutachtens war es Kriterien zu definieren, bei deren Erfüllung eine Testsubstanz geeignet für einen "kalten" Abbautest nach OECD TG 309 ist. Die Kriterien sollen erkennen, ob eine Testsubstanz in der Wasserphase keine ausgeprägte intrinsische aerobe biologische Abbaubarkeit aufweist und gleichzeitig aufgrund ihrer physikochemischen Eigenschaften weder an Schwebstoff, Sediment oder Glasoberfläche adsorbiert noch in die Gasphase übergeht, d. h., während der Testdauer in der Wasserphase verbleibt.

Das zweite Ziel war die Beurteilung von 1250 Befundstoffen hinsichtlich ihrer intrinsischen Eignung für einen „kalten“ Abbautest nach OECD TG 309. In diesem Sachverständigengutachten wurde also anhand der definierten Kriterien beurteilt, ob ein Befundstoff vermutlich für einen solchen Abbautests geeignet ist, jedoch nicht, ob dieser Test wissenschaftlich oder regulatorisch für diesen Befundstoff notwendig ist.

Für die Abschätzung der Sorptionsneigung wurden Verteilungskoeffizienten wie log K_{OC} und log D, für die Flüchtigkeit der Befundstoffe der Henry-Koeffizient (berechnet für 12 °C, die empfohlene Temperatur im Abbautest) verwendet. Für eine Abschätzung, ob für eine Testsubstanz eine ausreichende intrinsische Abbaubarkeit vermutet werden kann, wurde sowohl auf bereits vorliegende Bewertungen als auch auf verschiedene QSAR-Verfahren (Quantitative Struktur-Wirkungs-Beziehung) zurückgegriffen.

Die Liste der 832 für einen „kalten“ Abbautest nach OECD TG 309 priorisierten Befundstoffe wurde in zwei Prioritätsstufen unterteilt: Befundstoffe, die bereits in Trinkwasser, Grundwasser, Rohwasser oder Uferfiltrat nachgewiesen wurden (Kategorie A, 422 Befundstoffe) und Befundstoffe, die bislang ausschließlich in Kläranlagenablauf und/oder Oberflächenwasser nachgewiesen wurden (Kategorie B, 410 Befundstoffe).

Das dritte Ziel dieses Sachverständigengutachtens war es, Empfehlungen für eine einfache, kostengünstige und effiziente Durchführung eines testrichtlinienkonformen und validen „kalten“ Abbautests nach OECD TG 309 zu erarbeiten. Die Empfehlungen gelten ausschließlich für solche Testsubstanzen, für die im Testverlauf keine ausgeprägte und signifikante Konzentrationsabnahme in der Wasserphase erwartet wird:

- Testsubstanz nicht radioaktiv markieren und Variante „*pelagic test*“ durchführen.
- Testsubstanzen in Mischung testen und die Mischung der Testsubstanzen und die verwendeten analytischen Methoden aufeinander abstimmen.
- Zwei Testkonzentrationen pro Testsubstanz; Summe der Testkonzentrationen in einer Mischung maximal 10 µg/L und 50 µg/L.
- Referenzsubstanz direkt in die Testgefäße mit den Testsubstanzen applizieren und nach analytischer Kompatibilität auswählen.
- Die dotierte Konzentration der Referenzsubstanz entspricht dem Hundertfachen der analytischen Bestimmungsgrenze.
- Stamm- und Dotierlösungen in deionisiertem Wasser herstellen und die wasserlöslichen Salze der Testsubstanzen verwenden.
- Entnahmeort von Wasser und Sediment ist für die testdurchführende Institution relevant.
- Abbautest bei 12 °C und im Dunkeln über eine Testdauer von 60 Tagen durchführen.
- Testgefäße schütteln, nicht rühren.
- Dimensionierung der Testansätze und die Probenahmestrategie an die Variante des Abbautests und an die Anforderungen der Analytik anpassen.
- Bei einzelner Testsubstanz vier und bei Mischungen sechs technische Replikate.
- Auf eine sterile Kontrolle verzichten.
- Die Probenahme für die Analyse der Test-/Referenzsubstanz(en) nach 0, 3, 7, 14, 28, 42 und 60 Tagen durchführen.
- Proben einfrieren und in einer gemeinsamen Sequenz analysieren.

Die Empfehlungen sollen einem breiten Anwenderkreis, z. B. den Laboratorien von WVU und Behörden mit etablierter Analytik, die Durchführung eines „kalten“ Abbautests nach OECD TG 309 für Befundstoffe in den eigenen Wasserressourcen erleichtern. Um möglichst viele Chemikalien in möglichst kurzer Zeit testen zu können, ist es von entscheidender Bedeutung, den Aufwand für die Testdurchführung zu minimieren und eine einfache, kostengünstige und effiziente Durchführung zu gewährleisten. Die Empfehlungen zielen darauf ab, die Testbedingungen (Temperatur, Konzentrationsbereich der Testsubstanz, Inokulum) so zu wählen, dass für die Testsubstanz standardisierte, allgemeingültige, vergleichbare und umweltrelevante Ergebnisse erzielt werden.

1 Background

The threat to drinking water resources posed by persistent and mobile substances has been scientifically highlighted for decades (Loos et al., 2010; Reemtsma et al., 2016; Schwarzenbach et al., 2006). Chemicals with these two intrinsic properties are referred to as NaNa substances (non-degradable and non-adsorbable), polar persistent organic pollutants (PPOPs), persistent polar pollutants (PPPs, P3 substances), persistent and mobile organic pollutants (PMOCs) and persistent, mobile and toxic substances or very persistent and very mobile substances (PMT/vPvM substances) (e. g. Neumann & Schliebner, 2019; Reemtsma et al., 2016; Steinhäuser & Richter, 2006). Currently, short-chain per- and polyfluoroalkyl substances (PFAS) are referred to as mobile *forever chemicals*.

The occurrence of polar chemicals in the aquatic environment has been known since the 1980s (Giger et al., 1984). In the USA, it was pointed out decades ago that many of these chemicals are present in the environment mainly because they are not degraded during wastewater treatment (Kolpin et al., 2002). In Europe, about 90% of surface water samples are contaminated with persistent and mobile chemicals (Loos et al., 2010). Modern chromatographic techniques currently detect a wide range of polar, ionizable and ionic chemicals in drinking water resources (Neuwald et al., 2022; Scheurer et al., 2017).

At the same time, the chemical industry and its downstream users have been using persistent substances in increasing numbers and quantities for decades (UN, 2019). Lack of or insufficient intrinsic degradability (persistence) is scientifically assessed as the most problematic property of a chemical (Cousins et al., 2019; Persson et al., 2022; Schäffer et al., 2022). It increases the potential for bioaccumulation, causes accumulation in the environment, and prevents degradation of the contamination even when emissions cease. All of this increases exposure and the likelihood of effects occurring and makes quantitative risk assessment impossible (Scheringer, 2023).

Water utilities warn that drinking water production will require increasing effort (ERM Coalition, 2020). After extensive consultation, the EU Commission has therefore included the new hazard classes PMT and vPvM for raw water protection in the CLP Regulation (EC, 2022) as part of the Green Deal (EC, 2019) and the Chemicals Strategy for Sustainability (CSS) (EC, 2020). From November 2026, companies in Europe will have to assess their chemicals for persistence, mobility and toxicity. If a substance meets the criteria, companies using it will have to self-classify it as a PMT substance (EUH450, "Can cause long-lasting and diffuse contamination of water resources") and/or a vPvM substance (EUH451, "Can cause very long-lasting and diffuse contamination of water resources") (ECHA, 2023a).

However, for many contaminants in water resources, some of which have been detected for decades, there is still no conclusive assessment of their intrinsic degradability in the aquatic environment by the responsible companies (Arp & Hale, 2022). It is essential for water utilities, monitoring and regulatory agencies to know whether the chemicals detected in their own water resources are persistent and thus pose a threat to drinking water production.

2 The test for aerobic biodegradability in surface water according to OECD TG 309

For the final assessment of the intrinsic aerobic biodegradability of a chemical, three standardized OECD tests are available: for soil (TG 307), water/sediment (TG 308) and surface water (TG 309). These simulation tests must always be performed by the responsible companies if a chemical has not been cleared of suspicion of lacking or insufficient intrinsic degradability (persistence) in the screening. For chemicals that are not particularly relevant to soils or sediments, ECHA recommends that the OECD TG 309 degradation test should always be performed first as a standard (ECHA, 2023b).

The goal of the OECD TG 309 degradation test is to demonstrate intrinsic aerobic biodegradability and to derive a valid half-life for aerobic biodegradation (degradation half-life, $DegT_{50}$) in surface water. When assessing whether the result is valid and allows a scientifically sound statement to be made, two basic cases must be distinguished.

Case 1: A pronounced and significant decrease in the concentration of the test substance in the aqueous phase is observed during the test.

For a valid and reliable determination of the intrinsic aerobic biodegradability of the test substance, it must now be demonstrated beyond doubt that aerobic biodegradation was the dominant process in the sum of all processes contributing to the disappearance (dissipation) of the test substance from the aqueous phase. Abiotic degradation such as hydrolysis or pure partitioning processes such as volatilization or adsorption as well as the formation of non-extractable residues (NER) must be excluded as causes. Furthermore, it must be clarified whether only primary degradation to stable (possibly persistent) transformation products or complete degradation (i. e. transformation to inorganic compounds, mineralization) was observed.

In case 1, this is most reliably achieved by ^{14}C-labeling of the test substance. The volatilized, adsorbed, mineralized, NER-bound portions of the radioactivity and the ^{14}C-labeled transformation products are quantified. However, the production, handling, and disposal of the radioactive material require special safety precautions, handling permits, trained personnel, and appropriate laboratory equipment.

Without ^{14}C-labeling of the test substance (so-called "cold" degradation test), a reliable elucidation of the different processes in case 1 is only possible with enormous analytical effort. To quantify volatilized (e. g. after enrichment via a trap with paraffin oil-soaked glass wool) or adsorbed fractions of the test substance, a substance-specific analysis would have to be performed, which usually requires extraction, purification and, if necessary, enrichment prior to analysis. The mineralization of the test substance would also have to be identified and quantified. However, this quantification is practically impossible without ^{14}C-labeling of the test substance due to the low test concentrations. In the "*suspended sediment test*" it would be practically impossible to reliably exclude the formation of NER without ^{14}C-labeling of the test substance.

Case 2: No pronounced and significant decrease in the concentration of the test substance in the aqueous phase is observed during the test.

For a valid and reliable determination of lack of or insufficient intrinsic aerobic biodegradability and thus persistence of the test substance, it is only necessary in this case to demonstrate that a sufficiently high aerobic biodegradation potential (i. e. a vital inoculum) was present in the test system. This is ensured using a reference substance.

In case 2, a valid result of the degradation test according to OECD TG 309 can always be obtained without ^{14}C-labeling of the test substance. Analytically, only the quantification of the test substance itself and only in the aqueous phase is required. Since no pronounced and significant decrease in concentration is observed in case 2, it is not necessary to clarify and quantify different processes.

Case 2 is expected especially for persistent and mobile chemicals.

By omitting the ^{14}C-labeling of the test substance, a valid degradation test according to OECD TG 309 can also be performed easily, cost-effectively and efficiently by water utilities and authorities with appropriate laboratory infrastructure and established analytical methods for substances found in their own water resources. This has been demonstrated by the KWR Water Research Institute in the Netherlands in cooperation with the German Federal Environment Agency (UBA) using seven test substances (Hofman-Caris & Claßen, 2020).

3 Objectives

The first objective of this report was to define criteria which, if met, would make a test substance suitable for a "cold" degradation test according to OECD TG 309. The criteria should be suitable for determining whether a test substance does not exhibit pronounced intrinsic aerobic biodegradability in the aqueous phase and, at the same time, due to its physicochemical properties, neither adsorbs to suspended matter, sediment or glass surfaces nor passes into the gas phase, i. e. remains in the aqueous phase during the test. The criteria and procedure are described in Chapter 5.2 and can therefore be applied to chemicals not considered in this report (see second objective).

The second objective was to assess water contaminants with respect to their intrinsic suitability for a "cold" degradation test according to OECD TG 309. Therefore, this report assesses whether a contaminant is likely to be suitable for a "cold" degradation test according to OECD TG 309, but not whether this test is scientifically or legally required for that contaminant.

As a result, the list of contaminants in Chapter 6 presents the contaminants prioritized for "cold" degradation testing according to OECD TG 309 in two tables: Table 2 lists the prioritized contaminants that have already been detected in drinking water, raw water, bank filtration and/or groundwater (category A). Table 3 lists the prioritized contaminants that have only been detected in wastewater treatment plant effluent and/or surface water (category B).

As a second result, the list of contaminants in Chapter A.2 (Table 5) shows the deprioritized contaminants for a "cold" degradation test according to OECD TG 309. For a valid test result, ^{14}C-labeling would probably be required for these contaminants.

Both lists of contaminants – divided into three tables – including the evaluated intrinsic properties and additional information are available for download in MS Excel format.

The third objective of this report was to develop recommendations for a simple, cost-effective and efficient implementation of a valid "cold" degradation test according to OECD TG 309. The recommendations apply only to those test substances for which no pronounced and significant decrease in concentration in the aqueous phase is expected during the test (case 2), e. g. the prioritized contaminants in Table 2 and Table 3.

The recommendations in Chapter 4 are intended to make it easier for a wide range of users, e. g. water utility laboratories and authorities with established analytical facilities, to perform a "cold" degradation test according to OECD TG 309 for substances found in their own water resources. The focus is on reducing variability between test vessels (technical replicates), increasing statistical power, minimizing uncertainty and thus increasing the overall validity of the test result. To test as many chemicals as possible in as short a time as possible, it is essential to minimize the effort required to perform the test and to ensure simple, cost-effective and efficient implementation. The recommendations aim at selecting the test conditions (temperature, concentration range of the test substance, inoculum) in such a way that standardized, generally valid, comparable and environmentally relevant results are obtained for the test substance.

4 Recommendations for performing a “cold” degradation test for aerobic biodegradability in surface water according to OECD TG 309

The test for aerobic biodegradability in surface water must always be performed according to OECD TG 309 (OECD, 2004) and its specifications must be followed to obtain a valid test result.

The test guideline allows the test to be performed with and without ^{14}C-labeling of the test substance, as two basic variants of the test procedure with respect to the presence of a solid fraction (*pelagic test* or *suspended sediment test*), as well as further variations of the test conditions.

The following are recommendations for the simple, cost-effective and efficient performance of a valid "cold" degradation test according to OECD TG 309, divided into thematic focus areas and categorized according to the paragraphs of the test guideline.

It is important to note, that the recommendations apply only to case 2, i. e. to test substances which are unlikely to undergo significant intrinsic aerobic biodegradation and abiotic degradation (e. g. by hydrolysis) in the aqueous phase and which, due to their physicochemical properties, remain in the aqueous phase throughout the test.

Therefore, the following applies to all recommendations: If, contrary to expectations, case 2 does not occur in the OECD TG 309 degradation test, but a pronounced and significant decrease in the concentration of the test substance in the aqueous phase (case 1) is observed, the test result may be invalid. It may be ambiguous whether aerobic biodegradation was the dominant process or whether abiotic degradation by hydrolysis, other physical processes such as sorption or volatilization, or the formation of NER (particularly relevant for the *suspended sediment test* variant) was primarily responsible for the decrease in concentration in the water phase.

To obtain also in case 1 a valid test result without a ^{14}C-labeling of the test substance, it may be necessary to analytically identify the full degradation pathway of the test substance. Alternatively, the degradation test may need to be repeated under different conditions, e. g. with a ^{14}C-labeling of the test substance.

4.1 General principle of the test (paragraphs 5 and 6)

The following recommendations relate first to the general test principle, such as the type of degradation test (*pelagic test* or *suspended sediment test*), the number and concentrations of the test substance(s), and the synergy of the analysis and the composition of the test substance mixture.

4.1.1 Recommendation: Do not label the test substance radioactively

For test substances for which no pronounced and significant decrease in concentration in the water phase (case 2) is expected during the degradation test, e. g. the prioritized contaminants listed in Chapter 6, it is recommended not to label the test substance with ^{14}C. The degradation test according to OECD TG 309 can therefore be performed easily, inexpensively and efficiently in laboratories of water supply companies and authorities with established analytical equipment and temperature cabinets or temperature chambers.

4.1.2 Recommendation: Test substances in a mixture

The omission of ^{14}C-labeling of the test substance and the substance-specific analysis and quantification of the test substance in the aqueous phase allows parallel testing of several test

substances in one mixture. The OECD TG 309 degradation test can thus be performed for several test substances simultaneously, making it simple, cost-effective and efficient.

Studies show that the performance of a degradation test for the single test substance is not affected by the presence of other test substances, provided that the sum of the test concentrations is sufficiently low (Birch et al., 2023a, 2023b; Li et al., 2019; Li & McLachlan, 2020; Tian et al., 2022). The state of the art in trace analysis allows reliable quantification of low test concentrations even in mixtures. Mathematical modeling of degradation kinetics is then performed separately for each test substance in the mixture (see Chapter 4.4.4 and Chapter 4.5).

4.1.3 Recommendation: Coordinate mixture of test substances and analysis

Modern analytical multi-methods make it possible to quantify many different individual substances in a single analysis. It is recommended that the composition of the test substance mixture and the analysis be coordinated so that all test substances can be quantified in one or a maximum of two analyses. This reduces the analytical effort of the degradation test.

4.1.4 Recommendation: Two test concentrations per test substance; sum of the test concentrations in a mixture maximum 10 µg/L and 50 µg/L

According to OECD TG 309, two test concentrations are recommended with a factor of 5 to a maximum of 10 between the low and the high test concentrations per test substance. Both test concentrations should be set as low as possible and as high as analytically necessary (i. e. for test substances for which no pronounced and significant decrease in concentration in the aqueous phase is expected: test concentration ≥ 10 × limit of quantitation).

When testing a mixture of test substances, it is recommended to limit the sum of the test concentrations in the mixture to a maximum of 10 µg/L for the low test concentrations and 50 µg/L to a maximum of 100 µg/L for the high test concentrations. This principle thus determines the maximum number of test substances in the mixture.

4.1.5 Recommendation: Perform the “*pelagic test*” variant

For test substances for which no pronounced and significant decrease in concentration in the water phase (case 2) is expected during the degradation test, e. g. the prioritized contaminants listed in Chapter 6, it is recommended to perform the "*pelagic test*" variant. It requires fewer resources to perform than the “*suspended sediment test”*.

During preparation, the coarse particles are removed by filtration, for example, through a nylon filter with a mesh size of about 100 µm, through a coarse paper filter, or by sedimentation. Finer sediment particles are still present and are kept in suspension during the test by continuous shaking (see Chapter 4.3.5).

Evidence that a sufficiently high aerobic biodegradation potential is present in the test system due to a viable inoculum is critical for validity. This must be demonstrated by biodegradation of the reference substance (see Chapter 4.2).

Another advantage of the "*pelagic test*" is that the test results are easier to interpret because no sediment is added that could influence the course of concentration of the test substance. Even small amounts of suspended sediment can lead to relevant NER formation (Holzmann et al., 2021). Cationic test substances may sorb to clay minerals, organic matter (humus), or clay-humus complexes (Schaffer & Licha, 2015; Tian et al., 2024). Therefore, in the "*suspended sediment test*" it is necessary to exclude the formation of NER and sorption to the added sediment as

causal processes for a concentration decrease in the water phase. In practice, this may only be possible with ^{14}C-labeling of the test substance.

On the other hand, the addition of sediment usually leads to an increase in microbial activity, which can reduce the variability between replicates and strengthen the validity of the degradation test (Fenner et al., 2017; Seller et al., 2020). Therefore, if no pronounced and significant decrease in concentration is observed in the water phase (case 2), the "*suspended sediment test*" variant may, also without ^{14}C-labeling of the test substance, provide valid evidence of lack of or insufficient intrinsic degradability (persistence) of the test substance. Due to the low sorption tendency of anions, this is particularly of interest when testing organic acids (Schaffer & Licha, 2015).

4.2 Selection of the reference substance (paragraphs 12 and 31) and preparation of stock and spiking solutions (paragraphs 17 and 23)

A reference substance is used to demonstrate a sufficiently high level of microbial activity in the test system. Recommendations are given for the selection and use of the reference substance and, in general, for the preparation of stock and spiking solutions of the test and reference substance(s).

4.2.1 Recommendation: Apply reference substance directly to test vessels and select according to analytical compatibility

The use of modern analytical multi-methods makes it possible to quantify the reference substance together with the test substances in a single analysis. It is therefore advisable to add the reference substance directly to the test vessels (at low and at high test concentrations) together with the test substance or a mixture of test substances. Avoiding the need for a separate preparation into which only the reference substance is spiked reduces the operational effort of the degradation test.

Such an *in-situ* positive control also represents the highest level of quality assurance, as the microbial population exposed to the test substances is immediately checked for sufficiently high activity. If the expected degradation of the reference substance is detected, an inhibitory effect of the test substance(s) on the microbial activity can be reliably excluded.

Quantifying the reference substance together with the test substances in a joint analysis also reduces the analytical workload.

OECD TG 309 suggests two chemicals, aniline and benzoate, as reference substances. Due to the possibility of NER formation, the use of aniline in the "*suspended sediment test*" variant is not recommended (Shrestha et al., 2016).

If reversed phase liquid chromatography (RPLC) is used, benzoate is recommended. Highly polar test substances may require the use of special analytical methods (e. g. hydrophilic interaction chromatography (HILIC), supercritical fluid chromatography (SFC) or ion exchange chromatography (IC)). In this case, the use of an alternative reference substance with high analytical compatibility is recommended. This is acceptable if results of degradation studies are available for the alternative reference substance that demonstrate sufficiently rapid aerobic biodegradation of the substance. OECD TG 309 specifies a period of less than two weeks as the expected interval for aerobic biodegradation of a reference substance. It is also acceptable to use a reference substance for which there is no evidence of sufficiently rapid aerobic biodegradation in an OECD TG 309. In this case, however, the predominant aerobic biodegradability and thus the suitability of

the chemical as a reference substance must also be demonstrated by an additional sterile control (see Chapter 4.4.3).

The occurrence of diauxic growth can be detrimental to the validity of the recommended procedure. This term refers to the two-phase growth of chemotrophic organisms that have two different substrates (i. e., chemicals) as energy sources. The energy sources are used in strict sequence. A consequence of diauxic growth may be that the degradation of a test substance starts only after the degradation of the reference substance. Since reference and test substances are used at similarly low concentrations in the replicates (low µg/L range, see Chapter 4.1.4 and Chapter 4.2.2), the probability of diauxic growth is rather low. However, if diauxic growth is suspected (e. g. because of anomalies in the degradation kinetics of a test substance), the test substance or mixture of test substances should be tested separately from the reference substance.

4.2.2 Recommendation: The spiked concentration of the reference substance is one hundred times the analytical limit of quantification

To analytically demonstrate the rapid aerobic biodegradation of the reference substance with sufficient resolution, the spiked concentration must be sufficiently high at the start of the degradation test. However, if the reference substance is tested together with the test substance (see Chapter 4.2.1), diauxic growth must be avoided and therefore the spiked concentration must be set as low as possible. It is therefore recommended to limit the spiked concentration of the reference substance to one hundred times the analytical limit of quantification.

When testing a mixture of test substances, it is recommended not to add the spiked concentration of the reference substance to the maximum sum of the concentrations of the test substances (see Chapter 4.1.4). If there is a reasonable suspicion of diauxic growth, the test substance or mixture of test substances should be tested separately from the reference substance. In this case, the recommendation to limit the spiked concentration to one hundred times the analytical limit of quantification does not apply.

4.2.3 Recommendation: Prepare stock and spiking solutions in deionized water and use the water-soluble salts of the test substances

For test and reference substances with sufficient water solubility above 1 mg/L, it is recommended that stock and spiking solutions be prepared in deionized water. The use of an organic co-solvent is not required. This supports simple, cost-effective and efficient implementation by eliminating the need for solvent control.

The stock solutions of the reference and test substances are prepared as single-substance solutions, and the spiking solutions of the test substances are prepared as mixtures. The spiking solution of the reference substance is prepared as a single substance solution. To exclude errors in the preparation (weighing, calculation, pipetting, filling, etc.), it is recommended to check the solutions analytically before performing the degradation test.

To minimize dilution of the test water during spiking, the volume of the spiking solution(s) used to prepare test batches should be kept as small as possible (i. e. < 10% of the final volume of the water phase) according to OECD TG 309. If this cannot be achieved using deionized water as the solvent, it is recommended that the spiking solutions be prepared in autoclaved test water. If it is not possible to autoclave the test water, it is recommended that the spiking solutions be prepared in test water immediately prior to the preparation of the test replicates.

Since free acids and free bases may be poorly soluble in unbuffered water (e. g., deionized water), it is recommended that their water-soluble salts, if available, be used in the preparation of stock and spiking solutions. The respective counterion must be considered when preparing the

stock solution. If extreme pH values occur in the spiking solution, care must be taken to maintain the pH range specified in OECD TG 309 during the degradation test. However, due to the high dilution of the spiking solution in the test vessel, a relevant influence of the pH value is not expected.

If salts of the test substances are used, those with an inorganic counterion should preferably be selected, also to exclude diauxic growth. However, the low concentrations of typical organic anions of organic bases (e. g. acetate, citrate, etc.) are not considered a concern and are not expected to affect the degradation test. The same is true for concentrations of typical inorganic cations of organic acids such as Na^+ or K^+.

