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Capacity building for better water management



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Prioritisation process: Monitoring-based ranking

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I. Introduction

I.1. Background and overall prioritisation process

Article 16(4) of the Water Framework Directive (WFD, Directive 2000/60/EC) requires the Commission to identify priority substances that present a significant risk to or via the aquatic environment, including such risks to water used for the abstraction of drinking water. The first list of priority substances was established by Council Decision 2455/2001/EC. The Environmental Quality Standard Directive (EQSD, Directive 2008/105/EC) sets out the quality standards for the first list of priority substances. According to Article 8 of the EQSD, the Commission shall review the list of priority substances by 13 January 2011, at the latest.

According to Article 16(2) of the WFD, the substances should be prioritised for action on the basis of risk to or via the aquatic environment identified by

- risk assessment carried out under Regulation (EEC) No 793/93 (Existing Substances Regulation, replaced by REACH Regulation 1907/2006), Directive 91/414/EC (Pesticides Directive) and Directive 98/8/EC (Biocides Directive), or
- targeted risk-based assessment (following the methodology of Existing Substances Regulation) focusing solely on aquatic ecotoxicity and on human toxicity via the aquatic environment.

Alternatively, in absence of those assessments, a simplified risk assessment could be carried out, which involves the collection of evidences such as the widespread contamination of substances of concern based on monitoring data, production or use volumes, use patterns and aquatic ecotoxicity and human toxicity via exposure routes. The COMMPS¹ procedure is an example of this simplified risk assessment that was used as a basis to identify the first list of priority substances in 2001.

Since 2005, the INERIS/IOW consortium has provided technical and scientific support to DG Environment in the work to review the list of priority substances. The work builds on the previous experience with the COMMPS procedure and the comments made on the procedure by the Scientific Committee on Toxicity, Ecotoxicity and the Environment² (CSTEE, currently Scientific Committee for on Health and Environmental Risks). Along the process, extensive consultations and discussions have been held with experts from Member States, stakeholders and Commission Services at the Working Group E on Priority Substances under the WFD Common Implementation Strategy³. Since 2007, the European Chemicals Bureau⁴ of the European Commission's Joint Research Centre (JRC, Institute for Health and Consumer Protection) has been actively involved in the prioritisation work.

¹ Revised proposal for a list of priority substances in the context of the Water Framework Directive (COMMPS procedure). Fraunhofer-Institut, June 1999. Available at http://ec.europa.eu/environment/water/water-dangersub/pdf/commps_report.pdf. COMMPS stands for Combined Monitoring-based and Modelling-based Priority Setting Scheme.

² Opinion on the revised proposal for a List of Priority Substances in the Context of the Water Framework Directive (COMMPS Procedure) prepared by the Fraunhofer-Institut (Germany) - Final report Opinion adopted at the 11th CSTEE plenary meeting on the 28th of September 1999. http://ec.europa.eu/health/ph_risk/committees/sct/docshhtml/sct_out49_en.htm

³ Expert Advisory Forum on Priority Substances until 2006.

⁴ Currently "Chemical Assessment and Testing" Unit





After some initial discussions within the Working Group on Priority Substances, a background document was presented in March 2007 that extensively discussed the options for prioritisation (Bonnomet and Dulio, 2007⁵, from now on referred to as “Background Document” in the present report). As a conclusion from the discussions, it was decided to start the work by carrying out first a monitoring-based prioritisation. A data collection was launched for this purpose in 2008.

Based on the “Background document” and the discussions held so far at the Working Group, INERIS presented a methodology and a test run of the monitoring-based prioritisation exercise in March 2008. In October 2008, INERIS presented to the Working Group a more elaborated methodology for the monitoring-based prioritisation and a first ranking results based on the dataset available at that time (Bonnomet, 2008⁶, referred to from now on as “First stage ranking report”). Linked to this report, a document dedicated to the database and the treatment of data provided by the Member States was produced by IOW (Fribourg-Blanc, 2008⁷, referred to as the “Central database report”).

The October 2008 reports were extensively discussed and consulted with the Working Group E on Priority Substances. At the meeting in October 2008 it was also decided to do a supplementary data collection exercise to fill a number of gaps and improve the data available⁸. As a result, the database was substantially expanded (see section III for more details on the contents of the monitoring database).

Following discussions and written comments on the “First stage ranking report” and the “Central database report”, a thorough discussion on open issues was held at the Working Group meeting in March 2009, and an issue paper on general issues and substance specific issues related to PEC and PNEC calculations was produced and circulated for written comments in April 2009.

This report reflects the outcome of the monitoring-based prioritisation exercise that has been informed by the extensive consultation process described above.

In its opinion of 1999 on the COMMPS procedure, the CSTE^E stated that *“Monitoring data provide an excellent basis, from direct observation, to get information on European environmental conditions. However, monitoring data cannot be used as the single scoring method because the available information is incomplete and only covers a set of substances which were considered “relevant” in the past. Thus, the current monitoring information is biased by previous decisions on which substances should be monitored. Those decisions taken in the past: (1) mostly focused on Member States needs, knowledge and capacity; (2) do not necessarily address the same aims and goals of the List of Priority Substances under the Water Framework Directive, and (3) cannot faithfully represent the current water pollution problems. Therefore, it is important to incorporate a second system, to allow inclusion in the final list, of substances with a high potential risk for aquatic organisms for which no monitoring information is available to date”*.