4.3 Water and sediment sampling for the degradation test (paragraph 18) and test conditions (paragraphs 24, 25, and 26)

Regarding the selection of surface water for the collection of water and sediment for the degradation test, OECD TG 309 refers to the express purpose of the investigator. The CLP guidance also considers the use of an inoculum from a relevant aquatic system (ECHA, 2024; No. II.2.3.1 b). Recommendations for the choice of surface water and test conditions follow.

4.3.1 Recommendation: The sampling location for surface water and sediment is important to the entity conducting the test

For test substances that are not expected to undergo a pronounced and significant decrease in concentration in the water phase (case 2) during the degradation test, such as the prioritized contaminants listed in Chapter 6, it is recommended that the water for the degradation test be collected from a water body relevant to the institution conducting the test, even if this means that the water may be contaminated by the test substance. In this way, water suppliers and authorities can test for substances that have been detected in their own water resources.

If no pronounced and significant decrease in concentration is observed in the aqueous phase (case 2), this recommendation strengthens the validity of the degradation test. A microbial population potentially adapted to the test substance suggests an increased potential for aerobic biodegradation. Similarly, a test substance which shows no or insufficient intrinsic biodegradability in the aqueous phase using an adapted inoculum is likely to be non-degradable in the absence of a potentially non-adapted microbial population.

However, sampling in the immediate vicinity of major point sources (e. g. in the discharge area of industrial or municipal sewage treatment plants) must be avoided. In addition, the test water must be analyzed for the presence of the test substance(s) before the degradation test is carried out and the concentrations found, if any, must be considered in the preparation and/or addition of the spiking solution(s) (see Chapter 4.1.4 and Chapter 4.2.3). However, the test water should not be contaminated with the reference substance.

If, contrary to expectations, a pronounced and significant decrease in concentration is observed in the water phase (case 1), the use of anthropogenically influenced water (i. e. potentially adapted microbial population) may invalidate the test result. Although OECD TG 309 allows for a specific question regarding the degradability of a chemical in a previously exposed water body, including a sampling site with a corresponding exposure history, biodegradation by an adapted microbial population cannot be generalized to the aquatic environment.

If the objective is to obtain a generally valid test result, a section of watercourse should be selected which is unaffected by the test substance (i. e. without an adapted microbial population).

4.3.2 Recommendation: Perform the degradation test at 12 °C

It is recommended that the OECD TG 309 degradation test be performed at 12 °C. Although the test guideline recommends the field temperature of the sampled surface water as the test temperature, the ECHA Guidance on Information Requirements and Chemical Safety Assessment (Chapters R.7b (ECHA, 2023c) and R.11 (ECHA, 2023b)) specifies a temperature of 12 °C as the reference temperature for Europe. At a test temperature of 12 °C, the $DegT_{50}$ as a result of the degradation test can be directly compared with the CLP criteria for P and vP. If the test temperature is different, the determined $DegT_{50}$ would have to be normalized to 12 °C.

4.3.3 Recommendation: Perform the test in the dark

According to OECD TG 309, the test can be performed in the dark or in diffuse light. The test guideline recommends a dark environment, and this report follows that recommendation.

4.3.4 Recommendation: Test duration of 60 days

According to the CLP Regulation, a chemical is very persistent (vP) if less than 50% of the initial concentration in the aqueous phase has been aerobically biodegraded after 60 days. For test substances for which no clear and significant decrease in concentration in the aqueous phase is expected during the degradation test (case 2), e. g. the prioritized contaminants listed in Chapter 6, it is recommended to perform the degradation test according to OECD TG 309 over the test period of 60 days.

4.3.5 Recommendation: Shake test vessels, do not stir

Agitation of the test vessels is recommended. The use of a magnetic stirrer can result in continuous grinding of the added sediment or the solid fraction remaining after filtration/centrifugation, thus continuously creating new potential sorption sites for the test and reference substances (Shrestha et al., 2016).

4.4 Preparation of test replicates (paragraphs 28, 30, and 31) and specific chemical analysis (paragraph 41)

The dimensioning of the test approaches and the decision whether a replicate is sampled several times (i. e. at different times) for substance-specific analysis or is used in its entirety (e. g. for an extraction) during the ongoing degradation test depends, among other things, on the variant used ("*pelagic test*" or "*suspended sediment test*") and the analytical requirements. The recommendations should therefore be coordinated.

4.4.1 Recommendation: Adapt test replicates and sampling strategy to the degradation test variant and analytical requirements

The following recommendations for replicate sizing and sampling strategy apply to test substances for which no pronounced and significant decrease in concentration in the aqueous phase (case 2) is expected during the degradation test, e. g. the prioritized contaminants listed in Chapter 6. Three cases are distinguished based on the degradation test variant and the sample volume required for analysis per sampling time (see Table 1 and the following explanations).

According to the OECD TG 309 test guideline, at least 100 mL of water phase should be used, and the test vessel should not be filled more than one-third.

Case A1: It is recommended to perform the degradation test with a water volume of 300 mL in a bottle with a nominal volume of 1,000 mL. In many cases, this is a suitable compromise between the space required on the shaker and the volume of the sub-samples required for analysis.

Table 1: Recommendations for the size of test replicates and the sampling strategy for the three cases based on the degradation test variant and the sample volume required for analysis per sampling time

Case	Variant	Sample volume required for analysis at each sampling time	Dimensioning of the replicates	Sub-sample per sampling time
A1	*pelagic test*	≤ 25 mL	300 mL test water, bottle with 1,000 mL nominal volume	5 - 25 mL
A2	*pelagic test*	> 25 - 100 mL	100 mL test water, bottle with 300 mL nominal volume	entire replicate
B	*suspended sediment test*	≤ 100 mL	100 mL test water, bottle with 300 mL nominal volume	entire replicate

At each sampling time, a sub-sample of 5 - 25 mL is taken from a replicate for analysis (see Chapter 4.4.4). With a total of seven sampling times and a maximum sub-sample volume of 25 mL, it is ensured that a water volume of at least 100 mL is not undershot in the degradation test before the last sampling.

A replicate is not discarded after a sub-sample is taken, but the degradation test continues with that replicate. This eliminates a significant amount of additional work in preparing replicates.

Cases A2 and B: It is recommended to perform the OECD TG 309 degradation test with 100 mL of water in a 300 mL nominal volume bottle. The entire replicate is used for the analysis or, if a sub-sample is taken, the degradation test is terminated for the sampled replicate. This requires a significantly higher total number of replicates than in case A1.

When performing a "*suspended sediment test*", it is questionable whether it is possible, depending on the quality of the sediment, to take representative sub-samples and to keep the remaining suspension in the test vessel sufficiently constant with respect to its water/solid ratio over the entire test period. Therefore, in contrast to the *pelagic test*, this recommendation applies regardless of the sample volume required for analysis.

4.4.2 Recommendation: Four replicates for a single test substance and six replicates for mixtures

The OECD TG 309 test guideline requires at least two replicates per concentration of the test substance and recommends the use of at least three replicates per concentration. If a replicate is not further incubated after sampling (e. g. because the entire water phase is used for analysis, see Chapter 4.4.1), the recommendation applies to each sampling time (see Chapter 4.4.4).

Beyond the requirements of the test guideline, this report recommends that the OECD TG 309 degradation test be performed with four replicates for a single test substance and with six replicates when testing mixtures.

This recommendation increases the resource requirements but increases the statistical significance of the test results and thus their validity. With more replicates, outliers are more easily

identified, and test results are more reproducible. Especially when testing mixtures, the additional effort required for six replicates is justified, as the simultaneous testing of several chemicals in one approach already saves considerable resources.

4.4.3 Recommendation: No sterile control

For test substances which are not expected to undergo a pronounced and significant decrease in concentration in the aqueous phase (case 2) during the degradation test, e. g. the prioritized contaminants listed in Chapter 6, it is recommended to perform the OECD TG 309 degradation test without a sterile control.

Not using a sterile control makes it easier to perform the degradation test in a simple, cost-effective and efficient manner. In case 2, abiotic processes such as hydrolysis, volatilization and sorption can be excluded even without a sterile control, thus ensuring a valid result.

If there is any doubt about the physicochemical property data of a test substance, a sterile control must be performed. If, contrary to expectations, a pronounced and significant decrease in concentration is observed in the aqueous phase (case 1), this recommendation may invalidate the test result, since it is not possible to distinguish between biological and abiotic processes without a sterile control. In this case, the test must be repeated using a sterile control and, in the case of the variant "*suspended sediment test*", it may also be necessary to use ^{14}C-labeling of the test substance.

A fundamental exception to this recommendation is the use of a chemical as a reference substance whose suitability has not yet been demonstrated by available results from standardized degradation tests. A sterile control must be included to exclude abiotic processes such as hydrolysis, volatilization and sorption. In this case, it is recommended to include the test substance(s) in the sterile control as the additional effort is negligible due to the coordinated analysis.

4.4.4 Recommendation: Sample for analysis at 0, 3, 7, 14, 28, 42, and 60 days

For test substances for which no pronounced and significant decrease in concentration in the aqueous phase (case 2) is expected during the degradation test, e. g. the prioritized contaminants listed in Chapter 6, it is recommended to collect samples for analysis weekly at the beginning and every two weeks at the end of the test. Due to the application of the reference substance in the test vessel, an additional sampling on day 3, i. e. within the first week of exposure, is recommended.

In general, at least five sampling points are required during the degradation phase. Seven measurement points increase the probability of deriving a reliable rate constant and thus a valid $DegT_{50}$ by modeling the degradation kinetics.

4.4.5 Recommendation: Freeze samples and analyze in a common sequence

It is recommended that samples be frozen and analyzed in a common sequence. According to OECD TG 309, samples should be frozen below –18 °C or chemically preserved for prolonged storage.

This recommendation presupposes that the stability of the test substance(s) and reference substance(s) has been demonstrated by appropriate preliminary tests. For this preliminary test, the day 0 (c_0) sample can be used, which according to OECD TG 309 should be analyzed first in a timely manner (i. e. within 24 h) without prior freezing. One freeze-thaw cycle of the test substance(s) and reference substance(s) in the test water used is sufficient as a preliminary test to determine the storage stability, since these are the critical processes for this type of storage.

After the first analysis (c_0), the sample is frozen, thawed and analyzed on one of the next two days (i. e. before the next sampling). If all test substances are found to be stable (e. g. maximum deviation from the initially determined concentration of 10% (EC, 2023)), the recommendation can be applied to all further samples of the degradation test. The results of the preliminary tests should be documented and included in the technical justification report of the method.

This recommendation supports a simple, cost-effective and efficient implementation. Possible inter-day variations in the sensitivity of the measurement do not need to be considered in this procedure, which has a positive effect on the statistical evaluation of the measurement results.

If the samples are analyzed within 24 hours, they must be stored at 2 °C to 4 °C according to OECD TG 309.

4.5 Test data and reporting (paragraphs 43 to 53)

Specifications for kinetic evaluation of measurement data and reporting are described in the OECD TG 309 test guideline. Explanations are provided, for example, in the FOCUS guideline on estimating persistence and degradation kinetics from environmental fate studies (FOCUS, 2006).

Although this report does not make recommendations, the authors seek to establish a network of test facilities to provide support for kinetic evaluation of measurement data and reporting. Interested parties are invited to participate.

5 Procedure for the prioritization and deprioritization of contaminants for a “cold” degradation test according to OECD TG 309

5.1 List of 1250 contaminants

In 2023, the UBA published a literature review listing 1289 contaminants detected in the six matrices wastewater treatment plant effluent (WTPE, 442 contaminants), surface water (SW, 1021 contaminants), bank filtrate (BF, 114 contaminants), groundwater (GW, 338 contaminants), raw water (RW, 212 contaminants), and drinking water (DW, 385 contaminants) (Arp et al., 2023).

For this report, the identities of these contaminants were first checked, information was replaced and supplemented where necessary, and structural features (SMILES, InChI) were added. In addition, 45 duplicates were removed, and six additional contaminants were added from other sources. The resulting list contained 1250 contaminants.

Selected parameters describing adsorption tendency, volatility and degradation were researched or generated using QSAR (Quantitative/Qualitative Structure-Activity Relationships) for the 1250 contaminants and this information was added. Based on this data, the contaminants were evaluated for their suitability for a "cold" degradation test according to OECD TG 309. Contaminants identified as unsuitable for this variant of the degradation test are referred to as *deprioritized*.

5.2 Deprioritization and prioritization

The procedure was divided into three steps and is shown schematically in Figure 1.

In a first step, the data obtained were used to deprioritize those contaminants that are highly unlikely to remain in the aqueous phase of the degradation test due to their high adsorption potential and/or high volatility. This was the case for 269 contaminants.

In a second step, contaminants suspected of being biodegradable were deprioritized. This applied to 177 contaminants.

These two steps were carried out in parallel and resulted in 41 contaminants being deprioritized based on both their physicochemical properties and their predicted biodegradability.

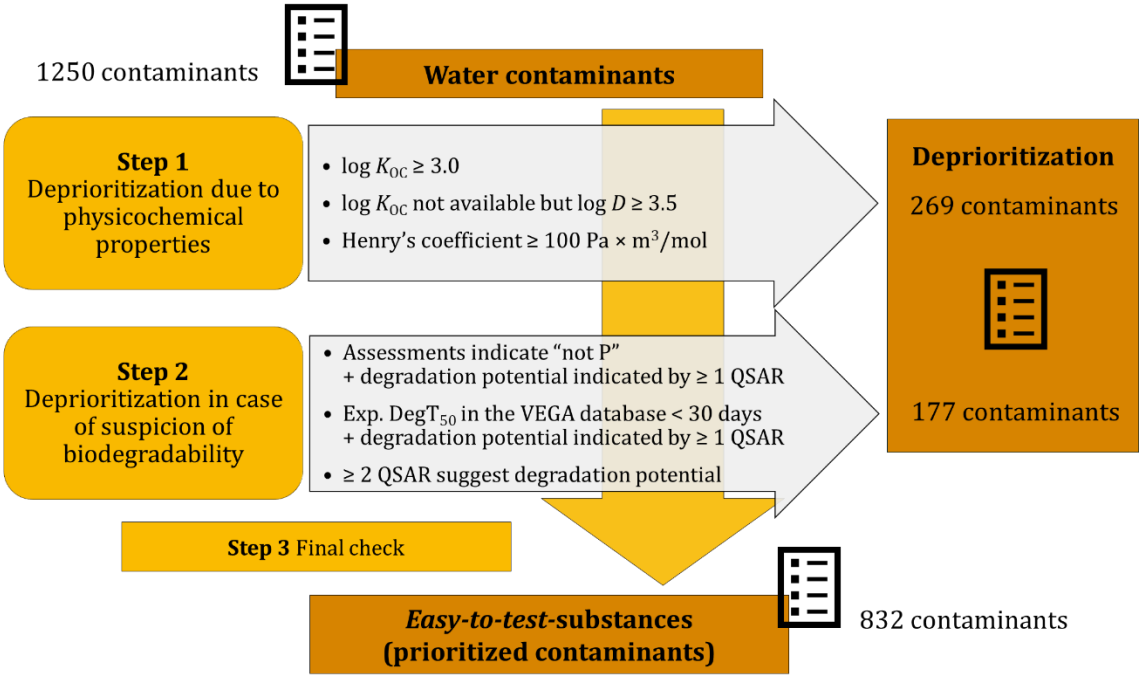
Finally, a third step involved a final review of the results.

The three steps are described in more detail below.

Step 1: The adsorption potential, e. g. on the test vessel wall and on the suspended sediment, was estimated, where available, using distribution coefficients such as the M/vM criterion log K_{OC} from Arp & Hale (2022) and Arp et al. (2023). A log $K_{OC} \geq 3.0$ resulted in deprioritization. If log K_{OC} was not available, log D at pH 7.4 was calculated as a measure of lipophilicity using two independent QSARs and the mean of these results was used for the assessment. The OPERA (Open (Quantitative) Structure-activity/property Relationship App) (Mansouri et al., 2018) and Percepta ACD/Labs Release 2022.2.3 (Build 3577, 7 Jun 2022, GALAS model) platforms were used to calculate the individual values of log D. A contaminant was deprioritized if the mean value of log $D \geq 3.5$. As log D was calculated in contrast to the log K_{OC} used, a potential uncertainty was considered with the value that was 0.5 units higher.

The Henry's coefficient as a measure of volatility was also calculated using the above mentioned ACD/Labs software (reference temperature 12 °C). A value of 100 Pa × m^3/mol or higher led to deprioritization. This value was taken from the OECD TG 309 specifications.

Figure 1: Deprioritization and prioritization of contaminants



Source: original figure, TZW: DVGW-Technologiezentrum Wasser.

Step 2: To assess whether a contaminant is likely to be sufficiently biodegradable for deprioritization in an OECD TG 309 degradation test, the assessments of Arp & Hale (2022) and Arp et al. (2023) were included. Furthermore, experimentally determined $DegT_{50}$ values stored in the VEGA database[1] were considered. In addition, different QSARs and their combinations were used, such as the approach within *hot-target-analysis* (BIOWIN combination from Nödler et al. (2019)) and the P score (Hartmann et al., 2023).

Modeled results from the two QSARs VEGA and a method under development by Hafner et al. (2023) were considered if the quality of the results was characterized as *moderate* or *good* (VEGA) or the log standard deviation of the calculated $DegT_{50}$ according to Hafner et al. (2023) was less than 0.75. In the context of this report, biodegradability is assumed to be relevant if the calculated $DegT_{50}$ is less than 30 days. The $DegT_{50}$ of the contaminants according to Hafner et al. (2023) was kindly calculated and provided by Jasmin Hafner for this report.

The BIOWIN combination of Nödler et al. (2019) incorporates models 1 through 6 of the US EPA's EPI suite. Using a calibration over 45 chemicals for which TZW had internal real-world data on their behavior during bank filtration and/or wastewater treatment, the result range ≥ 0.6 was derived for chemicals suspected to be sufficiently biodegradable (Nödler et al., 2019). The target value of the calibration performed was a prediction with at least 80% accuracy.

Researchers at the Dutch National Institute for Public Health and the Environment (RIVM) have developed a computer-based screening tool to identify persistent, mobile and toxic chemicals, known as the *PMT score* (Hartmann et al., 2023). The basic approach is to rank chemicals from 0 (low PMT potential) to 1 (high PMT potential). The PMT score is calculated from the individual

[1] https://www.vegahub.eu/

scores for P, M and T. The basis for the calculation of the P score is the result of the BIOWIN-3 model of the EPI suite of the US EPA. For this report, biodegradability is assumed to be achieved with a P score ≤ 0.09. This value was derived empirically from examples. The P scores of all contaminants considered were kindly calculated and provided by RIVM for this report.

Step 3: In the third step, a final review of the individual assessments was performed based on retrospectively defined criteria. Contaminants that are good indicators of untreated wastewater due to their known biodegradability (e. g. caffeine (Warner et al., 2019)) were retrospectively deprioritized (six contaminants: caffeine, paraxanthine, theobromine, theophylline, aniline, and ibuprofen). Seven inconclusive contaminants that did not meet the volatility criterion (calculated Henry's coefficient) for deprioritization were also deprioritized. These are 1,1,2,2-tetrachloroethane, 1,1,2-trichloroethane, 1,2,3-trichloropropane, dibromochloromethane, bromoform, 1,2-dibromoethane and dibromomethane. Based on experience, these seven contaminants are most likely to have an increased tendency to volatilize from the aqueous phase. The trihalomethanes mentioned are also disinfection by-products and their presence in drinking water is usually not related to raw water contamination.

Deprioritized contaminants: Deprioritization in this report does not mean that a valid test result could not be obtained for these contaminants without ^{14}C-labeling. However, compared to the prioritized contaminants, a "cold" degradation test according to OECD TG 309 with deprioritized contaminants is likely to require significantly more effort and carry an increased risk of a non-valid test result. The 418 deprioritized contaminants are listed in Table 5 in the Appendix.

Ranking within the lists: The contaminants in the two lists (Table 2, Table 3 and Table 5) were sorted by descending vPvM score. The vPvM score is calculated from the individual scores for P and M and can be regarded as a measure of the relevance of a contaminant for drinking water.

The vPvM scores of all contaminants were kindly generated and provided by RIVM for this report. A statistical comparison of the vPvM scores of the deprioritized and prioritized contaminants is presented in the Appendix, Chapter A.1.

6 List of contaminants prioritized for a “cold” degradation test according to OECD TG 309

The three steps described in Chapter 5.2 were used to identify and prioritize those contaminants that are not expected to have a pronounced and significant intrinsic aerobic biodegradability in an OECD TG 309 degradation test and that remain in the aqueous phase throughout the test due to their physicochemical properties.

The list of 832 contaminants prioritized for a "cold" degradation test according to OECD TG 309 has been divided into two priority levels: Table 2 contains contaminants that have already been detected in drinking water, groundwater, raw water or bank filtrate (category A). Table 3 contains contaminants that have only been detected in wastewater treatment plant effluent and/or surface water (category B).

The contaminants in both tables were sorted by descending vPvM scores.

The columns of the tables contain the following information:

- The **CAS No.**, **EC No.**, and **Name** columns contain the **identifying characteristics** of the contaminants. The *CAS No.* and *EC No.* are examples of chemicals listed in the CAS and REACH databases, respectively, which contain the contaminant (i. e. the organic species) considered in this report. Thus, the *CAS No.* and *EC No.* may represent salts of the contaminants (e. g., a sodium salt of an acid - but the investigated contaminant was the free acid or organic anion). The name of the free acid or base is given in the *Name* column, if applicable. For the sake of presentation, trivial names and, where appropriate, common abbreviations are used.

- The **vPvM** column lists the **vPvM scores** (dimensionless) of the contaminants. The *vPvM score* is calculated from the individual P and M scores and can be regarded as a measure of the relevance of a contaminant for drinking water production (from 0 = low to 1 = high).

- Columns **Ad1** and **Ad2** (Ad for adsorption) list the parameters used to estimate the **adsorption tendency** of the contaminants. The values are rounded to one decimal place for presentation purposes. Column *Ad1* lists the min log K_{OC} values from Arp & Hale (2022) or Arp et al. (2023), if available. An empty cell indicates that this information is not available. Column *Ad2* lists the means of the calculated log *D* values.

- The calculated **Henry coefficients** (in Pa × m^3/mol) of the contaminants are listed in the **V** column (V for volatilization). The values are rounded to whole numbers for presentation purposes.

- Columns **Deg1** to **Deg6** (Deg for degradation) list the parameters used to assess whether **biological degradability** is suspected.

  - The column *Deg1* contains the conclusions on persistence (P-conclusion) from Arp & Hale (2022) and Arp et al. (2023). An empty cell indicates that this information is not available.

  - The column *Deg2* contains the adjusted combination of different BIOWIN models (BIOWIN1 to BIOWIN6) according to Nödler et al. (2019) (dimensionless).

  - The column *Deg3* contains the calculated $DegT_{50}$ values (in days) of the contaminants according to Hafner et al. (2023), provided that a value of 0.75 was not exceeded for the logarithmic standard deviation of the calculated $DegT_{50}$ value. An empty cell indicates

that this quality criterion was not met. Values are rounded to whole numbers for presentation purposes.

- The column *Deg4* contains, if available, the experimental $DegT_{50}$ (in days) of the contaminants as stored in the VEGA database. An empty cell indicates that this information is not available.
- The column *Deg5* contains the VEGA-QSAR calculated $DegT_{50}$ (in days) of the contaminants, provided that the quality of the result was rated as *moderate* or *good* by the platform. An empty cell indicates that this quality criterion was not met.
- The column *Deg6* contains the P scores (dimensionless) of the contaminants according to Hartmann et al. (2023).

The lists of contaminants are also available for download in MS Excel format. In addition to the columns mentioned above, these files contain the structural characteristics of the contaminants (SMILES, InChI) and, based on the table by Arp et al. (2023), the maximum concentrations of the contaminants in the different water matrices (WTPE, SW, DW, GW, RW, BF) as well as the corresponding references in a separate sheet ("Ref Index").