⁵ Prioritisation of Substances: BACKGROUND DOCUMENT

(http://circa.europa.eu/Members/irc/env/wfd/library?!=working_groups/priority_substances/priority_substances/01st_meeting_2007/methodology-for-prioriti/ EN_1.0_&a=d)

⁶ WG-E(4)-08-05 - Prioritisation process-1st stage ranking

⁷ WG-E(4)-08-03 - The central database and associated data treatments

⁸ The main reasons to launch a supplementary data collection was to allow those countries that had not provided data to do so, improve the available data for sediment and biota, collect information for the substances included in Annex III of the EQSD and improve the available data for metals in the dissolved phase.





Despite the tremendous qualitative and quantitative jump from the COMMPS monitoring database (ca. 700 000 analysis of 314 substances from 15 countries) to the current monitoring database (ca. 14 000 000 analysis of 1 153 substances from 28 countries), the above statement by the CSTEЕ remains valid. Monitoring-based prioritisation provides an excellent basis for prioritisation but, as has been repeatedly raised at the Working Group E on Priority Substances, it overlooks substances that may pose a risk to or via the aquatic environment but are not monitored.

Since November 2007 an Expert Group working on Prioritisation (sub-group of the Expert Group on Environmental Quality Standards) was appointed and chaired by JRC. According to its mandate, the group is developing a modelling-based methodology that will complement the monitoring-based methodology presented in this report. The Expert Group is also discussing how to use the information from monitoring and how to combine the outcomes of both processes. This approach follows the opinion of the CSTEЕ, which recognised that *“monitoring and modelling based approaches have disadvantages and benefits”* and therefore *“must be run as parallel approaches before being combined in a final step”*⁹.

In order to provide a complete picture of the overall prioritisation process based on the two approaches run in parallel, a general scheme has been produced by the Expert Group on Prioritisation in May 2009 and is attached to this report (Annex I). The proposed scheme still has to be consulted and discussed within the Working Group E on Priority Substances.

I.2.Methodology based on monitoring data ranking

The prioritisation methodology based on monitoring data and produced by INERIS comprises the following major steps:

- Step 1: Establish the manageable list
- Step 2: Design procedures for data collection, data processing and data treatment
- Step 3: Choose relevant parameters to evaluate effects data
- Step 4: Develop mathematical algorithms for prioritisation of substances
- Step 5: Expert review and presentation of the results

The aim of this report is to describe the prioritisation methodology based on monitoring data developed by INERIS/IOW consortium and to present the results obtained following the methodology proposed. According to the scheme attached in Annex I, the list of substances will be delivered.

⁹ See opinion of the CSTEЕ of 28 September 1999 referred to in footnote 2.





1.2.1 General principles, including prioritisation algorithms

a. General principles

Art. 16 of the WFD is about setting priority for pollution control, including EQS derivation, and emission controls. In this context, a reliable assessment of risks is critical because costs due to unnecessary pollution control measures should be minimised. This implies that the selection of priority substances should rely on hard facts, and in particular strong evidences for risk should be demonstrated in order to get significant benefits from the pollution control measures.

The solution should be compatible with the objectives of art. 16 of the WFD. In particular according to art. 16(2), substances shall be prioritised on the basis of available risk assessments. In this article, 3 tiered categories of risk assessments are distinguished depending on their level of details and of confidence:

- The 1st tier category deals with risk assessments which were completed for substances explicitly cited by paragraph 16(2)a of the WFD: i.e. existing substances evaluated under Reg. (EEC) 793/93, pesticides evaluated under Dir. 91/414/EEC and biocides evaluated under Dir. 98/8/EC. Those substances must be considered as candidate priority substances when the risk assessment identifies a risk to or *via* aquatic environment.
- The 2nd tier category is based on paragraph 16.2(b, 1st §) of the WFD. Substances have to be considered as candidate priority substances if risks have been identified by targeted assessments focusing on ecotoxicity and human toxicity *via* the aquatic environment. This may include substances under still ongoing risk assessments (e.g. draft risk assessment reports if conclusions about risks to or *via* the aquatic environment are agreed). This may also embrace substances not covered by Reg. (EEC) 793/93, Dir. 91/414/EEC or Dir. 98/8/EC, but considered under other pieces of legislation (e.g. substances under Dir. 93/67/EEC, pharmaceuticals under Dir. 2001/82/EC or Dir. 2001/83/EC) or substances evaluated on a voluntary basis.
- The 3rd tier category is about a simplified risk-based procedure in accordance with paragraph 16.2(b, 2nd §) of the WFD. It addresses those substances for which a simplified assessment has indicated a potential high level of concern (high hazard and high exposure) to or *via* the aquatic environment. Any substance for which risk to or *via* the aquatic environment is suspected by several Member States (in particular, substances of concern identified after WFD art. 5 or Dir. 76/464/EEC art. 7 reports) could virtually belong to this category.

In principle, reporting for art. 7 Dir. 76/464/EEC or for art. 5 WFD should cover all the known relevant substances for each Member State. As a matter of fact, the list of priority substances is expected to be a subset of all these national relevant substances but have to be selected on the basis of criteria for EU relevance.





Indeed, priority substances should be substances for which a widespread risk at EU level can be demonstrated, or at least suspected¹⁰. By virtue of the subsidiary principle, substances that show only local risks are not relevant for Community wide actions and should not be included into the WFD priority list. In other words, local problems should be tackled locally, when EU wide problems should be covered by EU wide measures.

So, information like the number of Member States and river basin districts involved could serve as a basis for deselecting substances that are of local concern only. This approach was already used in the COMMPS procedure and is used as well in the monitoring-based prioritisation presented in this report.

1.2.2 Advantages of the monitoring-based methodology

The prioritisation presented in this report is underpinned by a monitoring database which is by far the best and most extensive ever compiled at European level. As recognised by the CSTE (see section 1.1), the monitoring-based approach is an excellent basis for prioritisation as provide direct evidence of the presence of substances in the environment.

In the absence of reliable and sufficient monitoring data, modelling can serve as a complementary approach to identify risks from substances.

1.2.3 Limitations of the monitoring-based methodology

a. How to cope with the lack of data?

Art. 16 of the WFD implies that substances cannot be prioritised if there are no available evidences of risk to or via the aquatic environment, either from completed, targeted or simplified risk assessments. It would not be possible to prioritise substances if there is no data available.

The fact is that data are lacking for numerous substances. This may precisely be seen as a purpose of concern, and it is now actually largely acknowledged that emerging pollutants will have to be regulated, sooner or later. Therefore, it would be definitively worthwhile to get data for such substances. But it is not under the scope of art. 16 to ask for the production of new data. This should be done under other contexts.

For example, pursuant to articles 5 and 8 of the WFD, Member States should identify and monitor substances liable to jeopardise the achievement of good status. Member States have therefore interest in developing knowledge in the identification and evaluation of emerging pollutants. Also, knowledge is expected to increase with the implementation of other pieces of legislation. For instance, Dir. 91/414/EEC and Dir. 98/8/EC require risk assessments (and therefore data) for active substances to be authorised in pesticide or biocide products, respectively. Finally, in replacement of Reg. EEC 793/93 and of Dir. 93/67/EEC, REACH will require submission of data and risk assessments for dangerous chemicals or for chemicals with significant production/importation volumes.

¹⁰ Monitoring data are preferable for demonstrating widespread contamination, though widespread occurrence can also be predicted from modelling results and substances' usage data.





b. Priority setting should rely on strong evidences for risk but how should we deal with time and resources constraints?

Time and resources are obviously essential to collect and validate data and evidences for demonstrating risk. Time is needed to retrieve the data. This depends principally on their format: are the data compiled in preformatted databases, reported in easily importable electronic format, or only available on paper documents? Time is also needed to check the reliability of the data. An in-depth risk assessment usually requires lots of time.

Data for substances identified under tier 1 or tier 2 assessment categories (see section I.2.1a) are easily available and have been thoroughly validated by competent authorities. But for substances under tier 3 category, data has to be retrieved from various sources with various formats and with diverse and sometimes unknown reliabilities. Then, the time required to collect and to check data for tier 3 substances can be substantial depending on the number of substances to be considered and the level of reliability required.

Due to available resources and time constraints, the number of substances to be simultaneously considered for the candidate list should therefore stay limited and manageable. Considering all substances of tiers 1, 2 and 3 would lead to a long list of candidate substances which would not be possible to process. Therefore, a compromise has been found to define a list of candidate substances which remains manageable.

c. How to cope with non monitored substances ?

The present prioritisation process will focus on candidate substances that are monitored and a modelling approach is expected to fill in the gap of non monitored substances, including emerging pollutants. Indeed, emerging substances of high concern may exist, but for which data and evidences are currently scarce or uncertain. The implementation of the WFD is expected to improve substantially the monitoring data that is currently available. In the future additional knowledge will be available from the risk assessments under REACH, Dir. 91/414/EEC, Dir. 98/8/EC and also from the scientific literature.

II. Step 1: Establishment of the manageable list of candidate substances

Aquatic ecosystems are facing with potentially thousands, if not millions, of chemical contaminants. In the absence of information on these contaminants, no scientific reasons can be invoked to *a priori* not consider all these substances as candidates for prioritisation. Unfortunately, the fact is that information is scarce or lacking for the vast majority of them. Indeed, it is not inconceivable that the identity of some of them is not even known.

When information exists, easy access to it is not guaranteed. It may be compiled in databases, reported in easily importable electronic format, but some data can only be retrieved from plain text format or paper. Furthermore, some information may not be publicly available. Actions have been initiated by the EC to promote the production of new data, easy access to information *via* centralised databases (e.g. WISE, E-PRTR, REACH-IT), and improved data-sharing. But for the time being, an interim solution is needed.





Relevant parameters were selected on the basis of risk to or via aquatic environment and accordingly to Article 16(2) of the WFD. Therefore, parameters had to be chosen in order to properly characterise together risk to organisms living in the water column, risk to benthic organisms, risk to predators *via* secondary poisoning and risk to human health *via* aquatic exposure routes as described in Section IV. of this report.

The final size of the manageable list of candidate substances was decided on the basis of the available time and resources. To this end, the manageable list is defined via the criterion of monitoring only: definition of the manageable list is based on the number of countries monitoring the substances¹¹ and it was decided to limit the candidate list to about 300 substances.

Identification of the manageable list is given in section III.3.2 (page 16).

III. Step 2: Data collection, associated data treatments and data processing

III.1. Introduction

For the monitoring-based prioritisation process, a data collection is needed. Reflections on how to proceed started with the identification of potential data sources that could be collected and gathered for use in the monitoring based part of the prioritisation as presented in the document *EAF(8)-04/02/INERIS Data collection and processing.doc*. This was completed by the definition of the minimum requirements for these data to make them useful in the process, gathered in a data collection template defined in the document "Common template for data collection" first proposed at the EAF (9) meeting of October 2006. The final template is reported in Annex II of this report.