Table 2: Prioritized contaminants for conducting a “cold” degradation test according to OECD TG 309, sorted by descending vPvM score, part 1

Category A: contaminants for which there are detections in at least one of the following compartments: drinking water, groundwater, raw water, bank filtrate

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
110871-86-8	629-019-8	Sparfloxacin	0.89		-0.9	0	n.a.	-0.15				0.97
73334-07-3	277-385-9	Iopromide	0.89		-2.6	0	n.a.	-0.26				0.85
1401-69-0	215-754-8	Tylosin	0.88		0.8	0	n.a.	-0.15				0.95
8025-81-8	232-429-6	Spiramycin	0.88		0.8	0	n.a.	-0.20				0.98
98079-51-7	619-317-6	Lomefloxacin	0.87	-1.5	-2.8	0	no conclusion/data	-0.05				0.94
79660-72-3	677-525-2	Fleroxacin	0.87	-1.4	-0.8	0	n.a.	-0.15				0.98
100-97-0	202-905-8	Methenamine	0.87		-1.3	0	vP	0.14				0.81
82419-36-1	680-263-1	Ofloxacin	0.86	-0.8	-4.0	0	n.a.	0.04				0.93
112398-08-0	638-772-1	Danofloxacin	0.85		-3.5	0	n.a.	0.00				0.92
57-62-5	200-341-7	Chlortetracycline	0.85		-2.1	0	n.a.	0.24				0.93
93106-60-6	618-911-2	Enrofloxacin	0.84		-4.7	0	n.a.	0.00				0.92
28179-44-4	248-887-5	Ioxitalamic acid	0.84		-2.0	0	vP	-0.26				0.85
98106-17-3	-	Diflofloxacin	0.84	0.9	-4.1	0	n.a.	-0.18				0.98
78649-41-9	-	Iomeprol	0.84		-3.1	0	n.a.	-0.13				0.74
60166-93-0	262-093-6	Iopamidol	0.83		-2.6	0	n.a.	-0.15				0.74
70458-92-3	274-611-8	Pefloxacin	0.83	-0.3	-1.9	0	n.a.	0.01				0.90
10118-90-8	800-277-5	Minocycline	0.83		-1.5	0	n.a.	0.26				0.89
80214-83-1	617-007-5	Roxithromycin	0.82		2.4	0	n.a.	-0.31				0.99

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
74011-58-8	-	Enoxacin	0.82	-1.6	-1.7	0	n.a.	0.08				0.87
98105-99-8	-	Sarafloxacin	0.82		-4.7	0	n.a.	-0.07				0.95
66108-95-0	266-164-2	Iohexol	0.82		-3.4	0	Potential P/vP++	-0.10				0.70
16846-24-5	240-871-6	Josamycin	0.82		2.2	0	n.a.	0.11				0.91
354812-41-2	-	Moxifloxacin	0.81	0.6	-2.7	0	n.a.	0.13				0.88
39405-35-1	-	Kitasamycin	0.80		0.5	0	n.a.	0.13				0.77
70458-96-7	274-614-4	Norfloxacin	0.80	-1.5	-2.9	0	n.a.	0.12				0.77
86386-73-4	627-806-0	Fluconazole	0.80	0.4	0.6	0	n.a.	-0.03				0.94
3922-90-5	223-495-7	Oleandomycin	0.79		0.9	0	n.a.	-0.09				0.86
85721-33-1	617-751-0	Ciprofloxacin	0.79	-1.7	-5.2	0	n.a.	0.11				0.78
117-96-4	204-223-6	Diatrizoic Acid	0.78		-0.6	0	Potential P/vP++	-0.32				0.89
81103-11-9	617-200-4	Clarithromycin	0.77		2.3	0	n.a.	-0.20				0.98
114-07-8	204-040-1	Erythromycin	0.76		1.9	0	n.a.	-0.13				0.97
79-57-2	230-540-4	Oxytetracycline	0.76		-2.9	0	n.a.	0.36				0.74
83905-01-5	617-500-5	Azithromycin	0.74		1.7	0	Potential P/vP++	-0.22				0.99
60-54-8	200-481-9	Tetracycline	0.74		-1.7	0	n.a.	0.30				0.81
-	-	1,3,5-Triazin-2-ol, 4,6-di-4-morpholinyl-	0.71		0.3	0	n.a.	0.11				0.80
62037-80-3	700-242-3	GenX (Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate)	0.71	1.1	-3.4	0	vP	-0.03				0.98
17090-79-8	241-154-0	Monensin	0.71		1.6	0	n.a.	-0.24				0.94
1893-33-0	606-172-9	Pipamperone	0.69		0.8	0	Pot. P/vP	0.05				0.98

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
375-73-5	206-793-1	PFBS (1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulphonic acid)	0.69		-4.8	0	vP	0.12				0.92
114311-32-9	601-305-7	Imazamox	0.68		-1.7	0	n.a.	0.29	30			0.65
111991-09-4	601-148-4	Nicosulfuron	0.68		-1.7	0	n.a.	0.49	27			0.79
90357-06-5	-	Bicalutamide	0.68		2.0	0	n.a.	0.03				0.99
2706-90-3	220-300-7	PFPeA (Perfluorovaleric acid)	0.68	0.8	-4.4	0	n.a.	0.18				0.83
375-85-9	206-798-9	PFHpA	0.67	1.6	-2.9	0	n.a.	0.12				0.93
76-57-3	200-969-1	Codeine	0.67	0.4	0.2	0	n.a.	0.49				0.71
30125-63-4	634-816-9	Desethylterbutylazin	0.67		1.8	0	n.a.	0.13	62			0.83
15676-16-1	239-753-7	Sulpiride	0.66	0.2	-1.1	0	Pot. P/vP	0.44				0.68
80370-57-6	688-302-4	Ceftiofur	0.66		-1.8	0	n.a.	0.32				0.62
2706-91-4	220-301-2	PFPS (C5-Sulfonate)	0.66	1.4	-4.1	0	n.a.	0.06				0.97
88040-23-7	643-019-5	Cefepime	0.65		-3.2	0	n.a.	0.38				0.54
27619-97-2	248-580-6	6:2 fluorotelomer sulfonic acid	0.65	1.3	-2.5	0	Potential P/vP++	-0.01				0.99
3682-35-7	222-965-9	TPTZ (2,4,6-tri(2-pyridinyl)-1,3,5-triazine)	0.65		2.9	0	n.a.	0.17				0.91
108-78-1	203-615-4	Melamine	0.65		-1.2	0	vP	0.18	108		13	0.53
140-08-9	205-397-6	(2-chlorethyl) phosphite	0.65		2.0	0	n.a.	0.26				0.68
1007-28-9	623-281-7	Deisopropylatrazine	0.64		1.2	0	Pot. P/vP	0.19	88		13	0.67
88-50-6	201-836-0	4-amino-2,5-dichlorobenzenesulphonic acid	0.63		-5.1	0	Pot. P/vP	0.13				0.54
21725-46-2	244-544-9	Cyanazine	0.63		2.3	0	n.a.	0.17	50			0.90

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
6190-65-4	622-793-8	Deethylatrazine	0.63	0.6	1.2	0	Pot. P/vP	0.16	74		141	0.69
56038-13-2	259-952-2	Sucralose	0.63		-0.9	0	n.a.	0.27				0.45
18467-77-1	242-348-8	Diprogulic acid	0.62		-3.4	0	n.a.	-0.02				0.52
15318-45-3	239-355-3	Thiamphenicol	0.62		-0.2	0	n.a.	0.41				0.48
138261-41-3	428-040-8	Imidacloprid	0.62		-1.4	0	Pot. P/vP	0.22				0.58
375-22-4	206-786-3	PFBA	0.62	0.4	-4.3	0	n.a.	0.24				0.62
3871-99-6	223-393-2	PFHxS-K	0.62	1.8	-4.9	0	n.a.	0.00				0.99
56-75-7	200-287-4	Chloramphenicol	0.61	0.3	1.0	0	Pot. P/vP	0.30				0.56
58-93-5	200-403-3	Hydrochlorothiazide	0.61	-0.0	-0.1	0	n.a.	0.16				0.59
914637-49-3	811-572-3	5:3 FTCA (2*H*,2*H*,3*H*,3*H*-Perfluorooc-tanoic acid)	0.61		0.2	1	n.a.	0.12				0.95
51940-44-4	257-530-2	Pipemidic acid	0.61	-1.0	-4.6	0	n.a.	0.28				0.43
914-00-1	213-017-5	Methacycline	0.61		-2.2	0	n.a.	0.41				0.55
738-70-5	212-006-2	Trimethoprim	0.61	0.4	0.8	0	n.a.	0.45				0.71
122-34-9	204-535-2	Simazine	0.61		2.2	0	Pot. P/vP	0.18	91			0.71
3737-09-5	223-110-2	Disopyramide	0.61	1.4	0.8	0	Pot. P/vP	0.21				0.87
152459-95-5	604-855-6	Imatinib	0.60		2.3	0	Potential P/vP++	-0.02				0.98
5011-34-7	225-690-2	Trimetazidine	0.60		-1.6	0	Pot. P/vP	0.64				0.58
42835-25-6	255-962-6	Flumequine	0.60		-1.3	0	n.a.	0.18				0.56
335-67-1	206-397-9	PFOA	0.60	2.1	-1.9	0	n.a.	0.00				0.99
84057-84-1	281-901-8	Lamotrigine	0.60	1.9	2.5	0	n.a.	0.07				0.77

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
5915-41-3	227-637-9	Terbuthylazine	0.60	2.1	3.1	0	n.a.	0.12	81			0.86
106266-06-2	600-733-1	Risperidone	0.59	1.6	2.5	0	n.a.	0.09				0.94
1912-24-9	217-617-8	Atrazine	0.59	1.4	2.6	0	Potential P/vP++	0.15	87			0.73
54-31-9	200-203-6	Furosemide	0.59	1.3	-1.4	0	n.a.	0.23				0.57
144689-63-4	604-433-1	Olmesartan medoxomil	0.59		1.2	0	n.a.	0.19				0.84
25953-19-9	247-362-8	Cefazolin	0.58	-0.8	-2.6	0	n.a.	0.55				0.44
27203-92-5	248-319-6	Tramadol	0.58	1.8	0.8	0	Pot. P/vP	0.31				0.67
144689-24-7	646-413-5	Olmesartan	0.58		0.0	0	Potential P/vP++	0.26				0.73
139-40-2	205-359-9	Propazine	0.58	1.7	3.0	0	Potential P/vP++	0.12	75		10	0.75
107534-96-3	403-640-2	Tebuconazol	0.57	2.4	3.3	0	Pot. P/vP	0.18	10			0.84
542-02-9	208-796-3	Acetoguanamine	0.57		0.4	0	vP	0.27				0.48
375-92-8	206-800-8	PFHpS	0.57	2.2	-4.1	0	n.a.	-0.06				1.00
66357-35-5	266-332-5	Ranitidine	0.57	-0.9	-1.1	0	Pot. P/vP	0.29				0.50
5786-21-0	227-313-7	Clozapine	0.57	2.3	2.4	0	n.a.	0.09				0.80
52722-86-8	258-132-1	Hydroxyethyl tetramethylpiperidinol	0.57		-0.8	0	P	0.45				0.42
846-49-1	212-687-6	Lorazepam	0.57	1.7	2.5	0	n.a.	0.33				0.60
1511-16-6	689-044-5	Haloperidol	0.57	2.6	3.1	0	Pot. P/vP	0.00				0.97
2008-58-4	214-787-5	2,6-Dichlorobenzamide	0.57	0.4	1.0	0	no conclusion/data	0.39	297			0.49
841-06-5	212-664-0	Methoprotryn	0.57		3.0	0	n.a.	0.11				0.68
515-64-0	208-204-3	Sulfisomidine	0.56	-0.2	-0.3	0	n.a.	0.27				0.50

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
13674-87-8	237-159-2	Tris[2-chloro-1-(chloromethyl)ethyl] phosphate (TDCPP)	0.56	2.2	3.7	0	vP	0.30				0.96
42399-41-7	255-796-4	Diltiazem	0.56	2.5	2.6	0	n.a.	0.53				0.70
104-23-4	203-187-9	4'-aminoazobenzene-4-sulphonic acid	0.56	2.4	-2.5	0	Pot. P/vP	0.13				0.51
115-96-8	204-118-5	Tris(2-chloroethyl) phosphate	0.56		1.6	0	Potential P/vP++	0.51				0.58
1812-30-2	217-322-4	Bromazepam	0.56	1.0	2.0	0	n.a.	0.32				0.67
93413-62-8	700-516-2	Desvenlafaxine	0.55		-0.2	0	Pot. P/vP	0.28				0.64
142459-58-3	604-290-5	Flufenacet	0.55		3.0	0	n.a.	0.10				0.96
375-95-1	206-801-3	PFNA	0.55	2.4	-1.4	0	n.a.	-0.06				1.00
96-88-8	202-543-0	Mepivacaine	0.55	1.2	1.4	0	n.a.	0.48				0.59
144-83-2	205-642-7	Sulfapyridine	0.55	0.2	-0.4	0	Not P	0.21				0.50
335-76-2	206-400-3	PFDA	0.55	2.8	-0.4	0	n.a.	-0.01				0.99
88-53-9	201-839-7	5-amino-2-chlorotoluene-4-sulphonic a-cid	0.54		-4.5	0	no conclusion/data	0.20				0.39
68-22-4	200-681-6	Norethisterone	0.54		2.9	0	Potential P/vP++	0.27				0.67
87674-68-8	618-045-5	Dimethenamid	0.54	1.8	2.3	0	n.a.	0.31	11			0.58
57-68-1	200-346-4	Sulfadimidine	0.54	0.7	0.0	0	Potential P/vP++	0.27				0.50
201668-32-8	-	Flufenacet ESA	0.54		-3.0	0	n.a.	0.26				0.49
63527-52-6	264-299-1	Cefotaxime	0.54		-2.8	0	no conclusion/data	0.56				0.38
74191-85-8	616-059-6	Doxazosin	0.54		2.2	0	Pot. P/vP	0.50				0.93
1014-69-3	213-800-1	Desmetryn	0.53		2.6	0	n.a.	0.19				0.58

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
886-50-0	212-950-5	Terbutryn	0.53	2.4	3.4	0	n.a.	0.15				0.77
1610-17-9	216-547-5	Atraton	0.53	1.1	2.6	0	n.a.	0.25				0.62
2062-84-2	218-172-2	Benperidol	0.53		3.1	0	n.a.	0.07				0.89
214217-88-6	-	*p*-Hydroxyatorvastatin	0.53		3.1	0	n.a.	0.28				0.62
13674-84-5	237-158-7	TCPP	0.53	2.2	2.6	0	vP	0.43				0.66
41859-67-0	255-567-9	Bezafibrate	0.53		1.1	0	n.a.	0.45				0.62
127-69-5	204-858-9	Sulfisoxazole	0.52	0.8	-1.7	0	n.a.	0.28				0.48
1610-18-0	216-548-0	Prometon (H)	0.52	1.6	2.9	0	n.a.	0.22				0.64
50563-36-5	256-625-6	Dimethachlor CGA 369873	0.52		2.5	0	n.a.	0.36			26	0.55
56773-42-3	260-375-3	PFOS Tetraethylammonium	0.52	2.6	-2.6	0	vP	-0.12				1.00
2447-57-6	219-504-9	Sulfadoxine	0.52	0.7	-0.5	0	n.a.	0.44				0.54
35255-37-9	-	*N*-Acetylsulfamethazine	0.52		0.7	0	n.a.	0.23				0.58
797-63-7	212-349-8	Levonorgestrel	0.52		3.1	0	n.a.	0.27				0.69
76824-35-6	-	Famotidine	0.52		-0.9	0	n.a.	0.28				0.38
137-58-6	205-302-8	Lidocaine	0.52	1.6	1.8	0	Pot. P/vP	0.51				0.57
57-53-4	200-337-5	Meprobamate	0.51	0.2	0.5	0	n.a.	0.49				0.41
834-12-8	212-634-7	Ametryn	0.51	2.1	3.0	0	vP	0.18				0.60
3144-16-9	221-554-1	2-oxobornane-10-sulphonic acid	0.51		-3.8	0	Pot. P/vP	0.51				0.40
80-08-0	201-248-4	Dapsone	0.51	1.8	1.0	0	vP	0.17				0.44
66753-07-9	634-744-8	Terbuthylazine-2-hydroxy	0.51		-0.3	0	n.a.	0.34				0.33

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
51218-45-2	257-060-8	Metolachlor (H)	0.51	1.8	3.2	0	n.a.	0.29	11			0.60
6145-73-9	228-150-4	Tris-2-chloropropyl phosphate	0.51		3.0	0	n.a.	0.43				0.66
19982-08-2	690-724-9	Memantine	0.51		0.3	0	n.a.	0.38				0.59
77732-09-3	-	Oxadixyl	0.51		1.0	0	n.a.	0.28				0.40
64-85-7	200-596-4	Desoxycortone	0.51		2.9	0	n.a.	0.36				0.62
69-81-8	200-717-0	Carbazochrome	0.50		-0.1	0	n.a.	0.37				0.30
126-86-3	204-809-1	2,4,7,9-tetramethyldec-5-yne-4,7-diol	0.50		2.8	0	P	0.27				0.52
4304-30-7	-	3'-*O*-Acetylthymidine	0.50		-4.9	0	n.a.	0.31				0.32
61-33-6	200-506-3	Benzylpenicillin	0.50		-0.8	0	n.a.	0.60				0.38
134523-00-5	-	Atorvastatin	0.50		1.8	0	n.a.	0.28				0.62
125-33-7	204-737-0	Primidone	0.50		0.8	0	n.a.	0.69				0.41
98-36-2	202-661-2	2-Chloroaniline-5-sulfonic acid	0.50		-4.2	0	n.a.	0.20				0.31
87-08-1	201-722-0	Phenoxymethylpenicillin	0.49		-0.8	0	n.a.	0.67				0.39
67129-08-2	266-583-0	Metazachlor	0.49	1.8	2.2	0	n.a.	0.50	16			0.58
7287-19-6	230-711-3	Prometryn	0.49		3.5	0	n.a.	0.16				0.63
826-36-8	212-554-2	Triacetonamine	0.49		-0.4	0	Pot. P/vP	0.47				0.39
127-79-7	204-866-2	Sulfamerazine	0.49	0.5	-0.3	0	n.a.	0.26				0.42
839705-03-2	445-750-3	*N*,*N*-Didesmethylvenlafaxine hoac salt	0.49		-0.4	0	no conclusion/data	0.58				0.48
34256-82-1	251-899-3	Acetochlor	0.49	1.9	3.0	0	n.a.	0.32	11			0.57
80-35-3	201-272-5	Sulfamethoxypyridazine	0.49	0.0	-0.1	0	n.a.	0.33				0.43

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
214217-86-4	-	*o*-Hydroxyatorvastatin	0.49		3.2	0	n.a.	0.28				0.62
63-05-8	200-554-5	Androst-4-ene-3,17-dione	0.49		2.8	0	Not P	0.31				0.67
56211-40-6	637-197-3	Torasemide	0.49	2.4	2.4	0	n.a.	0.14				0.73
3575-80-2	609-173-2	Melperone	0.49		2.2	0	Pot. P/vP	0.15				0.78
651-06-9	211-480-8	Sulfamethoxine	0.49		-0.1	0	n.a.	0.33				0.43
26787-78-0	248-003-8	Amoxicillin	0.48		-1.0	0	Potential P/vP++	0.63				0.33
100-90-3	-	*N*4-acetylsulfamethazine	0.48		0.0	0	n.a.	0.50				0.51
330-54-1	206-354-4	Diuron	0.48	2.6	2.7	0	vP	0.24	55			0.53
149289-30-5	-	*N*-Desmethylvenlafaxine	0.48		0.4	0	n.a.	0.56				0.51
144-82-1	205-641-1	Sulfamethizole	0.48	0.3	-1.3	0	n.a.	0.25				0.43
1897-45-6	217-588-1	Chlorthalonil M12	0.48		3.1	0	n.a.	0.34		7		0.91
58-15-1	200-365-8	Dimethylaminophenazone	0.48	0.2	0.6	0	n.a.	0.34	77			0.38
723-46-6	211-963-3	Sulfamethoxazole	0.48	0.6	-0.6	0	n.a.	0.27				0.40
69-53-4	200-709-7	Ampicillin	0.48	-1.7	-1.0	0	Pot. P/vP	0.63				0.33
93-76-5	202-273-3	2,4,5-T	0.48	2.5	-1.1	0	n.a.	0.33		23		0.49
37439-34-2	253-506-0	Sodium 3,5,6-trichloropyridin-2-olate	0.48		2.9	0	Pot. P/vP	0.21			2	0.74
519-65-3	208-274-5	AMDOHPH	0.48		-1.3	0	n.a.	0.55				0.28
122-11-2	204-523-7	Sulfadimethoxine	0.48	1.1	-0.0	0	n.a.	0.44				0.54
59-89-2	627-564-6	NMOR (*N*-nitrosomorpholine)	0.47	-0.4	-0.3	0	n.a.	0.22				0.31
72-14-0	200-771-5	Sulfathiazole	0.47		-0.0	0	n.a.	0.25				0.34

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
1220-83-3	624-483-8	Sulfamonomethoxine	0.47	0.5	-0.6	0	n.a.	0.33				0.43
21312-10-7	244-330-5	*N*4-Acetylsulfamethoxazole	0.47		-0.5	0	n.a.	0.50				0.41
205939-58-8	-	Dimethenamid ESA	0.47		-3.2	0	n.a.	0.49	56			0.37
1493-13-6	216-087-5	TFMSA (Trifluoromethanesulphonic a-cid)	0.47	-0.2	-5.8	0	Potential P/vP++	0.45				0.31
5205-93-6	226-002-3	DMAPMA (*N*-[3-(dimethylamino)pro-pyl]methacrylamide)	0.47		-1.5	0	Not P	0.55				0.33
110964-79-9	601-017-1	4-methanesulfonyl-2-nitrobenzoic acid	0.47		-4.7	0	Potential P/vP++	0.38	9			0.29
2855-13-2	220-666-8	Isophoronediamine	0.47		-3.2	0	P	0.48				0.38
330-55-2	206-356-5	Linuron	0.47	2.3	3.1	0	n.a.	0.23	46	23		0.56
389-08-2	206-864-7	Nalidixic acid	0.47	0.5	-1.4	0	n.a.	0.34				0.35
127-73-1	204-861-5	*N*-Acetylsulfamerazine	0.47		-1.8	0	n.a.	0.49				0.43
93-72-1	202-271-2	Fenoprop	0.46		-0.5	0	n.a.	0.29			6	0.51
15972-60-8	240-110-8	Alachlor	0.46	2.3	3.3	0	n.a.	0.29	13			0.57
58-22-0	200-370-5	Testosterone	0.46		3.2	0	Pot. P/vP	0.36				0.52
88150-42-9	425-820-1	Amlodipine	0.46	1.7	1.4	0	no conclusion/data	0.56				0.47
126924-38-7	-	Norfluoxetine	0.46		0.2	0	n.a.	0.33				0.72
120923-37-7	601-744-4	Amidosulfuron	0.46		-3.2	0	n.a.	0.48	17			0.53
126-54-5	204-792-0	TOSU (2,4,8,10-tetraoxaspiro(5,5)unde-can)	0.46		0.2	0	n.a.	0.18				0.27
1231710-75-0	-	Dimethachlor ESA	0.46		-3.5	0	n.a.	0.53	56			0.33
3337-71-1	222-077-1	Asulam	0.46		-2.2	0	n.a.	0.27	4			0.30

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
171118-09-5	812-484-8	Metolachlor ESA	0.46		-2.3	0	n.a.	0.47	67			0.38
67035-22-7	620-752-9	Dehydronifedipine	0.45		2.5	0	n.a.	0.50				0.60
76-99-3	200-996-9	Methadone	0.45	2.6	3.3	0	Pot. P/vP	0.27				0.69
154-21-2	205-824-6	Lincomycin	0.45		0.0	0	n.a.	0.44				0.26
144-80-9	205-640-6	Sulfacetamide	0.45	-0.8	-2.5	0	no conclusion/data	0.28				0.28
15307-79-6	239-346-4	Diclofenac-Na	0.45		1.6	0	Potential P/vP++	0.19				0.52
486-56-6	207-634-9	Cotinine	0.45		0.2	0	n.a.	0.57				0.31
439-14-5	207-122-5	Diazepam	0.45	2.3	3.1	0	n.a.	0.47				0.48
68-35-9	200-685-8	Sulfadiazine	0.45	0.3	-1.9	0	Potential P/vP++	0.25				0.33
53-86-1	200-186-5	Indometacin	0.45	2.7	3.1	0	Pot. P/vP	0.41				0.45
88-22-2	201-811-4	2-amino-3,5-xylenesulphonic acid	0.45	1.3	-4.3	0	Not P	0.30				0.26
172960-62-2	-	Metazachlor ESA	0.45		-4.8	0	n.a.	0.56	185			0.36
930-55-2	213-218-8	*N*-Nitrosopyrrolidin	0.44	-0.4	0.1	0	n.a.	0.31				0.28
88407-82-3	618-161-6	Atenolol (2E)-2-butenedioate (salt)	0.44	-0.7	-1.4	0	no conclusion/data	0.71				0.27
604-75-1	210-076-9	Oxazepam	0.44	1.3	2.1	0	n.a.	0.56				0.35
5165-97-9	225-948-4	AMPS (Sodium 2-methyl-2-[(1-oxoal-lyl)amino]propanesulphonate)	0.44		-6.5	0	Potential P/vP++	0.60				0.23
187022-11-3	-	Acetochlor ESA	0.44		-2.9	0	n.a.	0.50	59			0.36
142363-53-9	-	Alachlor ESA	0.44		-1.9	0	n.a.	0.47	45			0.36
37517-30-9	922-246-6	Acebutolol, 2-hydroxybenzoate	0.44	0.9	-0.2	0	no conclusion/data	0.69				0.34
50-06-6	200-007-0	Phenobarbital	0.44	0.9	1.2	0	no conclusion/data	0.41				0.35