In the "Background document" (Bonnomet and Dulio, 2007)¹², several options in relation with data collection (data sources, metadata for quality check) and data processing (plausibility check, data aggregation) were presented. The procedures finally applied for preparation and treatment of the central database envisaging as well the PEC calculation are described in "Central database report" (Fribourg-Blanc, 2008)¹³.

With the agreed template, a data collection tool to gather the datasets was developed and circulated (see for more information <http://www.oieau.fr/WISE-end-user-tool/>).

Monitoring data was collected in two periods, from February 2008 until July 2008 and from November 2008 until January 2009.

¹¹ This approach was also used in the monitoring-based part of the COMMPS procedure.

¹² Bonnomet, V. and Dulio, V. (2007). Prioritisation of Substances: Background document. Version 3 (March 2007).

¹³ WG-E(4)-08-03 - The central database and associated data treatments





III.2. Data collection

III.2.1 Tools and requirements

The data collection was defined with the minimum following characteristics:

- compartment: surface water,
- data from years 2000 to 2008,
- dangerous substances
- data with geo referenced stations, including RBD and water body category
- matrices: water, sediment and biota,
- clearly specified fractions (e.g. sediment fraction below 2mm, benthic invertebrates)

They were translated more precisely in a series of fields that lead to define the data collection template (for more details see Annex II), validated at the WG E(3) meeting. In addition flexibility was introduced during the data collection i.e. a dataset can still be acceptable in the absence of the following fields:

- name of laboratory,
- data source,
- type of station (considering that this labelling was not defined before end of 2006)
- LoQ or LoD using following rules:

Minimum information	LoD	LoD	LoQ	-
Value reported	<=LoD	>LoD and no LoQ	<=LoQ	>LoQ

A data collection tool was developed in Microsoft Access format with a dedicated function to allow the production of an exported file in XML format associated with summary information on problems found during the export. (for more information see <http://www.oieau.fr/WISE-end-user-tool/> and the End-user tool documentation available at the same place in the tool zip file: documentation-v8.pdf, where both the use of the tool is explained, and database and its data dictionary are clearly defined and described).

A central database tool was developed on the same basis with a dedicated function to allow the correction for regional characters and parsing of the files in XML format produced by the export function and import of them, and with different checking tools to allow feedback to the data providers.

With the increase of the central database size, the tool was re-developed in a different format on exactly the same basis and with the same functions using licence free software. This allowed adding direct link to a website showing summary statistics on each substance represented in the database.

III.2.2 Data collection steps

The data collection was then conducted using the following steps:

1. The consultant sends a request to each WG E representative with link to the tool.
2. WG E representative select relevant dataset(s), format them, download the tool and fill it with the prepared datasets, export the data, make additional checking based on the feedback provided by the tool, correct the dataset, export it again and send it to the consultant,





3. The consultant download the file, parse it and correct regional characters, then import it in an empty data collection tool, check the feedback provided by the import tool, make additional checking through a series of dedicated queries that assesses the files against the defined template, but also for quality and referential integrity, and report back all the results and questions to the data provider, asking for corrections, additions and confirmation of the summary figures on the dataset content.

WARNING: the content of the datasets provided is considered already checked by the data provider and except to check LoD is below LoQ, no plausibility check is made on the data.

4. WG E representative data provider checks and provides all necessary answers to the consultant. (Steps 3 and 4 can be repeated several times up to satisfaction of all requirements)

5. The consultant imports the validated files in the central database.

The following scheme illustrates the process described in this chapter.



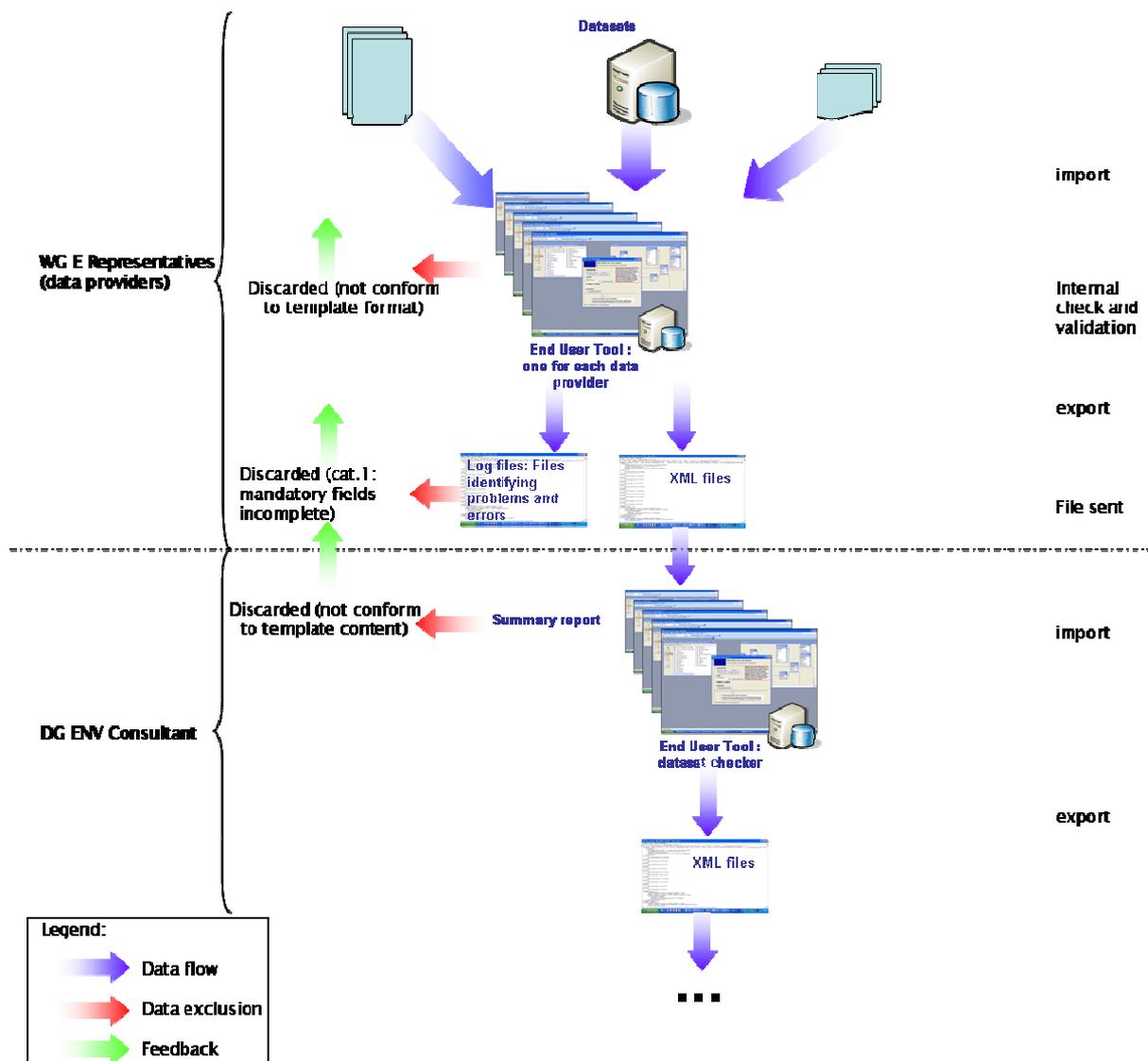


Figure 1: Data collection process

III.2.3 Data corrected during data collection

For absence of Latitude or Longitude, this is supplemented by position of the RBD centroid calculated by a GIS (mainly for Italian stations).

For incoherence between fraction and matrix (example: fraction of analysis on water when reported matrix of sampling is sediment), the data provider is consulted for correction.

When either $LoD > LoQ$, or a new fraction is provided, or analyses are provided with no sampling and/or sampling with no station, the data provider is consulted for correction.

In all cases, in the absence of answers, the data are excluded.





III.2.4 The data excluded during data collection

The following data are discarded:

- data measured before year 2000
 - data for groundwater (the database contains datasets for surface water only)
- nutrient substances (e.g. nitrates, phosphates) and other substances not relevant for priority and priority hazardous substances and listed in the following table (Note that excluded determinands are kept on purpose in the original language):

Table 1: List of excluded determinands

Substance Name	Comment
water temperature	in water sampling
pH-Wert	in water sampling
Total Nitrogen	delete (not relevant)
Phosphorus (total)	delete (not relevant)
Chemical Oxygen Demand (COD)	delete (not relevant)
Base-Neutral	delete (not relevant)
Total Organic Carbon (TOC)	for water sampling
Suspended Particulate Matter (SPM)	for water sampling
N-NH ₄ (Ammonium)	delete (not relevant)
Total organic carbon in dry sediment	delete (not relevant)
Inhibiteurs de cholinesterase	delete (not relevant)
N total (Azote)	delete (not relevant)
N-NH ₃ libre	delete (not relevant)
N-NO ₃ (Azote nitrique)	delete (not relevant)
P total (Phosphore)	delete (not relevant)
Substances tensioactives anioniques	delete (not relevant)
Substances tensioactives non-ioniques	delete (not relevant)
Estrogenic Activity	delete (not relevant)
Chemischer Sauerstoffbedarf	delete (not relevant)
Detergents	delete (not relevant)
Oil products hydrocarbons (index)	delete (not relevant)
N total Kj (Azote org + ammoniacal)	delete (not relevant)
Adsorbable organic halogen (AOX as Cl)	delete (non sufficiently specific derminand)

Note: where relevant, some data were transferred to the additional information for water sampling.

- datasets for which one or more of the following metadata is missing:
 - absence of RBD
 - absence of water body category (river, lake, transitional water, coastal water)
 - absence of date of sampling or date of analysis (at least one of the two must be provided)
 - matrix sample missing (water, sediment, biota), or not sufficiently detailed i.e. "Other" or "Other biota"
 - Fraction analysed:
 - missing,
 - not sufficiently detailed i.e. "Whole" (for matrix Other or Other biota), "Sediment other" (for sediment),





- Surface Particulate Matter (SPM) with no concentration level of SPM or with raw concentration value, not corrected / converted in $\mu\text{g/L}$ (taking into account the level of SPM in the sample)
- ambiguity on name of the determinand and CAS N^o, except for some groups of substances (DDT Total, Total PCBs)
- absence of Value + Unit
- absence of Limit of Detection or Limit of Quantification except where the data provider reports values of analyses above the Limit of Quantification (for all other cases at least one of the two LoD or LoQ must be provided and >0 , and they should be coherent: $\text{LoD} < \text{LoQ}$)

All discarded data were reported to each data provider with exact reason for discard, allowing the data provider to check and confirm or correct the dataset and report it back again.

III.3. Gathering data in a central database

Once the respective datasets are clean and ready, they are imported in the central database. Then the resulting updated main reference lists (fractions, substances and units) are checked and updated: various problems not already addressed in the previous treatments applied on each individual dataset are identified:

- different fractions that need to be harmonised (e.g. sieved sediments at different depth)
- substance specific units that can be transformed,
- same name or similar name with different CAS,
- absence of CAS,
- wrong CAS
- inconsistency in dates,
- type of monitoring station
- ...