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
14698-29-4	238-750-8	Oxolinic acid	0.43		-1.8	0	n.a.	0.66				0.28
143-24-8	205-594-7	Bis(2-(2-methoxyethoxy)ethyl) ether	0.43	-1.5	-0.4	0	vP	0.14				0.23
56070-16-7	634-681-6	Terbufos-sulfon	0.43		2.5	0	n.a.	0.52				0.39
6493-05-6	229-374-5	Pentoxifylline	0.43	0.0	0.6	0	n.a.	0.38				0.30
55-18-5	200-226-1	*N*-Nitrosodiethylamin	0.42	-0.0	0.5	0	n.a.	0.32				0.28
83-15-8	201-457-0	*N*-Acetyl-4-aminoantipyrin	0.42		1.3	0	n.a.	0.57				0.26
15545-48-9	239-592-2	Chlortoluron	0.42	1.7	2.5	0	n.a.	0.34	66		15	0.38
42017-89-0	255-626-9	Fenofibric acid	0.42		1.1	0	no conclusion/data	0.36				0.45
10595-95-6	621-991-1	*N*-Nitrosomethylethylamin	0.42	-0.4	0.1	0	n.a.	0.32				0.26
1698-60-8	216-920-2	Pyrazon	0.42		0.2	0	n.a.	0.48	42			0.28
62-75-9	200-549-8	*N*-Nitrosodimethylamine	0.42	-0.8	-0.3	0	n.a.	0.33				0.24
125-40-6	204-738-6	Butabarbital	0.42	0.6	1.5	0	n.a.	0.35				0.33
77-04-3	201-000-5	Pyrithyldione	0.42		0.7	0	n.a.	0.67				0.31
53-16-7	200-164-5	Estrone	0.42		3.2	0	Pot. P/vP	0.40				0.53
87-61-6	201-757-1	1,2,3-trichlorobenzene	0.42	2.9	4.0	61	Potential P/vP++	0.24		71		0.60
59277-89-3	261-685-1	Aciclovir	0.42		-0.8	0	n.a.	0.29				0.20
116-06-3	204-123-2	Aldicarb	0.41		1.0	0	n.a.	0.35		23		0.29
28721-07-5	249-188-8	Oxcarbazepine	0.41		1.8	0	n.a.	0.40				0.31
76-74-4	200-983-8	Pentobarbital	0.41	0.9	2.0	0	Pot. P/vP	0.34				0.35
108-60-1	203-598-3	2,2'-dichlorodiisopropyl ether	0.41	1.0	2.4	3	n.a.	0.25		23		0.37

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
105293-89-8	-	*N*,*N*-Dipropyl-1,4-benzenediamine	0.41		2.3	0	n.a.	0.26			16	0.43
66722-44-9	613-980-5	Bisoprolol	0.41	0.1	-0.1	0	no conclusion/data	0.30				0.28
17254-80-7	-	Chloridazon-methyldesphenyl	0.41		0.1	1	n.a.	0.47	84			0.21
1582-09-8	216-428-8	Trifluralin	0.41	1.8	5.2	0	n.a.	-0.07	90	71		0.96
57-41-0	200-328-6	Phenytoin	0.41	1.7	2.4	0	Potential P/vP++	0.47				0.36
36016-40-7	636-838-4	*o*-mesitylsulfonylhydroxylamine	0.41		1.1	0	n.a.	0.52				0.34
58-73-1	200-396-7	Diphenhydramine	0.40	2.5	2.0	0	Pot. P/vP	0.26				0.41
3060-89-7	221-301-5	Metobromuron	0.40	1.8	2.3	0	n.a.	0.33	29			0.35
50-27-1	200-022-2	Estriol	0.40	1.5	2.5	0	n.a.	0.58				0.29
1672-58-8	216-808-3	FAA (4-Formylaminoantipyrine)	0.40		-0.3	0	n.a.	0.58				0.24
3380-34-5	222-182-2	Triclosan	0.40	2.4	5.0	0	Potential P/vP++	0.25			19	0.77
76-22-2	200-945-0	Bornan-2-one	0.40	2.1	2.5	1	Not P	0.45				0.41
464-49-3	207-355-2	(+)-bornan-2-one	0.40	1.2	2.5	1	Not P	0.45				0.41
118-88-7	204-282-8	4-aminotoluene-2-sulphonic acid	0.40		-4.1	0	Pot. P/vP	0.29				0.20
38821-53-3	254-137-8	Cefradine	0.40		-3.5	0	n.a.	0.63				0.21
56681-55-1	-	Hydroxyalachlor	0.40		2.2	0	n.a.	0.52				0.28
374064-02-5	664-145-7	5-(2-Pyridinyl)-1*H*-pyrazole-3-carboxylic acid	0.40		-1.2	0	n.a.	0.60				0.24
1746-81-2	217-129-5	Monolinuron	0.40	1.6	2.2	0	n.a.	0.32				0.33
6339-19-1	-	Desphenyl chloridazon	0.39		-1.8	0	n.a.	0.49	62			0.20
63-74-1	200-563-4	Sulphanilamide	0.39	-0.7	-0.6	0	no conclusion/data	0.33	8			0.22

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
21087-64-9	244-209-7	Metribuzin	0.39		1.5	0	n.a.	0.26	8			0.33
150-68-5	205-766-1	Monuron	0.39	1.4	1.9	0	no conclusion/data	0.34	48			0.30
36507-30-9	641-693-5	10,11-Dihydro-10,11-Epoxycarbamaze-pine	0.39		1.4	0	n.a.	0.26				0.25
139481-59-7	604-138-8	Candesartan	0.39		-2.3	0	Potential P/vP++	0.47				0.54
30223-73-5	-	2-Ethylidene-1,5-dimethyl-3,3-diphe-nylpyrrolidine (EDDP)	0.39		2.4	0	n.a.	0.29				0.62
84-86-6	201-567-9	4-aminonaphthalene-1-sulphonic acid	0.39		-4.7	0	Pot. P/vP	0.24				0.20
84-89-9	201-571-0	5-aminonaphthalene-1-sulphonic acid	0.39		-4.5	0	no conclusion/data	0.24				0.20
82626-48-0	617-367-3	Zolpidem	0.39	2.2	3.2	0	Pot. P/vP	0.51				0.55
77-71-4	201-051-3	5,5-dimethylhydantoin	0.39	1.8	-0.6	0	vP	0.47				0.21
2706-56-1	220-295-1	2-pyridylethylamine	0.39		-2.1	0	n.a.	0.57				0.23
98-32-8	202-657-0	3-amino-4-hydroxybenzenesulphona-mide	0.39		0.1	0	Pot. P/vP	0.37				0.21
63659-18-7	613-310-1	Betaxolol	0.39	1.4	0.4	0	n.a.	0.49			6	0.30
882-09-7	212-925-9	Clofibric acid	0.39		-0.5	0	n.a.	0.49				0.26
6804-07-5	229-879-0	Carbadox	0.38		0.2	0	n.a.	0.36				0.26
95-51-2	202-426-4	2-chloroaniline	0.38		2.0	0	Pot. P/vP	0.31		7		0.29
81-81-2	201-377-6	Warfarin	0.38		1.1	0	P	0.69				0.33
51235-04-2	257-074-4	Hexazinone	0.38		1.4	0	n.a.	0.39				0.25
15686-71-2	239-773-6	Cefalexin	0.38		-1.9	0	n.a.	0.66				0.19
97-39-2	202-577-6	1,3-di-*o*-tolylguanidine	0.38		1.0	0	Potential P/vP++	0.31				0.43

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
50-36-2	200-032-7	Cocaine	0.38	1.4	1.4	0	n.a.	0.65				0.29
51-28-5	200-087-7	2,4-dinitrophenol	0.38	1.1	-1.0	0	Potential P/vP++	0.21			2	0.34
37350-58-6	253-483-7	Metoprolol	0.38	0.7	-0.9	0	n.a.	0.53			6	0.24
85441-61-8	-	Quinapril	0.38		1.1	0	n.a.	0.62				0.29
2163-68-0	-	Hydroxyatrazine	0.38		1.0	0	no conclusion/data	0.44				0.18
152019-73-3	690-353-2	Metolachlor-OA	0.37		-2.2	0	n.a.	0.46			26	0.19
64744-50-9	451-630-1	Gabapentin-lactam	0.37		1.9	0	Pot. P/vP	0.69				0.28
54063-53-5	258-955-6	Propafenone	0.37	2.3	2.1	0	no conclusion/data	0.67				0.35
1093205-95-8	700-837-8	3-hydroxy-2,2-dimethyl-*N*-propylpropa-namide	0.37		0.3	0	no conclusion/data	0.78				0.19
2760-98-7	220-425-7	Isophthalohydrazide	0.37		-1.7	0	no conclusion/data	0.38				0.17
112-49-2	203-977-3	1,2-bis(2-methoxyethoxy)ethane	0.37	-1.3	-0.3	0	no conclusion/data	0.24				0.17
551-92-8	209-001-2	Dimetridazole	0.37	0.1	0.4	0	n.a.	0.35				0.24
116-43-8	204-141-0	Succinylsulfathiazole	0.37		-2.5	0	n.a.	0.52				0.20
164265-78-5	-	Valsartan acid	0.36		-2.4	0	n.a.	0.56				0.21
1231244-60-2	-	Metazachlor OXA	0.36		-1.9	0	n.a.	0.65	89			0.18
100-88-9	202-898-1	*N*-cyclohexylsulphamic acid	0.36		-3.5	0	no conclusion/data	0.50				0.16
55589-62-3	259-715-3	Acesulfame-K	0.36		-0.8	0	n.a.	0.49				0.14
131341-86-1	603-476-3	Fludioxonil	0.36		3.2	0	n.a.	0.62	159			0.55
19988-24-0	-	Atrazin-desethyl-2-hydroxy	0.36		-2.3	0	n.a.	0.47				0.15
36894-69-6	253-258-3	Labetalol	0.36	1.2	2.1	0	Pot. P/vP	0.65				0.27

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
519-09-5	208-263-5	Benzoylecgonine	0.36		0.9	0	n.a.	0.60				0.15
171262-17-2	-	Alachlor OA	0.36		-2.0	0	n.a.	0.47	31			0.18
194992-44-4	-	Acetochlor OA	0.36		-2.4	0	n.a.	0.51	41			0.18
134-62-3	205-149-7	DEET	0.36	1.2	2.3	0	n.a.	0.67	61			0.24
58-25-3	200-371-0	Chlordiazepoxide	0.35	1.8	2.5	0	n.a.	0.30				0.46
121-57-3	204-482-5	Sulphanilic acid	0.35		-6.3	0	Pot. P/vP	0.29				0.15
87-62-7	201-758-7	2,6-xylidine	0.35	1.6	1.7	0	P	0.49		7		0.24
108-62-3	203-600-2	Metaldehyde	0.35		0.5	0	no conclusion/data	0.14	14			0.17
443-48-1	207-136-1	Metronidazole	0.35	-0.5	0.0	0	no conclusion/data	0.45				0.19
526-36-3	208-390-6	Xylometazoline	0.35	2.9	0.3	0	n.a.	0.38				0.57
133-64-2	-	5-Isopropyl-2-methylbenzenesulfonic a-cid	0.35		-5.0	0	n.a.	0.43				0.20
7313-54-4	-	Deisopropylhydroxyatrazine	0.35		-2.9	0	no conclusion/data	0.52				0.14
76-05-1	200-929-3	Trifluoroacetic acid	0.35	-0.8	-6.2	0	Potential P/vP++	0.37	2048			0.16
541-73-1	208-792-1	1,3-dichlorobenzene	0.35	2.4	3.4	68	Potential P/vP++	0.33		71		0.37
96-12-8	202-479-3	1,2-dibromo-3-chloropropane	0.35	2.3	2.9	7	Pot. P/vP	0.32				0.30
2164-08-1	218-499-0	Lenacil	0.35		2.0	0	n.a.	0.42	30			0.22
3930-20-9	-	Sotalol	0.35	-0.9	-0.9	0	n.a.	0.53				0.17
552-79-4	209-022-7	Methylephedrine	0.34		-0.4	0	n.a.	0.52				0.19
114798-26-4	601-329-8	Losartan	0.34		1.8	0	Potential P/vP++	0.28				0.39
103-83-3	203-149-1	Benzyldimethylamine	0.34	1.1	0.3	0	Not P	0.47				0.23

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
314-40-9	206-245-1	Bromacil	0.34	1.6	-0.6	0	no conclusion/data	0.31				0.24
25321-41-9	246-839-8	Dimethylbenzene sulfonic acid	0.34		-5.5	0	n.a.	0.49				0.17
665-66-7	211-560-2	Amantadine hydrochloride	0.34	1.6	-0.4	0	P	0.55				0.22
31431-39-7	250-635-4	Mebendazole	0.34		2.7	0	n.a.	0.47				0.34
27213-90-7	248-326-4	Diisobutylnaphthalenesulphonate	0.34	1.8	-1.1	0	P	0.24				0.35
121-82-4	204-500-1	Perhydro-1,3,5-trinitro-1,3,5-triazine	0.34	2.0	-2.7	0	Potential P/vP++	0.42				0.21
83-07-8	201-452-3	4-Aminoantipyrine	0.34	-0.3	1.2	0	n.a.	0.57				0.16
483-63-6	207-596-3	Crotamiton	0.33		2.5	0	n.a.	0.63				0.26
87333-19-5	642-904-3	Ramipril	0.33		1.3	0	n.a.	0.66				0.21
25057-89-0	246-585-8	Bentazone	0.33		0.4	0	n.a.	0.38	18			0.23
138402-11-6	604-078-2	Irbesartan	0.33		1.7	0	n.a.	0.36				0.52
791-28-6	212-338-8	Triphenylphosphine oxide	0.33	1.4	3.5	0	Pot. P/vP	0.54				0.24
70-55-3	200-741-1	Toluene-4-sulphonamide	0.33	0.3	0.9	0	Not P	0.53				0.19
5440-00-6	226-621-9	5,6-Diamino-1,3-Dimethyluracil	0.33		-2.0	0	n.a.	0.59				0.13
1707-03-5	216-948-5	Diphenylphosphinic acid	0.33		-2.4	0	n.a.	0.56				0.18
72-44-6	200-780-4	Methaqualone	0.33		2.5	0	n.a.	0.56				0.33
75-65-0	200-889-7	2-methylpropan-2-ol	0.33	-0.3	0.6	3	Potential P/vP++	0.60				0.15
80-39-7	232-465-2	*N*-ethyl-*o*-toluenesulphonamide	0.33		1.6	0	no conclusion/data	0.50	6			0.22
92-41-1	202-154-6	Naphthalene-2,7-disulfonic acid	0.33		-6.4	0	n.a.	0.24				0.14
102-06-7	203-002-1	1,3-diphenylguanidine	0.33	2.5	0.2	0	Potential P/vP++	0.46				0.25

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
479-92-5	207-539-2	Propyphenazone	0.32		2.5	0	n.a.	0.48				0.20
60-80-0	200-486-6	Phenazone	0.32	-0.8	1.4	0	Potential P/vP++	0.54				0.16
23031-25-6	245-385-8	Terbutaline	0.32	-0.9	-1.2	0	n.a.	0.66				0.17
298-46-4	206-062-7	Carbamazepine	0.32	2.4	2.2	0	n.a.	0.40				0.22
13523-86-9	236-867-9	Pindolol	0.32	1.4	0.1	0	n.a.	0.66				0.17
2465-59-0	219-570-9	Oxypurinol	0.32		-2.1	0	n.a.	0.52				0.13
123732-85-4	-	Propachlor ESA	0.32		-2.9	0	n.a.	0.59				0.16
1418095-19-8	-	Metolachlor NOA 413173	0.32		-4.4	0	n.a.	0.59				0.15
81-07-2	201-321-0	Saccharin	0.32		-4.0	0	Potential P/vP++	0.47	41			0.16
18559-94-9	242-424-0	Salbutamol	0.31	-0.9	-1.0	0	Potential P/vP++	0.68				0.14
15763-76-5	239-854-6	Sodium p-cumenesulphonate	0.31		-4.8	0	Not P	0.41				0.15
34123-59-6	251-835-4	Isoproturon	0.31	1.7	2.6	0	n.a.	0.46	12			0.23
111-96-6	203-924-4	Bis(2-methoxyethyl) ether	0.31	-1.2	-0.2	0	vP	0.33			26	0.13
4710-17-2	225-198-8	DMSA (Dichlofluanid metabolite)	0.31		1.4	0	n.a.	0.53	5			0.17
41394-05-2	255-349-3	Metamitron	0.31	0.8	0.8	0	n.a.	0.45	16			0.17
1125-21-9	214-406-2	Ketoisophorone	0.31		1.2	0	Not P	0.51				0.27
57775-29-8	260-945-1	Carazolol	0.31	2.6	1.3	0	n.a.	0.60				0.23
10605-21-7	234-232-0	Carbendazim	0.31	1.0	0.7	0	Pot. P/vP	0.51				0.19
3768-63-6	-	Tetramethylsulfamide	0.31		0.2	0	n.a.	0.51				0.13
34123-57-4	621-315-5	Isoproturon-monodemethyl	0.31		2.3	0	n.a.	0.49	13			0.21

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
1115-70-4	214-230-6	Metformin hydrochloride	0.30		-3.9	0	P	0.56				0.12
104-15-4	203-180-0	Toluene-4-sulphonic acid	0.30		-5.5	0	Not P	0.48				0.13
58955-93-4	-	10,11-Dihydro-10,11-Dihydroxy Carbamazepine	0.30		-0.3	0	n.a.	0.58				0.11
56-93-9	200-300-3	Benzyltrimethylammonium chloride	0.30		-2.7	0	Potential P/vP++	0.59				0.13
18691-97-9	242-505-0	Methabenzthiazuron	0.30		2.4	0	n.a.	0.41				0.21
333-41-5	206-373-8	Diazinon	0.30	2.7	3.8	0	n.a.	0.57	17	71		0.32
2634-33-5	220-120-9	1,2-benzisothiazol-3(2*H*)-one	0.30	1.0	0.8	0	Pot. P/vP	0.53				0.13
80-05-7	201-245-8	4,4'-isopropylidenediphenol	0.30	2.6	3.5	0	Not P	0.47				0.27
28657-80-9	249-133-8	Cinoxacin	0.30	0.5	-2.2	0	n.a.	0.77				0.14
2163-69-1	218-493-8	Cycluron	0.29		2.4	0	n.a.	0.48				0.18
17675-60-4	241-659-6	Amidinourea phosphate	0.29		-1.7	0	Pot. P/vP	0.61				0.10
130-14-3	204-976-0	Sodium naphthalene-1-sulphonate	0.29	1.3	-5.2	0	no conclusion/data	0.38				0.13
55-52-7	200-236-6	Pheniprazine	0.29		0.6	0	n.a.	0.49				0.15
1223748-39-7	-	3-[4-(Methoxycarbonyl)phenyl]-1-propanesulfonic acid	0.29		-3.2	0	n.a.	0.65				0.13
80-09-1	201-250-5	4,4'-sulphonyldiphenol	0.29	2.3	1.2	0	Pot. P/vP	0.52				0.18
3984-14-3	818-440-4	DMS (*N*,*N*-dimethylsulfamide)	0.29		-0.6	0	n.a.	0.57				0.11
332927-03-4	629-212-7	Acridin-9-carbonic acid	0.29		-0.5	0	n.a.	0.64				0.16
36993-94-9	-	Metamitron-Desamino	0.29		0.9	0	n.a.	0.64				0.18
132-57-0	205-066-6	7-hydroxynaphthalene-1-sulphonic acid	0.29		-3.6	0	no conclusion/data	0.43				0.12

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
93-01-6	202-209-4	6-hydroxynaphthalene-2-sulphonic acid	0.29		-3.5	0	Pot. P/vP	0.43				0.12
84-87-7	201-568-4	4-hydroxynaphthalene-1-sulphonic acid	0.29		-3.9	0	Pot. P/vP	0.43				0.12
58-61-7	200-389-9	Adenosine	0.29	-1.1	-1.1	0	Not P	0.38				0.11
22504-72-9	245-045-9	*N*,*N*'-dimethylsulfamide	0.29		-0.5	0	n.a.	0.57				0.11
98-95-3	202-716-0	Nitrobenzene	0.28	1.7	1.8	3	Potential P/vP++	0.45		71		0.17
1066-51-9	623-325-5	(aminomethyl)phosphonic Acid	0.28		-4.8	0	n.a.	0.66	85			0.10
5142-23-4	225-908-6	3-Methyladenine	0.28		-2.2	0	n.a.	0.52				0.13
92-27-3	202-142-0	6,7-Dihydroxy-2-naphthalenesulfonic a-cid	0.28		-3.4	0	n.a.	0.47				0.11
120-18-3	204-375-3	Naphthalene-2-sulphonic acid	0.28		-5.0	0	Pot. P/vP	0.38				0.13
2682-20-4	220-239-6	2-methyl-2*H*-isothiazol-3-one	0.28		-0.2	0	Not P	0.59				0.11
79-43-6	201-207-0	Dichloroacetic acid	0.28	0.4	-3.5	0	Not P	0.45				0.11
114-83-0	204-055-3	AMPH	0.28		0.9	0	n.a.	0.50				0.12
2212-67-1	218-661-0	Molinat	0.28	2.0	2.8	0	n.a.	0.58			8	0.19
60142-95-2	262-075-8	Gabapentin hydrochloride	0.28		-1.8	0	Pot. P/vP	0.69				0.09
1066-42-8	213-915-7	Dimethylsilanediol	0.28		-0.1	0	no conclusion/data	0.63				0.09
1068-90-2	213-952-9	Diethyl acetamidomalonate	0.28		-1.0	0	no conclusion/data	0.92				0.11
2465-65-8	-	*O*,*O*-Diethyl thiophosphate	0.27		-1.2	0	n.a.	0.51				0.15
29878-31-7	249-921-1	4-Methylbenzotriazole	0.27		1.9	0	n.a.	0.60				0.15
136-85-6	205-265-8	6-methylbenzotriazole	0.27		1.3	0	no conclusion/data	0.60				0.15
85-98-3	201-645-2	1,3-diethyldiphenylurea	0.27	2.5	3.4	0	Pot. P/vP	0.53				0.24

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
537-46-2	208-668-7	Methamphetamine	0.27	1.1	-0.6	0	n.a.	0.61			141	0.14
148-79-8	205-725-8	Thiabendazole	0.26		2.4	0	n.a.	0.45	22			0.18
55406-53-6	259-627-5	Iodopropynyl butylcarbamate	0.26	1.8	2.4	0	no conclusion/data	0.51				0.15
123-91-1	204-661-8	1,4-dioxane	0.26		-0.3	0	vP	0.43			23	0.09
2749-59-9	220-389-2	2,4-dihydro-2,5-dimethyl-3H-pyrazol-3-one	0.26		-0.0	0	no conclusion/data	0.60				0.10
108-79-2	203-617-5	4,6-dimethyl-2-hydroxypyrimidine	0.26		-0.3	0	n.a.	0.57				0.11
137862-53-4	604-045-2	Valsartan	0.26		-1.5	0	n.a.	0.50				0.14
95-16-9	202-396-2	Benzothiazole	0.26	1.3	2.1	1	Pot. P/vP	0.57				0.12
603-52-1	210-047-0	Ethyl diphenylcarbamate	0.25		3.3	0	no conclusion/data	0.57				0.23
10338-69-9	676-256-8	4-phenyl-1,2,3,6-tetrahydropyridine	0.25		-0.2	0	n.a.	0.65				0.12
78-40-0	201-114-5	Triethyl phosphate	0.25	-0.3	0.9	0	Potential P/vP++	0.71				0.10
108-80-5	203-618-0	Cyanuric acid	0.24	1.7	-1.3	0	vP	0.55				0.12
95-14-7	202-394-1	1*H*-benzotriazole	0.24	1.5	1.0	0	vP	0.60				0.11
1333-16-0	908-912-9	2,2'-Methylenediphenol	0.24		3.0	0	Pot. P/vP	0.60			4	0.16
288-88-0	206-022-9	1,2,4-triazole	0.24		-0.5	0	P	0.59				0.08
108-20-3	203-560-6	Diisopropyl ether	0.24		1.7	66	Potential P/vP++	0.41			10	0.10
22071-15-4	244-759-8	Ketoprofen	0.23		0.1	0	no conclusion/data	0.60				0.11
119-61-9	204-337-6	Benzophenone	0.23	2.7	3.0	0	Potential P/vP++	0.65				0.15
84-65-1	201-549-0	Anthraquinone	0.22	3.0	3.3	0	Not P	0.48				0.21
14260-98-1	238-141-7	2-Butoxyethyl dihydrogenphosphate	0.22		-3.3	0	n.a.	0.43				0.08

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
23386-52-9	245-629-3	Sodium 1,4-dicyclohexyl sulphonatosuccinate	0.21		-3.9	0	P	0.72				0.13
140-60-3	205-422-0	4-Decylbenzenesulfonic acid	0.20		0.5	0	n.a.	0.46				0.12
82571-53-7	919-112-4	Ozagrel	0.20		-1.8	0	n.a.	0.51				0.07
84238-45-9	282-500-0	Benzenesulfonic acid, 4-dodecyl-	0.19		1.2	0	Not P	0.45				0.14
3622-84-2	222-823-6	*N*-butylbenzenesulphonamide	0.18		1.8	0	vP	0.59				0.08
924-16-3	213-101-1	*N*-Nitrosodibutylamin	0.18	1.6	2.5	0	n.a.	0.49				0.07
67-43-6	200-652-8	DTPA	0.16		-8.4	0	vP	0.44				0.03
60-00-4	200-449-4	Edetic acid	0.13		-6.8	0	Pot. P/vP	0.53				0.02
538-75-0	208-704-1	Dicyclohexylcarbodiimide	0.11		3.3	1	Potential P/vP++	0.49				0.19

Table 3: Prioritized contaminants for conducting a “cold” degradation test according to OECD TG 309, sorted by descending vPvM score, part 2

Category B: contaminants that have so far only been detected in wastewater treatment plant effluent and/or surface water