They are corrected with the respective data providers.

Then, it is necessary to homogenise the data to allow calculation: same unit (for details, see Annex IV), treatment of the analyses with regards to their LoD and LoQ, and discarding of data with high LoD or LoQ.

The following scheme illustrates the process described in this chapter.



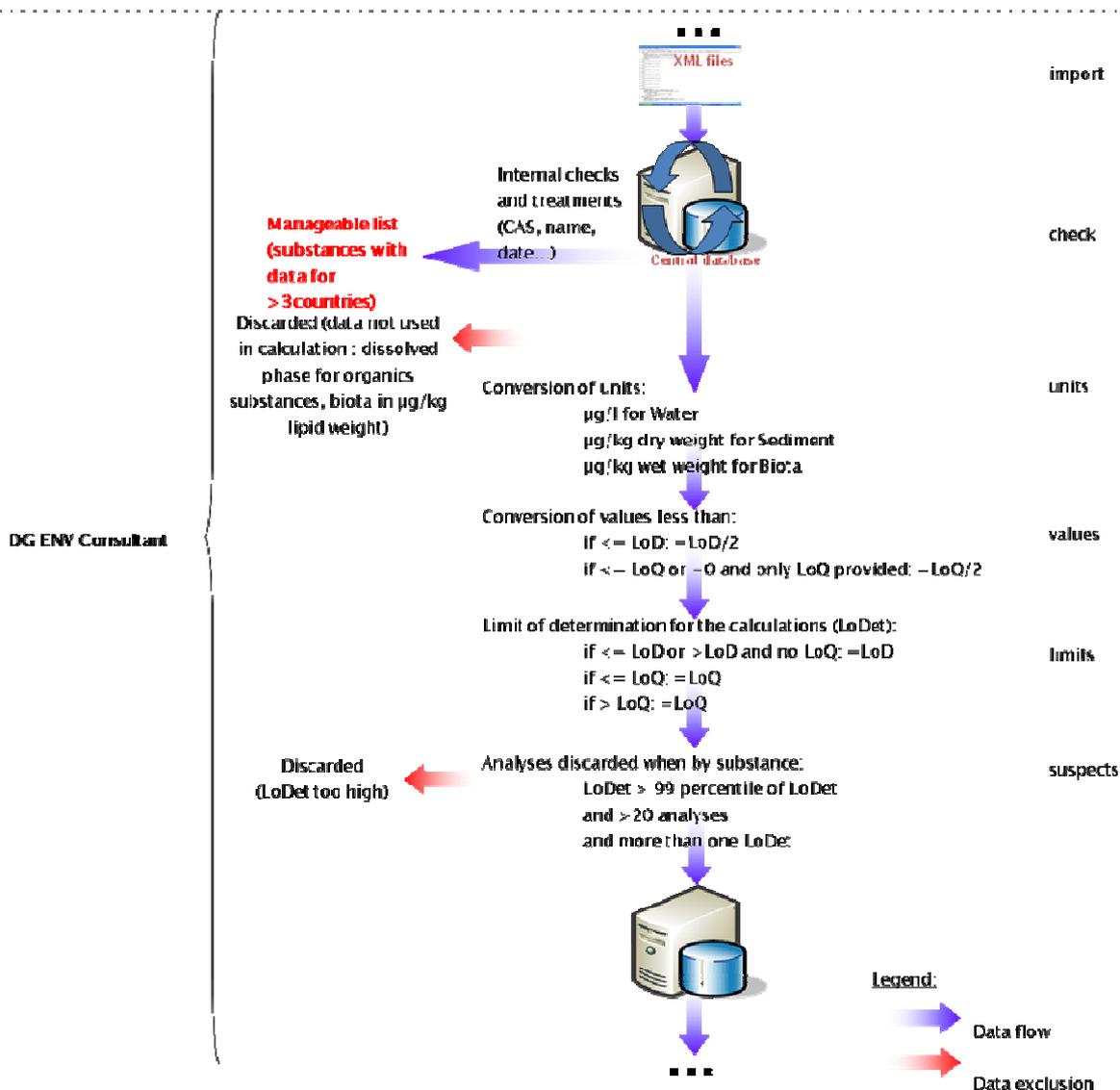


Figure 2: gathering of data in central database

III.3.1 Preliminary treatment of the datasets:

To allow better traceability, the treatments applied here on the analysis, were made by adding new fields in the database, referred to with same name completed by a “-correct”.

a. Homogenisation of units

In order to aggregate, compare or compute the measurements from different providers, care should be taken to convert all the measurements to a common unit for a given matrix. Conversion factors were used and applied on the value and on associated LoD and LoQ: linear changes of units from ng to µg or from mg to µg, changes taking into account molecular weight for tin compounds and nitrogen and phosphorus compounds where relevant (for more details, see Annex IV).





i. For water:

Conversion of the measurement unit was carried out as indicated in Table 2.

Table 2 : Unit conversion for water

Water – fractions analysed	Final measurement unit
Dissolved fraction	µg/L
Whole water with no separation of liquid and SPM phases	µg/L
Whole water with determination on each separate phase (sum of all phases)	µg/L
SPM	µg/kg

ii. For sediment:

It is assumed here that all values are expressed in dry weight by default, as confirmed by DE, CZ, FI, DK. Conversion of the measurement unit was carried out as indicated in Table 3.

Table 3 : Unit conversion for sediment

Sediment – fractions analysed	Final measurement unit
Fraction <2mm; <63µm; <50µm; <20µm	Regardless of the type of analysed fraction, all data for sediment will be expressed in µg/kg (dry weight)
<ul style="list-style-type: none"> If data are provided in µg/kg wet weight 	Data will be converted in µg/kg (dry weight) according to µg/kg (wet weight) x 4.6 ≈ µg/kg (dry weight). The conversion factor of 4.6, is based on the generic (i.e. according to TGD guidance using cited default values) assumption that the volume fraction of water in the whole (wet) sediment is 90% (volume fraction of solid is therefore 10%) and that the density of the solid fraction is 2500 kg/m ³ (and density of water is 1000 kg/m ³).
<ul style="list-style-type: none"> If data are provided in µg/kg without specification 	If information is lacking, it will be assumed by default that the measurements are reported in µg/kg dry weight (most common approach).

iii. For biota:

It is assumed here that all values are expressed in wet weight by default, as confirmed by DE, CZ, FI, DK. Conversion of the measurement unit was carried out as indicated in Table 4.

Table 4 : Unit conversion for biota.

Biota – species groups analysed	Final measurement unit
All fractions of Fish; Molluscs; Macrophyte	All final data will be expressed in µg/kg (wet weight)
<ul style="list-style-type: none"> If data are provided in µg/kg dry weight 	Measurements will be converted to µg/kg (wet weight) = µg/kg (dry weight) x % dry weight to wet weight ratio (when this information is provided). When the “dry weight to wet weight” ratio is not provided conversion factors of 0.2 dry/wet and 0.1 dry/wet will be applied for fish and molluscs, respectively and for macrophytes a conversion factor of 0.1 (Brix and the De Forest 2000).
<ul style="list-style-type: none"> If data are provided in µg/kg without specification 	By default, it will be assumed that the measurements are reported in µg/kg wet weight (most conservative approach)





Measurements reported in $\mu\text{g}/\text{kg}$ lipid weight are discarded (one country, 24 substances, 1612 analyses).

In addition, for Tin compounds, to allow their gathering in groups of substances, the conversion factor from the original substance with its unit to a value expressed respectively in $\mu\text{g Sn}^{+}/\text{l}$ for water in $\mu\text{g Sn}^{+}/\text{kg dw}$ for sediment and in $\mu\text{g Sn}^{+}/\text{kg ww}$ for biota is used. (See annex IV for complete table of conversion factors used).

b. Treatment of values depending on measurement limits

To homogenise the results, countries were asked to use the following rule:

Value reported	$\leq \text{LoD}$	$\leq \text{LoQ}$	$> \text{LoQ}$	$> \text{LoD}$ and no LoQ
Should be reported as	$\text{LoD}/2$	$\text{LoQ}/2$	Value	Value

When this rule was not implemented in all files, a post treatment was applied bi IOW.

In addition when the value is provided but =0:

- If only LOD is provided, then the value is replaced by $\text{LOD}/2$
- If only LOQ is provided, then the value is replaced by $\text{LOQ}/2$
- If both LOD and LOQ are provided, the value is replaced by $\text{LOD}/2$

c. Aggregation of data

To allow easier treatment, and as many datasets are provided with only one of the two limits LoD or LoQ, only one of them was finally used. In the database, a field called Limit of Determination (LoDet) was created. Then for all datasets the following rule was applied:

Value reported	$\leq \text{LoD}$	$\leq \text{LoQ}$	$> \text{LoQ}$	$> \text{LoD}$ and no LoQ
LoDet corresponds to	LoD	LoQ	LoQ	LoD

Some substances are also identified as highly relevant but with a relatively low number of analyses. This is especially the case for tin compounds and glyphosate. To allow their use in a reliable way, they are gathered under a single group as detailed in Table 5.

d. Selection of data

Once the dataset is updated with these elements, summary statistics are derived on the number of analyses by fraction, unit and substance to check if they all can be used for derivation of PECs.

This step allows the identification of organic substances where only the dissolved fraction in water is provided, and the 10 787 associated analyses that cannot be gathered with analyses on whole water and are discarded.





Table 5 : Substance groups.

CAS	Individual Substance Name	Substance Group
1071-83-6	Glyphosate (incl trimesium aka sulfosate)	Glyphosate
2439-99-8	Glyphosate	
818-08-6	Dibutyltin oxide	Dibutyltin compounds
683-18-1	Dibutyltin dichloride	
1002-53-5	Dibutylstannane	
14488-53-0	Dibutyltin cation	
1011-95-6	Diphenylstannane	Diphenyltin compounds
1118-46-3	Monobutyl tin trichloride	Monobutyltin compounds
78763-54-9	Monobutylstannane	
15231-57-9	Monooctylstannane	Monooctyltin compounds
2406-68-0	Monophenylstannane	Monophenyltin compounds
1461-25-2	Tetrabutyltin	Tetrabutyltin compounds
595-90-4	Tetraphenyltin	Tetraphenyltin compounds
56-35-9	Tributyltin hydrate	Tributyltin compounds
688-73-3	Tributylstannane	
36643-28-4	Tributyltin-cation	
6056-50-4	Tricyclohexylstannane	Tricyclohexyltin compounds
869-59-0	Trioctylstannane	Trioctyltin compounds
639-58-7	Triphenyltin chloride (Fentin chloride)	Triphenyltin compounds
76-87-9	Triphenyltin hydroxide (Fentin hydroxide)	
892-20-6	Triphenyltin hydride	
900-95-8	Triphenyltin acetate (Fentin acetate)	
668-34-8	Triphenyltin cation	

III.3.2 Identification of the manageable list

Once the dataset is updated with these elements, summary statistics are derived on the number of analyses by country and substance, to identify the “manageable list” (**Error! Reference source not found.**).