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
1404-90-6	215-772-6	Vancomycin	0.94		-6.9	0	n.a.	0.59				1.00
100986-85-4	-	Levofloxacin	0.86		-4.0	0	n.a.	0.04				0.93
59017-64-0	927-786-6	Ioxaglic acid	0.86		-2.2	0	Pot. P/vP	-1.09				1.00
113617-63-3	638-855-2	Orbifloxacin	0.85		-0.4	0	n.a.	-0.23				0.99
115550-35-1	640-416-5	Marbofloxacin	0.85		-1.3	0	n.a.	0.11				0.86
20830-75-5	244-068-1	Digoxin	0.85		1.3	0	n.a.	-0.02				0.87
79356-08-4	635-502-4	Maduramycin	0.85		1.4	0	n.a.	-0.82				1.00
112811-59-3	664-293-2	Gatifloxacin	0.82		-3.1	0	n.a.	0.14				0.86
66-28-4	200-626-6	Strophanthidin	0.82		0.7	0	n.a.	0.66				0.85
3089-11-0	221-422-3	Hexa(methoxymethyl)melamine	0.81		1.4	0	n.a.	-0.28				0.97
90566-53-3	-	Fluticasone	0.80		2.4	0	n.a.	0.16				0.93
3576-88-3	222-695-1	Melam	0.80		-0.6	0	vP	-0.03				0.93
97240-79-4	619-263-3	Topiramate	0.80		0.7	0	n.a.	-0.13				0.86
2276-90-6	218-897-4	Iotalamic acid	0.79		-1.4	0	Pot. P/vP	-0.32				0.89
73384-59-5	277-405-6	Ceftriaxone	0.78		-2.5	0	n.a.	0.22				0.67
76-42-6	200-960-2	Oxycodone	0.77	-0.4	0.2	0	n.a.	0.30				0.91
5250-39-5	-	Flucloxacillin	0.76		-1.3	0	n.a.	0.15				0.92
965-52-6	226-051-0	Nifuroxazide	0.76		-1.3	0	n.a.	0.15				0.92
13292-46-1	236-312-0	Rifampicin	0.75		1.5	0	n.a.	0.15				0.96

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
69377-81-7	-	Fluroxypyr	0.75		-2.4	0	n.a.	0.09	14			0.85
66258-76-2	262-811-8	Piperacillin	0.75		-1.4	0	n.a.	0.55				0.69
100286-90-6	691-567-9	Irinotecan	0.75		-0.2	0	n.a.	0.22				0.95
486460-32-6	690-730-1	Sitagliptin	0.74		-0.1	0	Pot. P/vP	-0.26				1.00
173159-57-4	605-666-1	Foramsulfuron	0.74		-1.0	0	n.a.	0.57	6			0.75
33069-62-4	-	Paclitaxel	0.73		2.5	0	n.a.	0.57				0.96
23893-13-2	-	Anhydroerythromycin	0.73		1.7	0	n.a.	-0.28				0.98
33419-42-0	251-509-1	Etoposide	0.72		0.6	0	n.a.	0.37				0.68
83799-24-0	801-893-7	Fexofenadine	0.72		3.1	0	Pot. P/vP	0.23				0.75
28797-61-7	249-228-4	Pirenzepine	0.72	-0.3	-0.1	0	Pot. P/vP	0.23				0.92
124-94-7	204-718-7	Triamcinolone	0.71	0.2	0.7	0	n.a.	0.34				0.79
53-03-2	200-160-3	Prednisone	0.71	0.7	1.6	0	n.a.	0.31				0.81
2135-17-3	218-370-9	Flumetasone	0.71		1.5	0	Pot. P/vP	0.27				0.88
83881-51-0	695-115-1	Cetirizine	0.71		-0.9	0	n.a.	0.11				0.73
71675-85-9	275-831-7	Amisulpride	0.71		-1.2	0	n.a.	0.27				0.80
1918-02-1	217-636-1	Picloram	0.71		0.2	0	n.a.	0.17				0.85
108050-54-0	639-676-2	Tilmicosin	0.70		0.1	0	n.a.	-0.15				0.94
35607-66-0	252-641-2	Cefoxitin	0.70		-3.0	0	n.a.	0.36				0.61
50-02-2	200-003-9	Dexamethasone	0.70		1.8	0	n.a.	0.28				0.86
378-44-9	206-825-4	Betamethasone	0.70		1.8	0	Pot. P/vP	0.28				0.86

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
82097-50-5	617-298-9	Triasulfuron	0.70		-1.4	0	n.a.	0.33	43			0.88
24560-70-1	-	Ethinylestradiol-3-sulfate	0.70		-0.3	0	n.a.	0.18				0.85
158062-67-0	605-127-0	Flonicamid	0.70		0.4	0	n.a.	0.38	2			0.83
127-33-3	200-592-2	Demeclocycline hydrochloride	0.69		-1.5	0	n.a.	0.34				0.74
36749-35-6	-	Deethylcyanazine acid	0.69		-4.5	0	n.a.	0.18				0.65
43200-80-2	256-138-9	Zopiclone	0.69	1.0	1.0	0	n.a.	0.15				0.92
129618-40-2	-	Nevirapine	0.69	1.5	2.0	0	n.a.	0.25				0.84
68-88-2	200-693-1	Hydroxyzine	0.69	2.2	2.7	0	n.a.	0.13				0.83
2013-58-3	217-938-3	Meclocycline	0.68		-1.5	0	n.a.	0.33				0.76
139-91-3	205-384-5	Furaltadone	0.68		-2.3	0	n.a.	0.06				0.70
61-72-3	200-514-7	Cloxacillin	0.68		-1.2	0	n.a.	0.38				0.74
76639-94-6	620-107-1	Florfenicol	0.67		0.6	0	n.a.	0.32				0.61
51333-22-3	257-161-7	Budesonide	0.66	2.2	2.4	0	n.a.	0.19				0.81
53-06-5	200-006-5	Cortisone	0.66	1.1	1.1	0	n.a.	0.34				0.87
2479-86-9	-	Androsterone sulfate	0.66		-1.0	0	n.a.	0.22				0.77
125-28-0	204-732-3	dihydrocodeine	0.66	0.8	0.2	0	n.a.	0.50				0.71
50-23-7	200-020-1	Hydrocortisone	0.66		1.7	0	Not P	0.37				0.71
34084-50-9	690-803-8	7-aminoflunitrazepam	0.66		1.9	0	n.a.	0.14				0.75
113844-99-8	-	Torasemide carbonic acid	0.65	2.4	-1.3	0		0.20				0.66
50-24-8	200-021-7	Prednisolone	0.65		1.6	0	Potential P/vP++	0.36				0.71

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
83-43-2	201-476-4	Methylprednisolone	0.65	0.9	1.7	0	n.a.	0.33				0.73
73-48-3	200-800-1	Bendroflumenthiazide	0.65	1.3	1.1	0	n.a.	0.04				0.92
98319-26-7	620-534-3	Finasteride	0.65		2.9	0	n.a.	0.30				0.90
25614-03-3	247-128-5	Bromocriptine	0.65		3.0	0	n.a.	0.03				1.00
35689-59-9	252-677-9	Doxycycline	0.64		-1.7	0	Pot. P/vP	0.41				0.61
120983-64-4	691-449-7	Prothioconazole-desthio	0.64		3.3	0	n.a.	0.15	21			0.90
303-81-1	216-023-6	Novobiocin	0.64		0.5	0	n.a.	0.30				0.90
66215-27-8	266-257-8	Cyromazine	0.64	0.2	0.4	0	n.a.	0.16	28		141	0.60
69477-29-8	614-977-1	2,6-bis-(Diethanolamino)-4,8-dipi-peridinopyrimido-(5,4-d)-pyrimi-dine, tosylat salt	0.64	1.1	1.6	0	Pot. P/vP	0.21				0.88
364-62-5	206-662-9	Metoclopramide	0.63	1.7	-0.4	0	Pot. P/vP	0.26				0.83
51481-65-3	257-233-8	Mezlocillin	0.63		-1.7	0	n.a.	0.44				0.68
6331-96-0	700-413-2	2-amino-4,5-dichlorobenzenesul-fonic acid	0.63		-4.7	0	Potential P/vP++	0.13				0.54
887-54-7	-	Dacthal monoacid	0.63		0.0	0	n.a.	0.30			7	0.79
676228-91-4	-	Thiacloprid amide	0.63		0.7	0	n.a.	0.21				0.60
27314-13-2	248-397-1	Norflurazon	0.63		2.9	0	n.a.	0.18				0.81
59-05-2	200-413-8	Methotrexate	0.63		-4.8	0	n.a.	0.15				0.47
126-07-8	204-767-4	Griseofulvin	0.62		2.5	0	n.a.	0.35				0.86
81403-80-7	617-230-8	Alfuzosin	0.62		1.1	0	Pot. P/vP	0.23				0.86
42028-21-7	-	Estriol-17-sulfate	0.62		-0.9	0	n.a.	0.36				0.55

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
211914-51-1	859-177-5	Dabigatran	0.62		0.1	0		0.19				0.65
76963-41-2	627-310-4	Nizatidine	0.61	-0.9	-0.7	0	n.a.	0.27				0.54
438-67-5	207-120-4	Estrone-3-sulfate	0.61		-1.1	0	n.a.	0.25				0.71
29094-61-9	249-427-6	Glipizide	0.61		0.1	0	n.a.	0.38				0.73
23214-92-8	245-495-6	Doxorubicin	0.61		0.3	0	n.a.	0.31				0.72
918-00-3	620-529-6	1,1,1-Trichloro-2-propanone	0.61		1.7	10	n.a.	0.28				0.67
125-29-1	204-733-9	Hydrocodone	0.60		0.5	0	n.a.	0.39				0.82
4205-90-7	224-119-4	Clonidine	0.60		1.3	0	n.a.	0.17				0.63
79277-27-3	616-673-4	Thifensulfuron-methyl	0.60		0.1	0	n.a.	0.42	9			0.66
126535-15-7	603-146-9	Triflusulfuron-methyl	0.60		1.6	0	n.a.	0.15	10			0.98
18323-44-9	242-209-1	Clindamycin	0.60		1.8	0	n.a.	0.30				0.55
503612-47-3	639-684-6	Apixaban	0.60		2.1	0		0.59				0.80
54143-55-4	685-650-9	Flecainide	0.59	1.6	1.8	0	Pot. P/vP	0.23				0.98
25122-46-7	246-634-3	Clobetasol	0.59		3.3	0	n.a.	0.24				0.95
481-95-8	-	Estriol-3-sulfate	0.59		-1.3	0	n.a.	0.40				0.47
466-99-9	207-383-5	Hydromorphone	0.59		-0.5	0	n.a.	0.34				0.73
37148-27-9	253-366-0	Clenbuterol	0.59		0.3	0	n.a.	0.20				0.73
848-75-9	212-700-5	Lormetazepam	0.59	1.9	3.0	0	n.a.	0.32				0.63
83066-88-0	617-435-2	Fluazifop-P	0.58	1.6	-2.8	0	no conclusion/data	0.29	12			0.74
34205-21-5	251-879-4	Dimefuron	0.58		1.9	0	n.a.	0.17				0.71

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
606-17-7	210-105-5	Iodipamide	0.58		1.1	0	n.a.	-1.14				1.00
55335-06-3	259-597-3	Triclopyr	0.58		1.2	0	n.a.	0.28	24			0.66
26839-75-8	248-032-6	Timolol	0.58		-0.6	0	n.a.	0.28				0.63
481-96-9	-	Estradiol-3-sulfate	0.58		-0.5	0	n.a.	0.32				0.57
18683-91-5	242-500-3	Ambroxol	0.58		1.6	0	Pot. P/vP	0.25				0.63
773058-82-5	415-180-1	Seroquel	0.58	1.8	2.6	0	no conclusion/data	0.21				0.55
110488-70-5	613-102-0	Dimethomorph(E)	0.58		2.4	0	n.a.	0.36	44			0.76
133-90-4	205-123-5	Chloramben (Amiben)	0.57		-1.9	0	n.a.	0.29			2	0.52
68-96-2	200-699-4	21-alpha-hydroxyprogesterone	0.57		3.2	0	n.a.	0.24				0.85
87848-99-5	618-080-6	Acrivastine	0.57		2.0	0	n.a.	0.25				0.55
61337-67-5	288-060-6	Mirtazapine	0.57	2.1	1.5	0	n.a.	0.14				0.84
21593-23-7	244-466-5	Cefapirin	0.57		-4.3	0	no conclusion/data	0.63				0.38
50-18-0	200-015-4	Cyclophosphamide	0.57		0.6	0	n.a.	0.29				0.52
66-79-5	200-635-5	Oxacillin	0.57		-1.3	0	n.a.	0.57				0.50
80-32-0	201-269-9	Sulfachloropyridazine	0.56		-0.7	0	n.a.	0.17				0.56
208465-21-8	606-653-3	Mesosulfuron-methyl	0.56		2.0	0	n.a.	0.50	35			0.66
976-71-6	213-554-5	Canrenone	0.56		2.5	0	n.a.	0.34				0.78
36322-90-4	252-974-3	Piroxicam	0.56	1.5	1.9	0	n.a.	0.23				0.54
4394-00-7	224-516-2	Niflumic acid	0.56	2.5	2.1	0	Pot. P/vP	0.17				0.84
5355-16-8	226-333-3	Diaveridin	0.56		0.6	0	n.a.	0.37				0.62

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
53774-07-5	-	Bifenox-acid	0.56		0.6	0	n.a.	0.24	43		7	0.78
68-89-3	256-627-7	Metamizole	0.56		-7.4	0	n.a.	0.43				0.36
139755-83-2	604-158-7	Sildenafil	0.56		1.6	0	no conclusion/data	0.09				0.91
3778-73-2	223-237-3	Ifosfamide	0.56		0.8	0	n.a.	0.29				0.52
2152-44-5	218-439-3	Betamethasone 17-Valerate	0.56		3.4	0	n.a.	0.39				0.73
75277-39-3	278-169-7	HEPES sodium salt	0.56		-4.7	0	Pot. P/vP	0.49				0.33
28159-98-0	248-872-3	Irgarol	0.56	2.6	3.0	0	n.a.	0.14				0.79
520-85-4	208-298-6	Medroxyprogesterone	0.56	2.6	3.6	0	n.a.	0.22				0.86
58-94-6	200-404-9	Chlorothiazide	0.55	-1.1	-0.7	0	n.a.	0.24				0.47
23950-58-5	245-951-4	Pronamide	0.55		3.4	0	n.a.	0.26				0.76
81335-37-7	-	Imazaquin	0.55		-1.0	0	n.a.	0.55	83			0.48
96525-23-4	619-224-0	Flurtamone	0.55		2.0	0	n.a.	0.17	13			0.76
54739-18-3	611-193-1	Fluvoxamine	0.55	2.0	2.3	0	n.a.	0.18				0.74
132539-06-1	-	Olanzapine	0.55	1.9	1.7	0	n.a.	0.15				0.70
56980-93-9	260-497-7	Celiprolol	0.55	0.6	0.8	0	n.a.	0.47				0.54
287714-41-4	689-191-5	Rosuvastatin	0.55		-0.8	0	n.a.	0.20				0.47
113096-99-4	619-020-1	Cyproconazole	0.55	2.2	3.0	0	n.a.	0.22	111			0.64
55268-75-2	259-560-1	Cefuroxime	0.54	-0.5	-3.9	0	n.a.	0.57				0.36
177406-68-7	605-799-5	Benthiavalicarb-isopropyl	0.54		1.2	0	n.a.	0.04				0.77
1622-61-3	216-596-2	Clonazepam	0.54	1.8	2.5	0	n.a.	0.21				0.69

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
85509-19-9	617-717-5	Flusilazole	0.54	3.0	3.9	0	n.a.	-0.01				0.89
36734-19-7	253-178-9	Iprodione	0.54		1.5	0	n.a.	0.16	22			0.70
564-35-2	-	11-Ketotestosterone	0.54		2.4	0	n.a.	0.37				0.57
53179-11-6	258-416-5	Loperamide	0.54	2.7	2.7	0	vP	0.13				0.97
60168-88-9	262-095-7	Fenarimol	0.54		3.3	0	n.a.	0.15				0.82
132-22-9	205-054-0	Chlorphenamine	0.54	2.2	1.3	0	n.a.	0.17				0.82
153719-23-4	428-650-4	Thiamethoxam DP	0.54		-1.5	0	n.a.	0.17				0.47
2164-17-2	218-500-4	Fluometuron	0.53	1.5	2.4	0	Pot. P/vP	0.22	98			0.61
60282-87-3	262-145-8	Gestoden	0.53		2.8	0	n.a.	0.26				0.69
106133-20-4	600-716-9	Tamsulosin	0.53		0.9	0	n.a.	0.58				0.68
73986-53-5	-	*O*-Desmethyltramadol	0.53		0.3	0	n.a.	0.28				0.56
59729-33-8	261-891-1	Citalopram	0.53	2.4	1.8	0	Pot. P/vP	0.03				0.93
23103-98-2	245-430-1	Pirimicarb	0.53	1.0	1.7	0	n.a.	0.35	48			0.57
13311-84-7	236-341-9	Flutamide	0.53	2.4	3.1	0	n.a.	0.15				0.82
38345-66-3	253-893-6	Chirald	0.52		1.0	0	n.a.	0.29				0.68
137-88-2	221-272-9	Amprolium	0.52		0.0	0	n.a.	0.29				0.44
6104-71-8	636-421-7	*N*-Desmethylclozapine	0.52		0.8	0	n.a.	0.20				0.59
647-29-0	-	PFOSi	0.52	2.6	-2.4	1	n.a.	-0.14				1.00
71758-44-6	-	2-(2-(Chlorophenyl)amino)benzal-dehyde	0.52		3.4	0	n.a.	0.10				0.77
119446-68-3	601-613-1	Difenoconazol I	0.52		3.4	0	n.a.	0.04	148			0.91

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
673-04-1	211-601-4	Simeton	0.52	0.6	2.3	0	n.a.	0.28				0.59
3572-43-8	222-684-1	Bromhexine	0.52		2.6	0	Pot. P/vP	0.09				0.88
1014-70-6	213-801-7	Simetryn	0.51	1.7	2.7	0	n.a.	0.21				0.58
73590-58-6	615-996-8	Omeprazole	0.51		2.2	0	Pot. P/vP	0.48				0.76
102625-70-7	600-331-6	Pantoprazole	0.51		1.4	0	Pot. P/vP	0.49				0.76
335104-84-2	608-879-8	Tembotrione	0.51		-0.6	0	n.a.	0.04	14			0.95
87392-12-9	618-004-1	S-Metolachlor	0.51		3.2	0	n.a.	0.29	11	71		0.60
7206-76-0	230-583-9	2-ethyl-2-phenylmalonamide	0.51		-0.3	0	n.a.	0.70				0.38
52-53-9	200-145-1	Verapamil	0.51	2.7	2.5	0	n.a.	0.54				0.96
61869-08-7	-	Paroxetine	0.51		1.9	0	n.a.	0.21				0.80
53994-73-3	258-909-5	Cefaclor	0.50		-2.5	0	n.a.	0.62				0.33
28981-97-7	249-349-2	Alprazolam	0.50	1.8	2.4	0	n.a.	0.30				0.54
135590-91-9	603-923-2	Mefenpyr-diethyl	0.50	2.8	4.3	0	Pot. P/vP	0.43				0.71
514-65-8	208-184-6	Biperiden	0.50	2.9	2.1	0	n.a.	0.25				0.69
139528-85-1	604-145-6	Metosulam	0.50		2.1	0	n.a.	0.25	10			0.89
38649-73-9	801-861-2	Talinolol	0.50		1.6	0	n.a.	0.49				0.50
10418-03-8	233-894-8	Stanozolol	0.50		3.5	0	n.a.	0.18				0.89
55219-65-3	259-537-6	Triadimenol	0.50	2.3	3.0	0	n.a.	0.35	74			0.56
71125-39-8	-	Meloxicam	0.50		1.8	0	n.a.	0.27				0.46
81777-89-1	617-258-0	Clomazone	0.50		2.5	0	n.a.	0.24	44			0.54

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
396-01-0	206-904-3	Triamterene	0.50	0.6	1.0	0	n.a.	0.11				0.54
2536-31-4	219-800-8	Chlorflurecol-methyl ester	0.49		2.2	0	n.a.	0.40				0.49
1867-66-9	217-484-6	Ketamine hydrochloride	0.49		1.6	0	no conclusion/data	0.33				0.54
599-79-1	209-974-3	Sulfasalazine	0.49		-2.3	0	n.a.	0.27				0.38
5902-51-2	227-595-1	Terbacil	0.49		0.3	0	n.a.	0.28				0.47
78-44-4	201-118-7	Carisoprodol	0.49	0.4	1.9	0	n.a.	0.40				0.49
90717-03-6	402-790-6	Quinmerac	0.49		-1.8	0	no conclusion/data	0.56	41			0.33
125-73-5	204-754-3	Dextrorphan	0.48		1.6	0	n.a.	0.27				0.63
169590-42-5	685-962-5	Celecoxib	0.48	3.0	3.2	0	n.a.	0.13				0.86
107868-30-4	643-090-2	Exemestane	0.48		3.3	0	n.a.	0.29				0.68
31430-15-6	250-624-4	Flubendazole	0.48		2.5	0	n.a.	0.15				0.71
125-71-3	204-752-2	Dextromethorphan	0.48		2.0	0	n.a.	0.30				0.73
210880-92-5	433-460-1	Clothianidin	0.48		0.0	0	no conclusion/data	0.27				0.39
122-16-7	-	Sulfanitran	0.48		1.9	0	n.a.	0.25				0.56
123312-89-0	602-927-1	Pymetrozin	0.48	1.0	0.2	0	n.a.	0.33	6			0.34
846-48-0	212-686-0	Boldenone	0.47		2.7	0	Not P	0.35				0.52
16773-42-5	240-826-0	Ornidazole	0.47		0.6	0	n.a.	0.30				0.38
1852-43-3	-	Androsterone-glucuronide	0.47		-1.4	0	n.a.	0.30				0.31
103577-45-3	627-144-2	Lansoprazole	0.47	1.9	2.6	0	n.a.	0.15				0.93
53003-10-4	258-290-1	Salinomycin	0.46		3.5	0	n.a.	-0.22				0.97

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
141854-21-9	-	4’-*O*-demethyl-PPZ sulfide	0.46		2.0	0		0.31				0.46
111988-49-9	601-147-9	Thiacloprid	0.46		1.3	0	n.a.	0.23				0.57
1180-25-2	634-203-6	Testosterone glucuronide	0.46		-1.3	0	n.a.	0.30				0.30
74222-97-2	277-780-6	Sulfometuron-methyl	0.46		-1.4	0	n.a.	0.51				0.43
19044-88-3	242-777-0	Oryzalin	0.46		2.1	0	n.a.	0.02	85			0.82
1639-60-7	207-420-5	Dextropropoxyphene hydrochlo-ride	0.46		2.8	0	n.a.	0.46				0.67
638-73-3	-	Chlorodiiodomethane	0.46		2.1	21	n.a.	0.24				0.46
437-38-7	207-113-6	Fentanyl	0.46	2.6	3.4	0	n.a.	0.48				0.65
136470-78-5	620-487-9	Abacavir	0.46		1.4	0	n.a.	0.23				0.38
152-62-5	205-806-8	Dydrogesterone	0.46		3.3	0	n.a.	0.28				0.71
626-43-7	210-948-9	3,5-dichloroaniline	0.46	2.2	2.9	0	Pot. P/vP	0.22	28		58	0.51
135062-02-1	629-921-1	Repaglinide	0.46		3.0	0	n.a.	0.49				0.82
846-50-4	212-688-1	Temazepam	0.46	2	2.2	0	n.a.	0.54				0.38
26225-79-6	247-525-3	Ethofumesate	0.46		2.4	0	n.a.	0.27	9			0.51
93479-97-1	642-919-5	Glimepiride	0.46		-0.1	0	n.a.	0.18				0.71
127-71-9	204-859-4	Sulfabenzamide	0.46	1.6	-0.9	0	n.a.	0.29				0.36
57-42-1	200-329-1	Pethidine	0.46	1.5	1.1	0	no conclusion/data	0.55				0.46
57-67-0	200-345-9	Sulfaguanidine	0.45	-0.9	-0.9	0	no conclusion/data	0.28				0.28
25451-15-4	247-001-4	Felbamate	0.45	0.4	0.5	0	n.a.	0.57				0.32
23696-28-8	245-832-7	Olaquindox	0.45		-0.2	0	n.a.	0.64				0.24

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
2479-90-5	-	Estrone glucuronide	0.45		-1.4	0	n.a.	0.48				0.27
104206-82-8	600-533-4	Mesotrione	0.45	-0.0	-0.7	0	n.a.	0.23	14			0.58
99102-04-2	-	Erythrohydrobupropion	0.45		0.3	0	n.a.	0.36				0.40
1122-58-3	214-353-5	*N*,*N*-dimethylpyridin-4-amine	0.45	0.8	0.0	0	no conclusion/data	0.33				0.37
55142-85-3	259-498-5	ticlopidine	0.45		2.3	0	n.a.	0.18				0.68
42200-33-9	255-706-3	Nadolol	0.45	-0.6	-1.4	0	n.a.	0.72				0.27
3337-62-0	222-075-0	3,5-dibromo-4-hydroxybenzoe a-cid	0.45		-1.7	0	n.a.	0.53	1			0.41
68157-60-8	-	Forchlorfenuron	0.44		3.0	0	n.a.	0.27				0.54
7681-76-7	231-675-1	Ronidazole	0.44		-1.7	0	n.a.	0.29				0.31
644-62-2	211-419-5	Meclofenamic acid	0.44		1.6	0	n.a.	0.23				0.73
67392-87-4	266-679-2	Drospirenone	0.44		3.4	0	n.a.	0.30				0.81
66085-59-4	266-127-0	Nimodipine	0.44	2.9	3.6	0	n.a.	0.41				0.48
37115-43-8	636-833-7	alpha-Hydroxyalprazolam	0.44		2.0	0	n.a.	0.34				0.38
64520-05-4	-	10-Hydroxy-amitriptyline	0.44		0.8	0	n.a.	0.32				0.44
513-88-2	208-175-7	1,1-dichloroacetone	0.44	0.7	0.9	10	no conclusion/data	0.38				0.31
140923-17-7	604-209-3	Iprovalicarb	0.44		3.0	0	n.a.	0.48	7			0.49
21187-98-4	244-260-5	Gliclazide	0.44		0.4	0	n.a.	0.27				0.41
1185255-09-7	815-493-5	Azoxystrobin acid	0.44		-0.4	0	n.a.	0.57	37			0.35
118134-30-8	601-505-4	Spiroxamine I	0.44		1.9	0	n.a.	0.08	59			0.82
15686-51-8	-	Clemastine	0.44		3.0	0	n.a.	0.10				0.85

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
15310-01-7	239-352-7	Benodanil	0.44		3.1	0	n.a.	0.15				0.41
58581-89-8	611-699-2	Azelastine	0.43		2.8	0	n.a.	0.13				0.83
220899-03-6	-	Metrafenone	0.43		3.2	0	n.a.	0.68	155			0.86
67018-85-3	266-544-8	Norverapamil	0.43		1.4	0	n.a.	0.66				0.90
76-73-3	200-982-2	Secobarbital	0.43	0.9	1.8	0	n.a.	0.33				0.37
1088-11-5	214-123-4	Nordazepam	0.43		2.8	0	no conclusion/data	0.49				0.45
100643-71-8	-	Desloratadine	0.43		1.8	0	n.a.	0.24				0.76
34970-00-8	-	Bromochloroiodomethane	0.43		1.7	98	n.a.	0.28				0.35
135410-20-7	603-921-1	Aacetamiprid	0.43		1.5	0	n.a.	0.24				0.52
99105-77-8	619-394-6	Sulcotrione	0.43		0.3	0	n.a.	0.29	21			0.59
121-14-2	204-450-0	2,4-Dinitrotoluene	0.43	1.6	2.0	0	n.a.	0.19		2		0.44
83-98-7	201-509-2	Orphenadrine	0.43	2.3	2.5	0	no conclusion/data	0.23				0.51
59-40-5	200-423-2	Sulfaquinoxaline	0.43	1.3	1.0	0	n.a.	0.21				0.42
51803-78-2	257-431-4	Nimesulide	0.43	2.3	1.8	0	n.a.	0.35				0.49
90982-32-4	618-690-2	Chlorimuron ethyl	0.43		-1.6	0	vP	0.45				0.62
95058-81-4	619-100-6	Gemcitabine	0.43		-2.1	0	n.a.	0.36				0.20
28343-61-5	881-469-6	Chlorothalonil-4-hydroxy	0.43		0.4	0	n.a.	0.49			4	0.78
131860-33-8	603-524-3	Azoxystrobin	0.42		2.7	0	n.a.	0.60	66			0.55
77-26-9	201-017-8	Butalbital	0.42	0.6	1.5	0	n.a.	0.33				0.35
83055-99-6	401-340-6	Bensulfuron methyl	0.42		-0.4	0	no conclusion/data	0.57	52			0.49

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
2403-88-5	219-291-2	2,2,6,6-tetramethylpiperidin-4-ol	0.42		-1.3	0	Potential P/vP++	0.56				0.26
634-03-7	211-204-6	Phendimetrazine	0.42		1.6	0	n.a.	0.27				0.32
149979-41-9	604-715-4	Tepraloxydim	0.42		3.2	0	n.a.	0.24				0.57
161326-34-7	605-252-0	Fenamidone	0.41		2.5	0	n.a.	0.33	10			0.47
23135-22-0	245-445-3	Oxamyl	0.41	-1.1	-1.5	0	n.a.	0.55	14			0.23
120375-14-6	-	Metolachlor-Morpholinon	0.41		2.6	0	n.a.	0.44	38		26	0.36
28249-77-6	248-924-5	Benthiocarb	0.41		3.3	0	n.a.	0.31	66			0.44
87857-41-8	804-562-5	Norsertraline	0.41		3.2	0	n.a.	0.25				0.67
35045-02-4	-	Metribuzin DA	0.41		1.8	0	n.a.	0.35	7			0.31
402-45-9	206-945-7	4-(Trifluoromethyl)phenol	0.41	1.8	2.7	2	n.a.	0.30				0.43
359-83-1	206-634-6	Pentazocine	0.41		2.1	0	n.a.	0.24				0.68
99-55-8	202-765-8	5-nitro-*o*-toluidine	0.41	1.5	1.7	0	Pot. P/vP	0.23			2	0.35
637-07-0	211-277-4	Clofibrate ethyl	0.41	2.5	3.5	0	n.a.	0.65				0.48
14214-32-5	238-068-0	Difenoxuron	0.41		2.6	0	n.a.	0.58				0.38
196618-13-0	-	Oseltamivir	0.41		-1.5	0	n.a.	0.60				0.26
34911-55-2	-	Bupropion	0.41	2.1	1.9	0	n.a.	0.30				0.54
34014-18-1	251-793-7	Tebuthiuron	0.40		1.7	0	n.a.	0.31				0.36
474-86-2	207-488-6	Equilin	0.40		3.2	0	n.a.	0.40				0.52
6988-21-2	230-253-4	Dioxacarb	0.40		0.7	0	n.a.	0.24	11			0.25
21829-25-4	244-598-3	Nifedipine	0.40	2.1	3.1	0	n.a.	0.55				0.35

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
532-03-6	208-524-3	Methocarbamol	0.40	-0.4	0.3	0	n.a.	0.79				0.23
23210-56-2	245-491-4	Ifenprodil	0.40		2.4	0	n.a.	0.42				0.43
91-53-2	202-075-7	Ethoxyquin	0.40		3.4	0	no conclusion/data	0.34				0.49
23887-31-2	245-926-8	Clorazepate	0.40		-1.4	0	n.a.	0.52				0.25
75-99-0	200-923-0	Dalapon	0.40		-3.3	0	n.a.	0.40			2	0.22
1918-16-7	217-638-2	Propachlor	0.40	1.6	2.2	0	n.a.	0.56	21			0.32
1709-59-7	216-970-5	4-Amino-*N*,*N*-dimethylbenzene-sulfonamide	0.39		0.7	0	n.a.	0.30				0.26
33089-74-6	861-087-6	Amitraz metabolite (Methanimi-damide, N-(2,4-dimethylphenyl)-*N*'-methyl-)	0.39		0.5	0	n.a.	0.40				0.30
1668-19-5	214-966-8	Doxepin	0.39		2.1	0	n.a.	0.34				0.53
102-77-2	203-052-4	2-(morpholinothio)benzothiazole	0.39	1.2	1.9	0	Pot. P/vP	0.27				0.25
10161-33-8	600-229-1	Trenbolone	0.39	1.5	2.7	0	n.a.	0.41				0.32
16118-49-3	240-286-6	Carbetamide	0.39		1.7	0	n.a.	0.60	11			0.27
88671-89-0	410-400-0	Myclobutanil	0.39		3.1	0	no conclusion/data	0.49	253			0.46
81-25-4	201-337-8	Cholic acid	0.39	1.7	0.1	0	n.a.	0.46				0.20
6164-98-3	228-200-5	Chlordimeform	0.39		2.0	0	n.a.	0.35				0.36
73-40-5	200-799-8	Guanine	0.39	-1.3	-1.0	0	no conclusion/data	0.35				0.19
51481-61-9	257-232-2	Cimetidine	0.39		-0.3	0	n.a.	0.41				0.29
106-47-8	203-401-0	4-chloroaniline	0.39	1.5	1.8	0	Potential P/vP++	0.31			6	0.29
1689-83-4	216-881-1	Ioxynil	0.38		1.5	0	n.a.	-0.08				0.53

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
137-17-7	205-282-0	2,4,5-Trimethylaniline	0.38	1.9	2.2	0	n.a.	0.50			6	0.31
102767-28-2	-	Levetiracetam	0.38		-1.2	0	n.a.	0.76				0.20
5352-88-5	688-804-3	1-(4-chlorophenyl)-3-methylurea	0.38	1.3	2.0	0	n.a.	0.35	52			0.28
83463-62-1	690-348-5	Bromochloroacetonitrile	0.38		1.7	10	n.a.	0.46				0.25
529-38-4	637-078-6	Cocaethylene	0.38		1.7	0	n.a.	0.64				0.31
1689-84-5	216-882-7	Bromoxynil	0.38	2.3	0.8	0	n.a.	0.54	2			0.51
2032-65-7	217-991-2	Methiocarb	0.38		2.5	0	n.a.	0.51	4			0.34
593-94-2	-	Dibromoiodomethane	0.38		2.1	8	n.a.	0.28				0.28
87-65-0	201-761-3	2,6-Dichlorophenol	0.38	2.0	2.5	0	n.a.	0.36		2		0.36
124750-92-1	-	Losartansäure	0.37		-0.4	0		0.35				0.47
517-09-9	208-230-5	Equilenin	0.37		3.3	0	n.a.	0.40				0.52
4065-45-6	223-772-2	Sulisobenzone	0.37	2.0	-1.7	0	P	0.54				0.24
101-21-3	202-925-7	Chlorpropham	0.37		3.4	1	n.a.	0.35	44		7	0.36
29331-92-8	-	10,11-Dihydro-10-hydro-xycarbamazepine	0.37		1.8	0	n.a.	0.50				0.20
129-03-3	204-928-9	Cyproheptadine	0.36		2.9	0	n.a.	0.25				0.50
17902-23-7	241-846-2	Tegafur	0.36	-0.7	-0.3	0	n.a.	0.30				0.19
75847-73-3	-	Enalapril	0.36		-0.9	0	n.a.	0.69				0.17
88-85-7	201-861-7	Dinoseb	0.36	2.9	0.1	0	vP	0.18			4	0.49
15299-99-7	239-333-3	Napropamide	0.36	2.5	3.6	0	n.a.	0.62	169			0.35
39809-25-1	663-371-3	Penciclovir	0.36		-1.8	0	n.a.	0.47				0.15

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
165252-70-0	605-399-0	Dinotefuran	0.36		-0.7	0	no conclusion/data	0.32				0.19
1806-98-0	-	17-beta-estradiol-17-glucuronide	0.36		-0.6	0	n.a.	0.34				0.19
938-73-8	213-346-4	Ethenzamide	0.36	0.5	1.0	0	n.a.	0.78				0.20
1491-59-4	216-079-1	Oxymetazoline	0.36	1.8	1.9	0	Pot. P/vP	0.43				0.55
2631-37-0	220-113-0	Promecarb	0.36		3.0	0	n.a.	0.53			7	0.31
69610-10-2	-	MDMA / Methylendioxyme-thamphetamine	0.35	1.3	-0.5	0	n.a.	0.72				0.27
33704-61-9	251-649-3	Cashmeran	0.35	2.3	4.1	1	Potential P/vP++	0.35				0.51
102-36-3	203-026-2	3,4-dichlorophenyl isocyanate	0.35		2.8	17	Pot. P/vP	0.28				0.45
52-01-7	-	Spironolactone	0.35		0.8	0	n.a.	0.63				0.23
30516-87-1	623-849-4	Zidovudine	0.35	-0.7	-0.4	0	n.a.	0.33				0.18
53112-28-0	414-220-3	Pyrimethanil	0.35	2.0	3.1	0	n.a.	0.45	43			0.35
1400-61-9	215-749-0	Nystatin	0.35		-1.3	0	n.a.	0.48				0.13
94-97-3	202-378-4	CBT (5-chloro-1*H*-benzotriazole)	0.35		2.2	0	n.a.	0.40				0.24
60397-77-5	-	2,4-dimethylphenylformamide	0.35		1.6	0	n.a.	0.71				0.23
950-81-2	213-452-0	4-formyl-antipyrine	0.34		1.1	0	n.a.	0.72				0.18
957-51-7	213-482-4	Diphenamid	0.34	1.5	2.6	0	n.a.	0.62				0.28
82801-81-8	-	MDEA (3,4-Methylenedi-oxyethamphetamine)	0.34		-0.9	0	n.a.	0.72				0.29
519-98-2	208-281-3	4-MAA (4-methylaminoantipy-rine)	0.34		1.2	0	n.a.	0.55				0.18
76608-88-3	278-498-6	Triapenthenol	0.34		2.5	0	n.a.	0.39				0.30

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
91-44-1	202-068-9	7-(diethylamino)-4-methyl-2-benzopyrone	0.34		2.8	0	Pot. P/vP	0.55				0.29
134678-17-4	-	Lamivudine	0.34		-1.1	0	n.a.	0.36				0.14
88768-40-5	641-006-9	Cilazapril	0.34		-0.1	0	n.a.	0.61				0.18
950-37-8	213-449-4	Methidathion	0.34	2.2	1.4	0	n.a.	0.54				0.22
78-59-1	201-126-0	Isoacetophorone	0.34	1.3	1.8	0	Not P	0.51				0.23
27503-81-7	248-502-0	Ensulizole	0.34		-2.4	0	Potential P/vP++	0.37				0.18
68011-66-5	809-752-1	2-hydroxycarbamazepine	0.34		1.8	0	n.a.	0.45				0.21
67306-00-7	614-049-6	Fenpropidin	0.33		3.4	0	n.a.	0.21	71			0.70
77-19-0	201-009-4	Dicycloverine	0.33		2.9	0	Pot. P/vP	0.43				0.60
3252-43-5	221-843-2	Dibromoacetonitrile	0.33		1.9	3	n.a.	0.42				0.19
6923-22-4	230-042-7	Monocrotophos	0.33		-0.3	0	n.a.	0.67				0.16
1852-50-2	633-751-3	Estriol-16-glucuronide	0.33		-1.2	0	n.a.	0.39				0.14
1077-56-1	214-073-3	*N*-Ethyl-*o*-toluenesulfonamide	0.33		1.6	0	n.a.	0.50	7			0.22
110235-47-7	432-140-7	Mepanipyrim	0.32		2.9	0	no conclusion/data	0.39				0.33
3376-94-1	-	Norpropoxyphene	0.32		2.0	0	n.a.	0.59				0.42
175217-20-6	605-752-9	Silthiopham	0.32		3.4	0	n.a.	0.55				0.42
99-99-0	202-808-0	4-nitrotoluene	0.32		2.4	1	Potential P/vP++	0.36		2		0.24
2479-91-6	-	Estriol-3-glucuronide	0.31		-2.1	0	n.a.	0.66				0.12
107-14-2	203-467-0	Chloroacetonitrile	0.31	0.0	0.5	1	no conclusion/data	0.73				0.17
13071-79-9	235-963-8	Terbufos	0.31	2.9	4.4	0	n.a.	0.54				0.34

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
99-88-7	202-797-2	4-isopropylaniline	0.31	1.7	2.4	0	Potential P/vP++	0.42			2	0.22
838-85-7	212-657-2	Diphenyl phosphate	0.31	0.1	-2.1	0	n.a.	0.53				0.22
98-53-3	202-678-5	4-tert-butylcyclohexanone	0.31		3.1	3	Not P	0.50				0.26
43210-67-9	256-145-7	Fenbendazole	0.30		3.1	0	n.a.	0.45				0.33
934-32-7	213-280-6	2-aminobenzimidazole	0.30		0.6	0	no conclusion/data	0.39	13			0.17
14769-73-4	238-836-5	Levamisole	0.30		1.1	0	n.a.	0.54				0.17
10265-92-6	10265-92-6	Methamidophos	0.30		-0.8	0	n.a.	0.53				0.13
16752-77-5	240-815-0	Methomyl	0.30		0.6	0	n.a.	0.50	11			0.14
26093-31-2	247-454-8	7-Amino-4-methylcoumarin	0.30		1.3	0	n.a.	0.59				0.15
4184-79-6	224-058-3	Xtri (5,6-dimethyl-1*H*-benzotria-zole)	0.30		1.9	0	n.a.	0.60				0.20
16051-77-7	240-197-2	Isosorbide mononitrate	0.30		-1.1	0	n.a.	0.32				0.11
1134-23-2	214-482-7	*S*-ethyl *N*-cyclohexylthio-carbamate	0.30	2.5	3.8	0	no conclusion/data	0.53			8	0.22
94-24-6	202-316-6	Tetracaine	0.30	2.4	2.7	0	n.a.	0.48			7	0.23
13392-18-2	680-817-2	Fenoterol	0.30		0.0	0	no conclusion/data	0.64				0.16
116539-59-4	-	Duloxetine	0.29		3.0	0	n.a.	0.55				0.34
3094-09-5	-	Doxifluridine	0.29		-1.6	0	n.a.	0.41				0.10
92-67-1	202-177-1	4-Aminodiphenyl	0.29	2.3	2.8	0	n.a.	0.44				0.20
835-31-4	212-641-5	Naphazoline	0.29	1.9	-0.3	0	no conclusion/data	0.46				0.23
491-80-5	207-744-7	Biochanin A	0.29	2.4	2.7	0	n.a.	0.72				0.31

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
76547-98-3	278-488-1	Lisinopril	0.29		-1.1	0	n.a.	0.69				0.10
101-42-8	202-941-4	Fenuron	0.29	0.5	1.2	0	no conclusion/data	0.58			4	0.14
934-34-9	213-281-1	2-Hydroxybenzothiazole	0.29		1.5	0	no conclusion/data	0.58				0.15
98-10-2	202-637-1	Benzenesulphonamide	0.29	-0.1	0.4	0	Pot. P/vP	0.59				0.13
82834-16-0	617-394-0	Perindopril	0.28		-1.1	0	n.a.	0.70				0.14
486-66-8	207-635-4	Daidzein	0.28	2.0	2.7	0	n.a.	0.66				0.23
497-18-7	207-837-2	Carbonohydrazide	0.28	1.3	-2.5	0	Pot. P/vP	0.49				0.09
256-96-2	205-970-0	Iminostilbene	0.28		3.5	0	Pot. P/vP	0.32				0.25
2814-20-2	220-561-7	2-Isopropyl-6-methyl-pyrimidin-4-ol	0.28		0.6	0	n.a.	0.50				0.13
26725-51-9	625-298-5	4-hydroxybenzotriazole	0.28		-0.5	0	n.a.	0.59				0.13
154361-50-9	-	Capecitabine	0.28		-1.0	0	n.a.	0.45				0.10
88-75-5	201-857-5	2-nitrophenol	0.28	1.4	1.5	0	Potential P/vP++	0.40			2	0.17
17804-35-2	241-775-7	Benomyl	0.27		2.3	0	n.a.	0.50		7		0.16
87269-97-4	807-772-5	Ramiprilate	0.27		-0.2	0		0.64				0.09
52888-80-9	401-730-6	Prosulfocarb	0.27	2.7	4.4	0	no conclusion/data	0.54	15			0.26
31218-83-4	250-517-2	Propetamphos	0.27		3.4	0	n.a.	0.55				0.20
120-75-2	204-423-3	2-methylbenzothiazole	0.27		2.5	0	n.a.	0.57				0.16
2592-95-2	219-989-7	1-hydroxybenzotriazole	0.26		-0.9	0	no conclusion/data	0.56				0.12
73573-88-3	700-442-0	Mevastatin	0.26		3.4	0	no conclusion/data	0.71				0.17
51-64-9	200-112-1	Dexamphetamine	0.26	0.9	-0.8	0	no conclusion/data	0.63				0.13

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
479-13-0	207-525-6	Coumesterol	0.26		2.8	0	n.a.	0.67				0.14
61676-87-7	262-890-9	Cymiazole	0.25		1.5	0	n.a.	0.49	57			0.29
446-72-0	207-174-9	Genistein	0.25	2.3	2.6	0	n.a.	0.68				0.22
74103-06-3	616-049-1	Ketorolac	0.25	1.7	1.2	0	no conclusion/data	0.61				0.11
50512-35-1	-	Isoprothiolane	0.25		3.2	0	n.a.	0.69				0.14
119-65-3	204-341-8	Isoquinoline	0.25		2.0	0	Pot. P/vP	0.59			31	0.12
615-22-5	210-417-1	2-(methylthio)-benzothiazol	0.25		1.7	0	n.a.	0.48				0.16
109-87-5	203-714-2	Dimethoxymethane	0.25	-0.4	0.2	6	no conclusion/data	0.43				0.09
3878-19-1	223-404-0	Fuberidazole	0.24		2.6	0	n.a.	0.48	12			0.16
7786-34-7	206-051-7	Mevinphos	0.24		0.3	0	n.a.	0.76				0.09
50-33-9	200-029-0	Phenylbutazone	0.23	2.5	1.6	0	n.a.	0.55				0.14
64228-79-1	-	Atracurium	0.23		-0.8	0	n.a.	0.71				1.00
1143-72-2	214-540-1	2,3,4-trihydroxybenzophenone	0.20		2.6	0	no conclusion/data	0.68				0.14
56354-06-4	690-035-3	THC-COOH	0.20		2.6	0	n.a.	0.61				0.19
133040-01-4	-	Eprosartan	0.16		-0.3	0	n.a.	0.55				0.13

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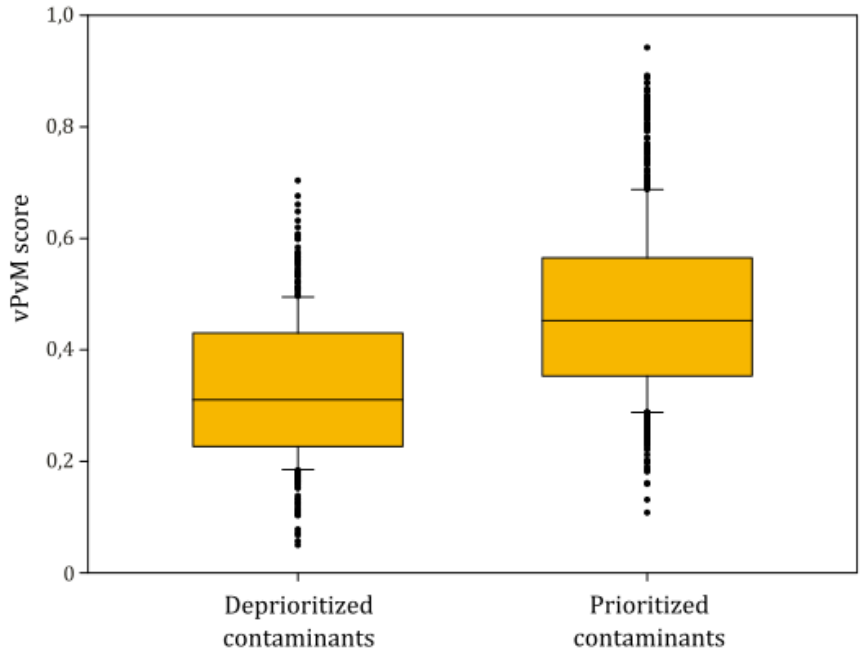
A Appendix

A.1 Statistical comparison of the vPvM scores of deprioriziced and prioritized contaminants

The distributions of the vPvM scores of the deprioritized and prioritized contaminants are shown in Figure 2. The minimum, maximum, and median values of the two groups are listed in Table 4.

Figure 2: Distributions of the vPvM scores of the deprioritized and prioritized contaminants



Source: original figure, TZW: DVGW-Technologiezentrum Wasser.

Table 4: The minimum, maximum, and median values of the vPvP scores of the deprioritized and prioritized contaminants

	Deprioritized contaminants	Prioritized contaminants
Minimum	0.049	0.108
Maximum	0.703	0.942
Median	0.310	0.453

On average, lower vPvM values are calculated for deprioritized contaminants than for contaminants for which no pronounced and significant decrease in concentration in the aqueous phase is expected in an OECD TG 309 degradation test. A Mann-Whitney rank sum test (SigmaPlot 12.5 software) was performed on the two groups (deprioritized and prioritized contaminants). The difference in median values between the two groups is statistically significant ($p < 0.001$).

A.2 List of contaminants deprioritized for a “cold” degradation test according to OECD TG 309

The deprioritized contaminants are listed in Table 5. The column descriptions are the same as in Chapter 6. In addition, the criteria that led to the deprioritization of each contaminant are highlighted in fuchsia. Contaminants that were deprioritized in Step 3 (see Chapter 5.2) are highlighted in ochre.

Table 5: Deprioritized contaminants

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
70288-86-7	274-536-0	Ivermectine	0.70		5.3	0	n.a.	-0.43	28			0.97
71486-22-1	-	Vinorelbine	0.68		3.9	0	n.a.	0.01				1.00
117704-25-3	601-490-4	Doramectin	0.66	3.9	5.1	0	n.a.	-0.43	26			0.98
19794-93-5	243-317-1	Trazodone	0.65	3.0	2.3	0	no conclusion/data	0.03				0.90
361377-29-9	606-301-9	Fluoxastrobin	0.63		3.8	0	n.a.	0.10	36			0.94
57-27-2	200-320-2	Morphine	0.62	3.0	-0.2	0	n.a.	0.43				0.60
69-23-8	200-702-9	Fluphenazine	0.61	3.2	3.9	0	n.a.	0.00				0.98
58-39-9	200-381-5	Perphenazine	0.61	3.2	3.4	0	n.a.	0.08				0.94
2709-56-0	220-304-9	Flupentixol	0.60		3.9	0	n.a.	0.06				0.96
188425-85-6	606-143-0	Boscalid (Nicobifen)	0.60		3.9	0	n.a.	0.19				0.86
35367-38-5	252-529-3	Diflubenzuron	0.58	3.1	3.9	0	n.a.	-0.06	6.9			0.94
93413-69-5	618-944-2	1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol	0.58	3.1	1.5	0	Potential P/vP++	0.31				0.74
53772-83-1	258-758-5	Zuclopenthixol	0.57		3.7	0	n.a.	0.14				0.86
133855-98-8	406-850-2	(2RS,3RS)-3-(2-chlorophenyl)-2-(4-fluorophenyl)-[(1*H*-1,2,4-triazol-1-yl)methyl]oxirane	0.57		3.6	0	Pot. P/vP	-0.01	280			0.90
56-23-5	200-262-8	Carbon tetrachloride	0.57	1.9	2.8	1443	Potential P/vP++	0.23		71		0.76
125116-23-6	603-031-3	Metconazole	0.57		3.9	0	n.a.	0.17	127			0.85

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
112281-77-3	407-760-6	(+/-) 2-(2,4-dichlorophenyl)-3-(1*H*-1,2,4-triazole-1-yl)propyl-1,1,2,2-tetrafluoroethylether	0.56		3.7	0	Pot. P/vP	0.07	2092			0.89
3562-63-8	222-628-6	Megestrol acetate	0.56		3.6	0	n.a.	0.22				0.86
79-34-5	201-197-8	Tetrachlorethan, 1,1,2,2-	0.56		2.6	38	n.a.	0.24		71		0.64
76-13-1	200-936-1	Trichlorotrifluoroethane	0.56	2.1	3.1	21243	n.a.	0.21				0.82
84-97-9	201-578-9	Pernazine	0.55		3.9	0	Pot. P/vP	0.09				0.89
60207-90-1	262-104-4	Propiconazole	0.55	3.2	3.6	0	n.a.	0.05	147			0.84
55-56-1	200-238-7	Chlorhexidine	0.54	3.9	-1.9	0	vP	-0.04				0.95
374726-62-2	609-434-0	Mandipropamid	0.54		3.6	0	n.a.	0.36	32			0.83
71-55-6	200-756-3	1,1,1-trichloroethane	0.54		2.5	638	Potential P/vP++	0.28			25	0.61
1918-00-9	217-635-6	Dicamba	0.54		-1.6	0	n.a.	0.57	6.8	23		0.48
75-69-4	200-892-3	Trichlorofluoromethane	0.54		2.4	10586	n.a.	0.27		708		0.62
280-57-9	205-999-9	1,4-diazabicyclooctane	0.53	3.4	-1.7	0	Potential P/vP++	0.34				0.39
55297-95-5	259-580-0	Tiamulin	0.53		3.6	0	n.a.	0.23				0.94
52485-79-7	257-950-6	Buprenorphine	0.53		4.3	0	n.a.	0.00				0.99
470-90-6	207-432-0	Chlorfenvinphos	0.52		3.8	0	n.a.	0.40				0.75
112410-23-8	412-850-3	*N*-tert-butyl-*N*'-(4-ethylbenzoyl)-3,5-dimethylbenzohydrazide	0.52		4.0	0	Pot. P/vP	0.19	72			0.74
57-63-6	200-342-2	Ethinylestradiol	0.52		3.7	0	n.a.	0.28				0.72

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
52169-36-5	610-790-4	5-chloro-*N*-[2-[4-(cyclohe-xylcarbamoylsulfamoyl)phe-nyl]ethyl]-2-methoxybenzamide; potassium	0.52	3.4	2.6	0	Pot. P/vP	0.30				0.88
126833-17-8	422-530-5	Fenhexamid	0.51		4.2	0	n.a.	0.28	0.83			0.79
125225-28-7	603-038-1	Ipconazole	0.51		4.1	0	n.a.	0.19	153			0.75
3734-33-6	223-095-2	Denatonium benzoate	0.51	3.4	1.7	0	Pot. P/vP	0.55				0.51
65277-42-1	265-667-4	Ketoconazole	0.51		3.9	0	n.a.	-0.03				0.99
154598-52-4	620-492-6	Efavirenz	0.50		4.3	0	n.a.	0.10				0.93
72-33-3	200-777-8	Mestranol	0.50		4.2	0	n.a.	0.32				0.80
54-11-5	200-193-3	Nicotine	0.50	3.6	0.4	0	n.a.	0.30				0.44
83164-33-4	617-446-2	Diflufenican	0.49	3.8	4.5	0	n.a.	-0.10	71			1.00
79-00-5	201-166-9	1,1,2-trichloroethane	0.49	1.7	2.0	78	Potential P/vP++	0.31			25	0.43
83366-66-9	-	Nefazodone	0.49	3.7	4.1	0	n.a.	0.13				0.95
114369-43-6	406-140-2	4-(4-chlorophenyl)-2-phenyl-2-[(1H-1,2,4-triazol-1-yl)methyl]bu-tanenitrile	0.49		3.5	0	Pot. P/vP	0.42	154			0.79
5630-53-5	227-069-1	Tibolone	0.49		3.6	0	n.a.	0.26				0.69
54910-89-3	611-209-7	Fluoxetine	0.49	3.2	0.4	0	n.a.	0.32				0.74
530-78-9	208-494-1	Flufenamic acid	0.49	4.0	1.6	0	Pot. P/vP	0.21				0.72
594-04-7	-	Dichloroiodomethane	0.48		1.7	648	n.a.	0.27				0.43
427-51-0	207-048-3	Cyproterone	0.48		3.8	0	n.a.	0.23				0.92

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
113665-84-2	601-269-2	Clopidogrel	0.48		3.7	0	n.a.	0.28				0.67
60-57-1	200-484-5	Dieldrin	0.48		5.0	0	n.a.	-0.09		708		1.00
72-20-8	200-775-7	Endrin	0.48		5.0	0	n.a.	-0.09		708		1.00
58-89-9	200-401-2	Lindane	0.48		3.8	7	n.a.	0.12				0.93
96-18-4	202-486-1	1,2,3-trichloropropane	0.48	1.9	2.2	17	Potential P/vP++	0.31		71		0.46
144-11-6	205-614-4	Trihexyphenidyl	0.48	3.8	2.4	0	Pot. P/vP	0.26				0.67
75-71-8	200-893-9	Dichlorodifluoromethane	0.48	1.2	2.1	36248	Potential P/vP++	0.32				0.44
1563-66-2	216-353-0	Carbofuran	0.48		1.9	0	n.a.	0.54	19	7		0.49
15165-67-0	403-980-1	R-(+)-2-(2,4-dichlorophen-oxy)propionic acid	0.48		-1.7	0	no conclusion/data	0.40	10		6	0.29
79983-71-4	413-050-7	(RS)-2-(2,4-dichlorophenyl)-1-(1*H*-1,2,4-triazol-1-yl)hexan-2-ol	0.48		3.7	0	Pot. P/vP	0.22				0.60
1861-32-1	217-464-7	DCPA mono/di-acid degradate	0.47	3.3	4.3	0	n.a.	0.31	25		6	0.78
67-66-3	200-663-8	Chloroform	0.47	2.0	2.0	569	Potential P/vP++	0.31		71		0.41
7082-99-7	806-361-8	Chlorbenside sulfone	0.47		3.7	0	n.a.	0.19				0.65
24219-97-4	246-088-6	Mianserin	0.47	3.2	3.4	0	n.a.	0.18				0.71
116-29-0	204-134-2	Tetradifon	0.47		4.8	0	n.a.	0.07				0.92
19666-30-9	243-215-7	Oxadiazon	0.47		4.2	0	n.a.	0.17	278			0.86
101-77-9	202-974-4	4,4'-methylenedianiline	0.47	3.8	1.6	0	Pot. P/vP	0.21		9		0.41
95-76-1	202-448-4	3,4-dichloroaniline	0.47	2.3	2.7	0	Potential P/vP++	0.22	4.4		13	0.51
141517-21-7	604-237-6	Trifloxystrobin	0.47		4.6	0	n.a.	0.19	0.33			0.78

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
71-58-9	200-757-9	Medroxyprogesterone acetate	0.47		3.8	0	n.a.	0.30				0.84
709-98-8	211-914-6	Propanil	0.47		3.2	0	n.a.	0.36	1.6		22	0.55
303-49-1	206-144-2	Clomipramine	0.47	4.1	4.0	0	Pot. P/vP	0.11				0.90
24579-73-5	607-406-2	Propamocarb	0.47		-1.2	0	n.a.	0.42	22		2	0.36
127-18-4	204-825-9	Tetrachloroethylene	0.46	2.1	3.4	448	vP	0.25		23		0.63
72509-76-3	620-472-7	Felodipine	0.46	3.5	4.4	0	n.a.	0.54				0.61
18181-80-1	242-070-7	Bromopropylate	0.46		5.2	0	n.a.	0.26				0.79
155213-67-5	-	Ritonavir	0.46		3.8	0	n.a.	0.27				0.94
82560-54-1	-	Benfuracarb	0.46		4.1	0	n.a.	0.49	0.8			0.67
82-68-8	201-435-0	Pentachloronitrobenzene	0.46		4.7	0	n.a.	-0.03				0.96
2058-94-8	218-165-4	PFUnDA	0.46	3.3	-0.5	1	n.a.	-0.18				1.00
79-01-6	201-167-4	Trichloroethylene	0.46	2.1	2.6	304	P	0.31		23		0.43
130-95-0	205-003-2	Quinine	0.45	3.6	1.9	0	n.a.	0.40				0.48
42874-03-3	255-983-0	Oxyfluorfen	0.45		4.6	0	n.a.	0.12	138			0.95
71-43-2	200-753-7	Benzene	0.45	1.5	2.1	329	Not P	0.74		7		0.39
521-18-6	208-307-3	Androstanolone	0.45		3.6	0	Pot. P/vP	0.36				0.53
120068-37-3	424-610-5	fipronil (ISO); (±)-5-amino-1-(2,6-dichloro-α,α,α-trifluoro-para-tolyl)-4-trifluoromethylsulfinyl-pyrazole-3-carbonitrile	0.45		3.6	0	Pot. P/vP	-0.13	119			1.00
50-48-6	200-041-6	Amitriptyline	0.44	4.0	0.0	0	Potential P/vP++	0.59				0.44
53-41-8	200-173-4	Androsterone	0.44		3.7	0	n.a.	0.36				0.53

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
481-29-8	207-563-3	Epiandrosterone	0.44		3.7	0	n.a.	0.36				0.53
81-15-2	201-329-4	Musk xylene	0.44		4.6	0	n.a.	-0.01				0.89
205650-65-3	803-116-7	Fipronil desulfinyl	0.44		3.5	0	n.a.	-0.10				1.00
67564-91-4	266-719-9	Fenpropimorph	0.44		4.6	0	n.a.	0.12	24			0.75
119168-77-3	601-585-0	Tebufenpyrad	0.44		4.6	0	n.a.	0.24	44			0.79
50-53-3	200-045-8	Chlorpromazine	0.44	4.3	4.0	0	Pot. P/vP	0.12				0.85
55134-13-9	611-230-1	Narasin	0.44		3.6	0	n.a.	-0.23				0.97
57-83-0	200-350-6	Progesterone	0.44	3.0	3.7	0	Pot. P/vP	0.28				0.71
2315-61-9	621-341-7	octylphenol diethoxylate	0.43		4.6	0	n.a.	0.39				0.57
2955-38-6	220-975-8	Prazepam	0.43	3.2	3.6	0	n.a.	0.44				0.55
79794-75-5	935-907-9	Loratadine	0.43		5.2	0	P	0.16				0.87
74070-46-5	277-704-1	Aclonifen	0.43		3.9	0	n.a.	0.18	47		7	0.69
70630-17-0	615-135-6	Mefenoxam	0.43		1.7	0	n.a.	0.62	16		7	0.34
57837-19-1	260-979-7	Metalaxyl	0.43		1.7	0	n.a.	0.62	16		7	0.34
101-20-2	202-924-1	Triclocarban	0.43	3.7	4.7	0	vP	0.14			22	0.80
60-87-7	200-489-2	Promethazine	0.43	3.8	3.5	0	Pot. P/vP	0.16				0.69
106700-29-2	600-765-6	Pethoxamid	0.43		3.5	0	n.a.	0.33	9.5			0.48
67906-42-7	206-401-9	PFDS	0.43	3.5	-2.8	0	n.a.	-0.25				1.00
2921-88-2	220-864-4	Chlorpyrifos	0.43		4.9	0	n.a.	0.35		7		0.87

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
58594-72-2	261-351-5	1-[2-(allyloxy)ethyl-2-(2,4-dichlorophenyl)-1*H*-imidazolium hydrogen sulphate	0.43		3.5	0	vP	0.16	36			0.65
64249-01-0	264-756-5	Anilofos	0.43		3.9	0	n.a.	0.51				0.52
77-10-1	621-588-0	PCP / Phencyclidine	0.43	3.7	2.4	0	n.a.	0.30				0.57
569-65-3	209-323-3	Meclozine	0.42		5.1	0	n.a.	0.08				0.92
175013-18-0	605-747-1	Pyraclostrobin	0.42		4.0	0	n.a.	0.24				0.68
75-27-4	200-856-7	Bromodichloromethane	0.42		2.1	238	n.a.	0.31		23		0.33
120-82-1	204-428-0	1,2,4-trichlorobenzene	0.42	3.3	4.0	82	Potential P/vP++	0.24		71		0.60
87-86-5	201-778-6	Pentachlorophenol	0.42	4.2	3.6	0	n.a.	0.12		23		0.90
81-14-1	201-328-9	4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone	0.41		4.1	0	Pot. P/vP	0.10				0.83
299-84-3	206-082-6	Fenchlorphos	0.41	4.1	5.0	0	n.a.	0.40			33	0.72
120014-06-4	-	Donepezil	0.41	3.5	2.5	0	n.a.	0.47				0.79
91-20-3	202-049-5	Naphthalene	0.41	2.6	3.3	31	Pot. P/vP	0.66		7		0.48
754-91-6	212-046-0	FOSA	0.41		3.7	0	n.a.	-0.15				1.00
307-55-1	206-203-2	PFDoDA	0.41	3.6	0.6	2	n.a.	-0.24				1.00
38083-17-9	253-775-4	Climbazole	0.41	3.8	3.0	0	Potential P/vP++	0.29				0.70
118-74-1	204-273-9	Hexachlorobenzene	0.41	4.5	5.6	0	n.a.	0.03		2292		0.96
1665-48-1	216-777-6	Metaxalone	0.41		2.3	0	n.a.	0.65			6	0.38
140-31-8	205-411-0	2-piperazin-1-ylethylamine	0.41	4.6	-4.3	0	P	0.60				0.21
108-70-3	203-608-6	1,3,5-trichlorobenzene	0.41	3.3	4.1	155	Pot. P/vP	0.24		71		0.60

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
113-59-7	204-032-8	Chlorprothixene	0.41		4.2	0	n.a.	0.18				0.71
120067-83-6	930-638-3	Fipronil-sulfide	0.40		3.6	0	Pot. P/vP	-0.12				1.00
1918-11-2	-	Terbucarb	0.40		4.0	0	n.a.	0.26				0.71
96-83-3	202-539-9	Iopanoic acid	0.40	4.1	2.3	0	n.a.	-0.52				0.76
66063-05-6	266-096-3	Pencycron	0.40		4.4	0	n.a.	0.27	63			0.51
87130-20-9	617-968-0	Diethofencarb	0.40		2.9	0	n.a.	0.64	8.0			0.38
107-06-2	203-458-1	1,2-dichloroethane	0.39		1.6	105	P	0.44		71		0.25
79617-96-2	616-708-3	Sertraline	0.39	4.3	3.4	0	n.a.	0.24				0.69
55179-31-2	259-513-5	Bitertanol I	0.39		4.0	0	n.a.	0.50	11			0.45
75-09-2	200-838-9	dichloromethane; methylene chloride	0.39		1.3	323	vP	0.45		71		0.23
31329-57-4	250-572-2	Naftidrofuryl	0.39		3.9	0	Pot. P/vP	0.24				0.62
78-87-5	201-152-2	1,2-dichloropropane	0.38	1.7	2.0	361	Potential P/vP++	0.39		71		0.27
94-82-6	202-366-9	DB, 2,4- (4-(2,4-dichlorophen-oxy)butyric acid)	0.38	2.6	0.1	0	n.a.	0.44	5.2		7	0.31
15574-96-6	239-632-9	Pizotifen	0.38		3.6	0	n.a.	0.23				0.63
2008-39-1	217-915-8	Dimethylammonium 2,4-dichlo-rophenoxyacetate	0.38		-1.5	0	no conclusion/data	0.46	9.2	2		0.27
99-09-2	202-729-1	3-nitroaniline	0.38	1.2	1.4	0	no conclusion/data	0.23	1.5		7	0.28
113-53-1	204-031-2	Dosulepin	0.38		3.7	0	n.a.	0.23				0.51
542-75-6	208-826-5	1,3-dichloropropene	0.38	1.6	2.1	102	Pot. P/vP	0.40	16		28	0.27
10061-01-5	233-195-8	(Z)-1,3-dichloropropene	0.38		2.1	102	Pot. P/vP	0.40	16		28	0.27

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
75-34-3	200-756-3	1,1-Dichloroethane	0.38	1.2	1.8	358	no conclusion/data	0.39			25	0.25
2315-67-5	264-520-1	4-tert-Octylphenol mo-noethoxylate	0.38		4.9	0	n.a.	0.54				0.48
49562-28-9	256-376-3	Fenofibrate	0.38		5.2	0	Pot. P/vP	0.43				0.71
1563-38-8	216-350-4	Carbofuran-7-phenol	0.37		2.2	0	n.a.	0.67	0.2			0.31
40487-42-1	254-938-2	Pendimethalin	0.37	3.8	4.8	0	n.a.	0.06	212		4	0.76
114-26-1	204-043-8	Propoxur	0.37	1.3	1.2	0	n.a.	0.59	13	23		0.25
36315-01-2	252-969-6	4,6-dimethoxypyrimidin-2-amine	0.37		0.4	0	no conclusion/data	0.64	22			0.27
68359-37-5	269-855-7	Cyfluthrin I	0.37		6.0	0	n.a.	0.19	22			0.97
72629-94-8	276-745-2	PFTriDA	0.37	4.1	1.8	3	n.a.	-0.31				1.00
156-59-2	205-859-7	cis-1,2-Dichloroethene	0.37	1.3	1.9	565	no conclusion/data	0.41			25	0.25
156-60-5	205-860-2	trans-dichloroethylene	0.37	1.4	1.9	565	Potential P/vP++	0.41			25	0.25
10262-69-8	233-599-4	Maprotiline	0.37	3.8	2.3	0	n.a.	0.39				0.48
124-48-1	204-704-0	Dibromochloromethane	0.37	1.7	2.2	87	n.a.	0.32				0.26
129-00-0	204-927-3	Pyrene	0.37		4.9	0	vP	0.21		71		0.76
50-28-2	200-023-8	Estradiol	0.36		3.6	0	Not P	0.50				0.38
57-91-0	200-354-8	17-alpha-Estradiol	0.36		3.6	0	n.a.	0.50				0.38
75-35-4	200-864-0	1,1-dichloroethylene	0.36	1.4	2.2	1973	Potential P/vP++	0.41			25	0.25
32598-11-1	630-497-5	PCB #70	0.36	5.2	6.1	0	n.a.	0.12			2292	0.87
95-68-1	202-440-0	2,4-xylidine	0.36	1.0	1.8	0	Pot. P/vP	0.49	0.3		6	0.24
95-50-1	202-425-9	1,2-dichlorobenzene	0.35		3.3	107	vP	0.33		71		0.37

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
61-68-7	200-513-1	Mefenamic acid	0.35	4.0	2.6	0	n.a.	0.52				0.37
60348-60-9	251-084-2	PBDE 99	0.35		7.0	0	n.a.	0.15				0.97
106-46-7	203-400-5	1,4-dichlorobenzene	0.35	2.4	3.4	105	Not P	0.33		71		0.37
120-12-7	204-371-1	Anthracene	0.35	4.5	4.6	0	P	0.59		23		0.57
1222-05-5	214-946-9	1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylin-deno[5,6-c]pyran	0.35	3.8	5.9	0	vP	0.18				0.65
32388-55-9	251-020-3	[3R-(3α,3aβ,7β,8aα)]-1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methano-azulen-5-yl)ethan-1-one	0.35	3.5	5.3	0	Pot. P/vP	0.30				0.58
5436-43-1	-	PBDE 47	0.35	6.6	6.6	0	n.a.	0.21				0.93
189084-62-6	620-888-9	PBDE 71	0.35		6.4	0	n.a.	0.21				0.93
122-14-5	204-524-2	Fenitrothion	0.35	2.9	3.3	0	no conclusion/data	0.47	3.1		21	0.35
143390-89-0	417-880-0	Kresoxim-methyl	0.35	2.5	3.3	0	n.a.	0.62	1.5			0.33
6452-71-7	229-257-9	Oxprenolol	0.35	0.99	0.0	0	n.a.	0.76			7	0.22
77-93-0	201-070-7	Triethyl citrate	0.34	0.13	0.5	0	Not P	0.92				0.16
58-08-2	200-362-1	Caffeine	0.34	-0.64	-0.3	0	Not P	0.45				0.17
37680-73-2	621-393-0	PCB101	0.34	5.7	6.1	0	n.a.	0.05			2292	0.95
22832-87-7	245-256-6	Miconazole nitrate	0.34	4.5	6.1	0	Pot. P/vP	-0.03				0.95
206-44-0	205-912-4	Fluoranthene	0.34	4.3	5.1	0	n.a.	0.21		71		0.76
83-67-0	201-494-2	Theobromine	0.34	-1.2	-0.4	0	Not P	0.47				0.16

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
87820-88-0	618-075-9	Tralkoxydim 1	0.34		3.8	0	n.a.	0.43				0.64
79902-63-9	616-751-8	Simvastatin	0.34		4.2	0	n.a.	0.65				0.34
64359-81-5	264-843-8	DCOIT	0.34		4.3	1	n.a.	0.33				0.32
1506-02-1	216-133-4	HHCB	0.34	3.1	5.6	0	Potential P/vP++	0.29				0.66
54464-57-2	259-174-3	OTNE	0.34		5.0	0	Potential P/vP++	0.32				0.56
128-37-0	204-881-4	2,6-di-tert-butyl-p-cresol	0.33		5.0	11	Pot. P/vP	0.35				0.53
74-97-5	200-826-3	Bromochloromethane	0.33	1.1	1.5	189	Pot. P/vP	0.40		23		0.18
113-45-1	204-028-6	methylphenidate	0.33	1.1	-1.2	0	n.a.	0.73			7	0.16
611-59-6	210-271-9	Paraxanthine	0.33	-1.0	-0.5	0	no conclusion/data	0.47				0.16
74-11-3	200-805-9	4-Chlorobenzoate	0.33		-0.7	0	no conclusion/data	0.67	3.8			0.19
58-55-9	200-385-7	Theophylline	0.33		0.0	0	Not P	0.47				0.16
120-32-1	204-385-8	Clorofene	0.33		3.9	0	Pot. P/vP	0.48				0.33
298-00-0	206-050-1	Parathion-methyl	0.33	2.0	2.8	0	n.a.	0.47	1.2	23		0.27
88-04-0	201-793-8	4-chloro-3,5-xylenol	0.33	2.1	3.3	0	Not P	0.55			3	0.30
10540-29-1	234-118-0	Tamoxifen	0.32	5.4	5.0	0	Pot. P/vP	0.43				0.66
31508-00-6	621-375-2	PCB118	0.32	5.9	6.7	0	n.a.	0.05			2292	0.95
60-51-5	200-480-3	Dimethoate	0.32	0.24	1.0	0	n.a.	0.68	4.1			0.16
95-53-4	202-429-0	*o*-toluidine	0.32	1.9	1.4	0	Not P	0.48			6	0.18
1634-04-4	216-653-1	tert-butyl methyl ether	0.32		1.2	200	Potential P/vP++	0.43				0.17
485-72-3	207-623-9	7-hydroxy-3-(4-methoxyphenyl)-4-benzopyrone	0.32		2.7	0	Not P	0.70				0.32

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
121552-61-2	601-785-8	Cyprodinil	0.32	3.0	3.8	0	n.a.	0.42	31			0.39
10287-53-3	233-634-3	Ethyl 4-dimethylaminobenzoate	0.32	2.7	3.0	0	no conclusion/data	0.60			6	0.24
25812-30-0	247-280-2	Gemfibrozil	0.31	3.0	1.6	0	no conclusion/data	0.69				0.28
63-25-2	200-555-0	Carbaryl	0.31	1.8	2.3	0	n.a.	0.51	16	7		0.21
75-45-6	200-871-9	Chlorodifluoromethane	0.31	0.64	1.0	21472	Potential P/vP++	0.47				0.15
72-69-5	200-788-8	Nortriptyline	0.31	3.4	1.5	0	n.a.	0.49				0.35
35065-28-2	621-377-3	PCB138	0.31	6.1	7.1	0	n.a.	-0.02			2292	0.98
101205-02-1	405-230-9	Cycloxydim	0.31		4.0	0	n.a.	0.36				0.39
91465-08-6	415-130-7	Cyhalothrin	0.31		6.6	0	n.a.	0.34	39			0.96
75-25-2	200-854-6	Bromoform	0.31		2.5	34	no conclusion/data	0.33		71		0.20
94-81-5	202-365-3	MCPB	0.31		-0.1	0	n.a.	0.66			7	0.20
637-92-3	211-309-7	2-ethoxy-2-methylpropane	0.31	0.57	1.6	234	Pot. P/vP	0.43				0.18
994-05-8	213-611-4	2-methoxy-2-methylbutane	0.31	0.72	1.7	117	Pot. P/vP	0.43				0.18
189084-64-8	-	PBDE 100	0.31		7.0	0	n.a.	0.15				0.97
39300-45-3	-	Dinocap I	0.31		4.5	0	n.a.	0.18			230	0.65
1929-86-8	217-683-8	Mecoprop	0.30		-0.3	0	no conclusion/data	0.60		7		0.18
16484-77-8	240-539-0	Mecoprop-P	0.30		-0.3	0	n.a.	0.60		7		0.18
28291-75-0	844-374-0	*N*-cyclohexyl-2-benzothiazole-a-mine	0.30		3.8	0	n.a.	0.29				0.31
89-57-6	201-919-1	5-aminosalicylic acid	0.30		-2.3	0	no conclusion/data	0.67			4	0.13
96-76-4	202-532-0	2,4-di-tert-butylphenol	0.30	3.7	4.9	0	P	0.35				0.44

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
25013-16-5	246-563-8	tert-butyl-4-methoxyphenol	0.30	3.1	3.3	0	Not P	0.64				0.28
52315-07-8	276-458-2	Cypermethrin	0.30		6.3	0	n.a.	0.52	25			0.87
51-03-6	200-076-7	2-(2-butoxyethoxy)ethyl 6-propy-lpiperonyl ether	0.30		4.3	0	P	0.31				0.32
140-66-9	205-426-2	4-(1,1,3,3-tetramethylbutyl)phe-nol	0.30	4.0	4.5	0	P	0.37		60		0.44
1330-78-5	809-930-9	Tris(methylphenyl) phosphate	0.30	4.3	4.9	0	Not P	0.54				0.49
37594-64-2	807-571-2	Clotrimazole	0.30		5.1	0	Pot. P/vP	0.25				0.69
72-54-8	200-783-0	*p*,*p*'-DDD	0.29		6.1	0	n.a.	0.12			800	0.90
1119449-37-4	687-832-3	nonylphenol monoethoxylate	0.29		5.2	0	n.a.	0.63				0.34
60-27-5	200-466-7	2-imino-1-methylimidazolidin-4-one	0.29		-1.3	0	Not P	0.60				0.10
85-41-6	201-603-3	Phthalimide	0.29	0.86	1.2	0	Not P	0.54	3.0			0.13
94-74-6	202-360-6	MCPA	0.29		-0.9	0	n.a.	0.67			7	0.17
119515-38-7	423-210-8	Icaridine	0.29		1.4	0	Pot. P/vP	0.63			10	0.16
82657-04-3	617-373-6	Bifenthrin	0.29		6.4	0	n.a.	0.16	61			0.94
103-33-3	203-102-5	Azobenzene	0.29		4.0	1	n.a.	0.35				0.31
531-95-3	208-522-2	Equol	0.29		3.1	0	n.a.	0.65			7	0.29
103-90-2	203-157-5	Paracetamol (Acetaminophen)	0.29	1.3	0.4	0	Pot. P/vP	0.72			2	0.13
216667-08-2	-	Amidosulfobetaine-14	0.29		5.4	0	n.a.	0.57				0.20
74-87-3	200-817-4	chloromethane; methyl chloride	0.28	0.75	1.2	6324	Not P	0.62				0.12
17109-49-8	241-178-1	Edifenphos	0.28		3.8	0	n.a.	0.60				0.20

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
176969-34-9	700-093-4	3-(difluoromethyl)-1-methyl-1*H*-pyrazole-4-carboxylic acid	0.28		-2.7	0	Pot. P/vP	0.61	7.8			0.12
59777-72-9	611-882-7	Ethyl 2-sulfamoylbenzoate	0.28		1.0	0	n.a.	0.65	3.4			0.15
75-00-3	200-830-5	Chloroethane	0.28	0.83	1.5	2843	Potential P/vP++	0.61		71		0.13
106-93-4	203-444-5	1,2-dibromoethane	0.28	0.13	2.1	52	Potential P/vP++	0.39				0.14
105-59-9	203-312-7	2,2'-methyliminodiethanol	0.28	-1.6	-2.3	0	Potential P/vP++	0.77				0.09
69770-45-2	274-110-4	Flumethrin	0.28		6.7	0	n.a.	0.13				0.98
525-66-6	208-378-0	Propranolol	0.28	2.0	1.0	0	no conclusion/data	0.65			6	0.18
68140-48-7	268-799-0	1-[2,3-dihydro-1,1,2,6-tetrame-thyl-3-(1-methylethyl)-1H-inden-5-yl]ethan-1-one	0.28		5.4	0	Pot. P/vP	0.33				0.55
759-94-4	212-073-8	EPTC	0.28	3.0	3.2	0	Pot. P/vP	0.60		7		0.19
74-95-3	200-824-2	Dibromomethane	0.28	1.3	1.9	0	Pot. P/vP	0.39				0.13
62-53-3	200-539-3	Aniline	0.28	1.6	1.1	0	Not P	0.56		7		0.13
122-20-3	204-528-4	1,1',1''-nitrilotripropan-2-ol	0.28	-0.86	-1.6	0	Potential P/vP++	0.69				0.09
105-60-2	203-313-2	ε-caprolactam	0.28		0.0	0	Not P	0.77				0.12
56392-14-4	641-558-0	Metoprolol acid	0.28		-0.1	0	n.a.	0.72			6	0.08
599-64-4	209-968-0	4-Cumylphenol	0.28	3.4	4.0	0	n.a.	0.52				0.27
207-08-9	205-916-6	Benzo[k]fluoranthene	0.28	5.7	5.7	0	n.a.	0.16		71		0.82
94-09-7	202-303-5	Benzocaine	0.27		1.8	0	no conclusion/data	0.64			3	0.14
75-01-4	200-831-0	Chloroethylene	0.27	0.86	1.5	4674	Potential P/vP++	0.59		23		0.13
3739-38-6	223-121-2	3-Phenoxybenzoate	0.27		0.7	0	no conclusion/data	0.81	12		7	0.17

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
100-02-7	202-811-7	4-nitrophenol	0.27	1.4	1.5	0	Not P	0.40	5.1			0.17
108-90-7	203-628-5	Chlorobenzene	0.27	2.5	2.7	435	Potential P/vP++	0.58		71		0.18
309-00-2	206-215-8	Aldrin	0.27	5.3	6.3	0	n.a.	-0.02		708		0.99
149-30-4	205-736-8	Benzothiazole-2-sulfonate	0.27	3.0	1.0	0	no conclusion/data	0.50				0.15
51263-08-2	257-093-8	Sodium hydrogen [6R-(6α,7β)]-3-(acetoxymethyl)-7-[(5-amino-5-carboxylato-1-oxopentyl)amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate	0.26		-2.3	0	Not P	0.80				0.07
75330-75-5	616-212-7	Lovastatin	0.26		3.7	0	n.a.	0.69				0.19
122-39-4	204-539-4	Diphenylamine	0.26	3.4	3.3	0	Potential P/vP++	0.51		2		0.19
3965-55-7	223-578-8	Sodium dimethyl 5-sulphonato-isophthalate	0.26		-5.5	0	P	0.73				0.09
83-34-1	201-471-7	3-methylindole	0.26	2.6	2.6	0	vP	0.62	0.8		6	0.15
19395-41-6	243-020-7	Ritalinic acid	0.25		0.8	0	n.a.	0.67			4	0.08
107-07-3	203-459-7	2-chloroethanol	0.25		0.1	0	Not P	0.73				0.09
72-55-9	200-784-6	*p*,*p*'-DDE	0.25		6.6	0	n.a.	0.13		2292		0.87
95-63-6	202-436-9	1,2,4-trimethylbenzene	0.25	2.6	3.8	345	Not P	0.69		23		0.21
105-67-9	203-321-6	2,4-xylenol	0.25	1.6	2.3	0	Not P	0.72	1.5	2		0.15
115-86-6	204-112-2	Triphenyl phosphate	0.25	3.5	4.4	0	Not P	0.61				0.21
2078-54-8	218-206-6	Propofol	0.25		3.8	6	n.a.	0.59			4	0.20
461-58-5	207-312-8	Cyanoguanidine	0.25	-1.1	-1.7	4	vP	0.65				0.09

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
18507-89-6	242-389-1	Decoquinate	0.25		6.1	0	n.a.	0.73				0.39
112830-95-2	-	HU-210	0.25		6.9	0	n.a.	0.54				0.50
57-88-5	200-353-2	Cholesterol	0.25		5.4	0	Pot. P/vP	0.26				0.68
61566-34-5	262-853-7	ibuprofen methyl ester	0.24		4.3	0	n.a.	0.64			7	0.21
89-83-8	201-944-8	Thymol	0.24	3.1	3.2	0	Not P	0.65			2	0.17
121-75-5	204-497-7	Malathion	0.24	1.8	2.5	0	n.a.	0.82	1.0	2		0.12
360-68-9	206-638-8	5-beta-coprostanol	0.24		6.8	0	n.a.	0.26				0.68
76420-72-9	278-459-3	Enalaprilat	0.24		-2.0	0	n.a.	0.66				0.07
126-71-6	204-798-3	Triisobutyl phosphate	0.24		3.7	0	Not P	0.57				0.18
108-94-1	203-631-1	Cyclohexanone	0.24		0.9	1	Not P	0.71		7		0.10
131-57-7	205-031-5	Oxybenzone	0.24	3.2	3.9	0	vP	0.69				0.22
106-42-3	203-396-5	p-xylene	0.24	2.3	3.2	368	Not P	0.69		23		0.15
50-78-2	200-064-1	*O*-acetylsalicylic acid	0.24	0.74	-2.0	0	Not P	0.88			6	0.08
95-47-6	202-422-2	*o*-xylene	0.24	2.4	3.2	272	Not P	0.69		23		0.15
50-29-3	200-024-3	*p,p*'-DDT	0.24	6.0	6.6	0	n.a.	0.05		229		0.98
52556-42-0	258-004-5	Sodium 3-(allyloxy)-2-hydroxyp-ropanesulphonate	0.24		-4.4	0	Potential P/vP++	0.61				0.06
13826-35-2	237-525-1	3-phenoxybenzylic alcohol	0.24	3.0	2.7	0	Pot. P/vP	0.73			3	0.13
22204-53-1	244-838-7	Naproxen	0.24		0.6	0	Pot. P/vP	0.67			7	0.11
102-71-6	203-049-8	2,2',2''-nitrilotriethanol	0.24	-1.9	-1.8	0	Not P	0.85				0.07
108-38-3	203-576-3	*m*-xylene	0.24	2.3	3.2	351	Not P	0.69		23		0.15

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
83-32-9	201-469-6	Acenaphthene	0.24	3.4	3.9	3	P	0.55		23		0.21
5495-84-1	226-827-9	2-isopropyl-9*H*-thioxanthen-9-one	0.24	4.0	5.0	0	no conclusion/data	0.41				0.31
120-72-9	204-420-7	Indole	0.24	2.0	2.3	0	no conclusion/data	0.61			6	0.11
74-83-9	200-813-2	Bromomethane	0.24	0.68	1.3	1013	Pot. P/vP	0.49	1.8			0.08
515815-48-2	485-140-4	Telmisartan Hydrochlorid	0.24	6.2	5.8	0	Pot. P/vP	0.29				0.73
55285-14-8	259-565-9	Carbosulfan	0.24		4.8	0	n.a.	0.52	5.2			0.27
70628-36-3	634-740-6	Propachlor-OXA	0.24		-2.8	0	n.a.	0.70				0.07
24280-93-1	246-119-3	Mycophenolic acid	0.23		1.8	0	n.a.	0.76				0.09
98-86-2	202-708-7	Acetophenone	0.23	1.3	1.6	0	Not P	0.70		7		0.11
142-68-7	205-552-8	Tetrahydropyran (THP)	0.23	0.38	1.0	18	n.a.	0.53			19	0.09
75-05-8	200-835-2	Acetonitrile	0.23	-0.55	-0.2	9	Not P	0.81				0.08
109-99-9	203-726-8	Tetrahydrofuran	0.23	1.3	0.6	10	Not P	0.55			23	0.08
78-93-3	201-159-0	Butanone	0.23	-0.19	0.4	4	Not P	0.73			6	0.08
67-64-1	200-662-2	Acetone	0.23		0.0	8	Not P	0.74			3	0.08
90-82-4	202-018-6	Pseudoephedrine	0.23	0.17	-0.8	0	n.a.	0.70				0.08
299-42-3	206-080-5	Ephedrine	0.23		-0.8	0	n.a.	0.70				0.08
1137-42-4	214-507-1	4-hydroxybenzophenone	0.23	-1.9	3.0	0	Not P	0.63	17			0.15
1561-92-8	216-341-5	Sodium 2-methylprop-2-ene-1-sulphonate	0.23	1.3	-5.1	0	P	0.64				0.07
1217465-10-5	-	metolachlor CGA 357704	0.23		-0.9	0	n.a.	0.67				0.06

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
60-29-7	200-467-2	Diethyl ether	0.23		1.1	87	no conclusion/data	0.54			23	0.08
13194-48-4	236-152-1	Ethoprophos	0.23		3.4	0	n.a.	0.66	28			0.15
106-44-5	203-398-6	*p*-cresol	0.22	1.7	2.0	0	Not P	0.72		1		0.11
95-48-7	202-423-8	*o*-cresol	0.22	1.3	2.0	0	Not P	0.72		1		0.11
31879-05-7	250-850-3	Fenoprofen	0.22		0.5	0	n.a.	0.69			7	0.11
14838-15-4	207-755-7	Norephedrine	0.22		-1.0	0	n.a.	0.72				0.07
77521-29-0	-	2-amino-3-(5-methyl-3-oxo-1,2-oxazol-4-yl)propanoic acid	0.22		-5.8	0	n.a.	0.62				0.05
581-42-0	209-464-0	2,6-Dimethylnaphthalene	0.22	3.4	4.3	20	n.a.	0.60			10	0.21
51276-47-2	257-102-5	Glufosinate	0.22		-1.9	0	n.a.	0.65				0.05
123-72-8	204-646-6	Butyraldehyde	0.22		0.9	10	Not P	0.90			3	0.07
83-46-5	-	Beta-Sitosterol	0.22		6.4	0	n.a.	0.23				0.72
99-87-6	202-796-7	*p*-cymene	0.22	3.7	4.2	490	Not P	0.63			16	0.18
108-88-3	203-625-9	Toluene	0.22	1.9	2.7	599	Not P	0.73		23		0.11
5975-78-0	637-367-7	Zearalanone	0.22		3.5	0	n.a.	0.68			7	0.24
5466-77-3	629-661-9	Octyl methoxy cinnamate	0.21		5.2	0	n.a.	0.74				0.25
3039-83-6	221-242-5	Sodium ethylenesulphonate	0.21		-6.0	0	Not P	0.67				0.06
54-21-7	200-198-0	Sodium salicylate	0.21	0.25	-1.4	0	Not P	0.83		2		0.08
19466-47-8	243-087-2	beta-Stigmastanol	0.21		7.2	0	n.a.	0.23				0.72
288-13-1	206-017-1	Pyrazole	0.21	-0.40	-0.2	0	Pot. P/vP	0.70				0.08
75-15-0	200-843-6	Carbon disulphide	0.21	1.1	1.9	3689	Not P	0.67				0.08

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
61789-40-0	224-292-6	(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammonium hydroxide	0.21		0.4	0	Not P	0.80				0.08
101-84-8	202-981-2	Diphenyl ether	0.21	3.3	4.0	2	Potential P/vP++	0.73		23		0.16
15687-27-1	239-784-6	Ibuprofen	0.21	2.8	0.9	0	P	0.57			8	0.10
979-32-8	213-559-2	Estradiol-17-valerate	0.21		5.6	0	n.a.	0.60				0.31
86-73-7	201-695-5	Fluorene	0.21	3.5	4.1	9	Pot. P/vP	0.53	37	23		0.18
1071-83-6	213-997-4	glyphosate	0.21		-8.7	0	n.a.	0.69	11			0.05
77-73-6	201-052-9	3a,4,7,7a-tetrahydro-4,7-methanoindene	0.21	2.5	2.8	145	Potential P/vP++	0.57			10	0.12
86-74-8	201-696-0	Carbazole	0.21	3.4	3.4	0	Pot. P/vP	0.52				0.15
84-66-2	201-550-6	Diethyl phthalate	0.21	2.3	2.6	0	Not P	0.86		7		0.09
90-12-0	201-966-8	1-methylnaphthalene	0.21	3.1	4.1	15	Pot. P/vP	0.60		7		0.16
90-43-7	201-993-5	Biphenyl-2-ol	0.21	2.5	3.1	0	Not P	0.64			4	0.12
100-41-4	202-849-4	Ethylbenzene	0.21		3.1	383	Pot. P/vP	0.67		23		0.12
84-69-5	201-553-2	Diisobutyl phthalate	0.21	3.0	4.2	0	Not P	0.76			7	0.13
131-11-3	205-011-6	Dimethyl phthalate	0.21	1.9	1.8	0	Not P	0.86		7		0.08
90-15-3	201-969-4	1-naphthol	0.20	2.3	2.9	0	Not P	0.64			2	0.11
66069-34-9	266-104-5	[2R-(2α,3Z,5α)]-3-(2-hydroxyethylidene)-7-oxo-4-oxa-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, compound with tert-butylamine (1:1)	0.20	1.3	-4.3	0	Not P	0.71				0.04

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
5728-52-9	227-233-2	Felbinac	0.20		0.4	0	n.a.	0.62				0.08
139110-80-8	691-117-1	Zanamivir	0.20		-6.9	0	n.a.	0.66				0.04
103-26-4	203-093-8	Methyl cinnamate	0.20		2.6	0	Not P	0.78				0.09
102-76-1	203-051-9	Triacetin	0.20	-0.73	0.4	0	Not P	0.96				0.06
13048-33-4	235-921-9	Hexamethylene diacrylate	0.20		2.7	0	Not P	0.90			6	0.10
98-82-8	202-704-5	Cumene	0.20		3.7	641	Pot. P/vP	0.67		23		0.13
521-35-7	689-788-0	CBN / Cannabinol	0.20	5.6	6.1	0	n.a.	0.57				0.38
89-78-1	201-939-0	Menthol	0.20	2.0	3.2	0	Not P	0.64			2	0.09
56-53-1	200-278-5	Diethylstilbestrol	0.20		4.6	0	n.a.	0.52				0.20
103-65-1	203-132-9	*n*-Propylbenzene	0.20		3.7	616	n.a.	0.67		23		0.13
26530-20-1	247-761-7	octhilinone (ISO); 2-octyl-2*H*-iso-thiazol-3-one	0.19	1.3	2.7	0	no conclusion/data	0.63				0.08
148553-50-8	-	Pregabalin	0.19		-0.9	0	n.a.	0.71				0.04
120-51-4	204-402-9	Benzyl benzoate	0.19	3.8	3.7	0	Not P	0.72			7	0.12
108-95-2	203-632-7	Phenol	0.19	1.5	1.6	0	Not P	0.76			2	0.07
132-64-9	205-071-3	Dibenzofuran	0.19	3.5	3.9	8	n.a.	0.51		7		0.15
100-42-5	202-851-5	Styrene	0.19		3.1	182	Not P	0.69		7		0.09
208-96-8	205-917-1	Acenaphthylene	0.19	3.2	3.9	0	n.a.	0.54			10	0.13
65059-42-9	265-332-2	Trimethyloctylammonium methyl sulphate	0.19		-2.1	0	Not P	0.72				0.06
99-76-3	202-785-7	Methyl 4-hydroxybenzoate	0.19		2.1	0	Not P	0.81				0.07

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
141-78-6	205-500-4	Ethyl acetate	0.19		0.8	18	Not P	0.85			3	0.06
120-47-8	204-399-4	Ethyl 4-hydroxybenzoate	0.19		2.5	0	Not P	0.81			3	0.08
110-83-8	203-807-8	Cyclohexene	0.19	2.0	2.8	3484	Potential P/vP++	0.71		7		0.08
4247-02-3	224-208-8	Isobutyl 4-hydroxybenzoate	0.19		3.2	0	Not P	0.76			7	0.10
26538-44-3	247-769-0	A-zearalanol	0.19		3.7	0	n.a.	0.72			6	0.15
94-13-3	202-307-7	Propyl 4-hydroxybenzoate	0.19		2.9	0	Not P	0.81			3	0.09
120-40-1	204-393-1	*N*,*N*-bis(2-hydroxyethyl)dodecanamide	0.18		3.7	0	Not P	0.94				0.06
3598-16-1	222-746-8	Sodium phenoxyacetate hemihydrate	0.18		-2.4	0	Not P	0.84			13	0.05
142-78-9	205-560-1	*N*-(2-hydroxyethyl)dodecanamide	0.18		3.9	0	Not P	0.89				0.07
123-03-5	204-593-9	Cetylpyridinium chloride	0.18	4.8	3.2	0	Pot. P/vP	0.65				0.15
501-52-0	207-924-5	3-phenylpropionic acid	0.18	3.3	-0.9	0	no conclusion/data	0.73			5	0.05
119-36-8	204-317-7	Methyl salicylate	0.18	1.6	2.5	0	Not P	0.81			3	0.07
92-52-4	202-163-5	Biphenyl	0.18	2.9	3.9	22	Not P	0.65			10	0.12
57-09-0	200-311-3	Cetrimonium bromide	0.18		1.8	0	Not P	0.68				0.13
81093-37-0	689-360-3	Pravastatin	0.18		1.0	0	n.a.	0.76				0.04
62-49-7	200-535-1	Choline	0.17		7.6	0	Not P	-0.41				1.00
70434-92-3	804-093-6	Cannabicyclohexanol	0.17		7.3	0	n.a.	0.58				0.22
110-82-7	203-806-2	Cyclohexane	0.17		3.3	3039	Not P	0.72		23		0.09
104273-73-6	806-797-9	Trinexapac acid	0.17		-1.9	0	n.a.	0.72	10			0.05

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
68411-44-9	270-126-0	Benzene, butyl-, branched and linear	0.17	3.2	4.3	535	no conclusion/data	0.67			16	0.14
154826-10-5	833-627-0	Octylphenoxy acetic acid	0.17		1.8	0	n.a.	0.64			8	0.08
5989-27-5	227-813-5	(R)-*p*-mentha-1,8-diene	0.16	3.2	4.5	817	Not P	0.58			16	0.12
26636-32-8	257-203-4	Diethoxyoctylphenol	0.16		5.1	0	n.a.	0.83			19	0.10
106807-78-7	631-246-2	Nonylphenoxyethoxy acetic acid	0.16		2.3	0	n.a.	0.63			8	0.09
1241-94-7	214-987-2	2-ethylhexyl diphenyl phosphate	0.16		5.4	0	Not P	0.62				0.12
26027-38-3	500-045-0	4-Nonylphenol, ethoxylated	0.16	2.6	5.5	0	no conclusion/data	0.82			19	0.11
15935-54-3	-	Carboxyibuprofen	0.16		-2.5	0	n.a.	0.62			4	0.04
1643-20-5	216-700-6	Dodecyldimethylamine oxide	0.16	2.5	4.6	0	Not P	0.70				0.09
99-66-1	202-777-3	2-propylvaleric acid	0.15		0.6	0	Not P	0.74			4	0.04
209414-07-3	635-711-0	JWH-018	0.15		6.5	0	n.a.	0.42				0.20
110-62-3	203-784-4	Valeraldehyde	0.14	0.39	1.3	5	Not P	0.93			3	0.03
85-68-7	201-622-7	Benzyl butyl phthalate	0.13	3.4	4.7	0	Not P	0.82		7		0.06
6197-30-4	228-250-8	Octocrilene	0.13	4.5	5.8	0	Potential P/vP++	0.70				0.16
104-40-5	203-199-4	*p*-nonylphenol	0.13	4.6	5.9	0	Pot. P/vP	0.70				0.09
1806-26-4	217-302-5	octylphenol	0.12	4.2	5.3	0	n.a.	0.70				0.08
107-66-4	203-509-8	Dibutyl hydrogen phosphate	0.12	0.50	-1.3	0	Potential P/vP++	0.67				0.03
94-26-8	202-318-7	Butyl 4-hydroxybenzoate	0.11	2.6	3.3	0	Not P	0.85			7	0.04
71-36-3	200-751-6	Butan-1-ol	0.11	0.11	0.8	1	Not P	0.87			3	0.02
139-13-9	205-355-7	Nitrilotriacetic acid	0.11		-7.4	0	Not P	0.71				0.01

CAS No.	EC No.	Name	vPvM	Ad1	Ad2	V	Deg1	Deg2	Deg3	Deg4	Deg5	Deg6
78-51-3	201-122-9	Tris(2-butoxyethyl) phosphate	0.10	2.5	3.4	0	Not P	0.55				0.03
7173-51-5	230-525-2	Didecyldimethylammonium chloride	0.10	2.8	5.4	0	Not P	0.74				0.07
109-66-0	203-692-4	Pentane	0.10		3.7	15645	Not P	0.80		23		0.03
84-74-2	201-557-4	Dibutyl phthalate	0.08		4.6	0	Not P	0.93		7		0.02
117-81-7	204-211-0	DEHP	0.07	5.7	7.5	0	n.a.	0.83		7		0.05
13560-89-9	236-948-9	1,6,7,8,9,14,15,16,17,17,18,18-dodecachloropentacyclo[12.2.1.16,9.02,13.05,10]octadeca-7,15-diene	0.07		10.4	0	vP	-0.48				1.00
126-73-8	204-800-2	Tributyl phosphate	0.06	1.8	3.7	0	Not P	0.82				0.01
123312-54-9	404-050-8	*N*,*N*-dimethyl-*N*,*N*-dioctadecylammonium hydrogen sulfate	0.05		10.1	0	no conclusion/data	0.62	28			0.29