There are 430, respectively 316 substances for which monitoring data (in water, sediment or biota) are available for more than 2 countries, respectively 3 countries (see **Error! Reference source not found.**). Dealing with a list of 430 substances was deemed not manageable. Therefore, **the 316 substances monitored by 4 countries and more were chosen to constitute the manageable list for the 2009 monitoring-based prioritisation process** and the number of countries monitoring the substance was the only criteria used in the selection of candidate substances.



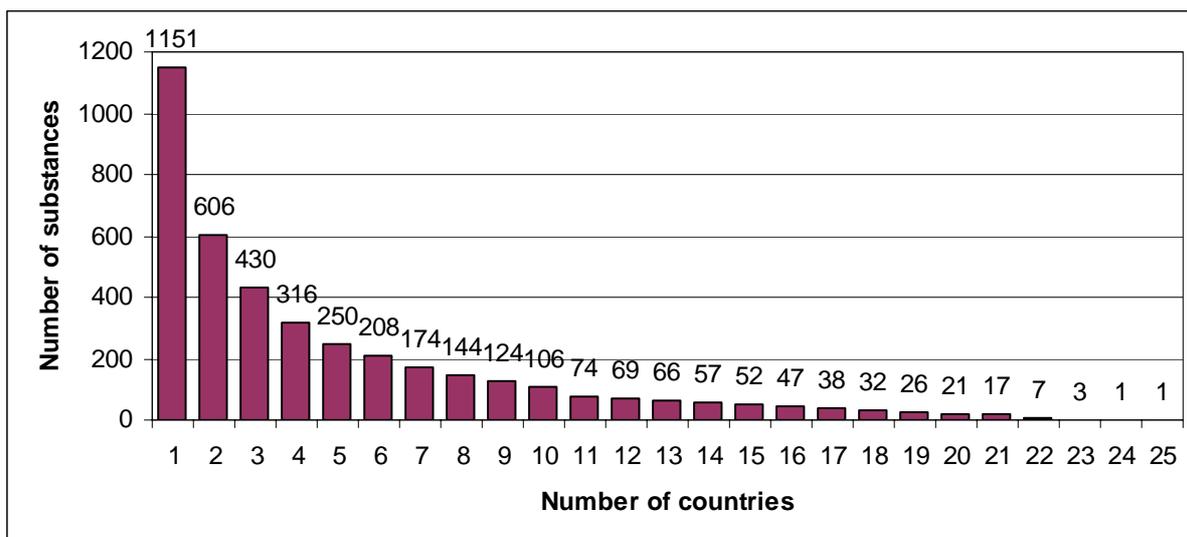


Figure 3: Substances reported by number of country (update 25/06/2009)

III.3.3 Identification and treatment of high determination limits

In the database, the distribution of determination limits vary widely and some values reach a very high level. Non quantified analyses (<DL) associated with high determination limits increase uncertainty in the risk evaluation. This may reflect measurements obtained from very poor analytical method.

As the rule for not quantified values is to replace the value by $LoDet/2$, high $LoDet$ can highly influence the results (in particular the calculation of PEC_2 , see section III.4.1). Therefore, a test was introduced to discard these analyses from the prioritisation process.

To apply the test it is first necessary to check that minimum requirements on the datasets tested are met. For all analyses on the same substance and fraction, two conditions should be met:

- more than 20 non quantified analyses;
- more than one $LoDet$ value.

On all datasets that meet the above conditions, a threshold value is calculated that is the 99 percentile of all $LoDet$ values for the substance X and the fraction in which it is measured.

Then, for each analysis :

- If $LoDet >$ threshold value, the corresponding analyses will be considered as suspect and not used in the calculation of $PECs$.
- If $LoDet <$ threshold value, the corresponding analyses are kept for use in the calculation of $PECs$.

The following table summarises the number of analyses discarded.





Table 6: Number of analysis considered suspect by country (updated 26/06/09)

Country	Number of total analyses	Number of suspect analyses
AUSTRIA	251265	211
BELGIUM	210174	
BULGARIA	920	
CYPRUS	6066	78
CZECH REPUBLIC	721143	1760
DENMARK	102264	225
ESTONIA	3396	
FINLAND	20442	
FRANCE	9500916	185971
GERMANY	660455	4187
GREECE	17322	
HUNGARY	24061	11
IRELAND	51198	
ITALY	352802	3264
LATVIA	593	
LITHUANIA	6632	48
LUXEMBOURG	16519	12
THE NETHERLANDS	20526	
NORWAY	424	1
POLAND	1451	
PORTUGAL	140066	635
ROMANIA	24152	451
SPAIN	300097	8
SLOVAKIA	7150	
SLOVENIA	41685	
SWEDEN	7315	59
SWITZERLAND	11974	
UNITED KINGDOM	2102041	6802
Total	14603049	203723

The analyses considered suspect with this treatment will not be used for the PECs calculation.

III.4.Calculation of PECs: treatments applied and results

Before applying the calculation steps needed to obtain the PECs for each substance, various treatments were necessary.

It is assumed at that level that all outliers, i.e. very high or very low results in national datasets, have been already checked by the data providers and validated.

The following scheme illustrates the process described in this chapter.



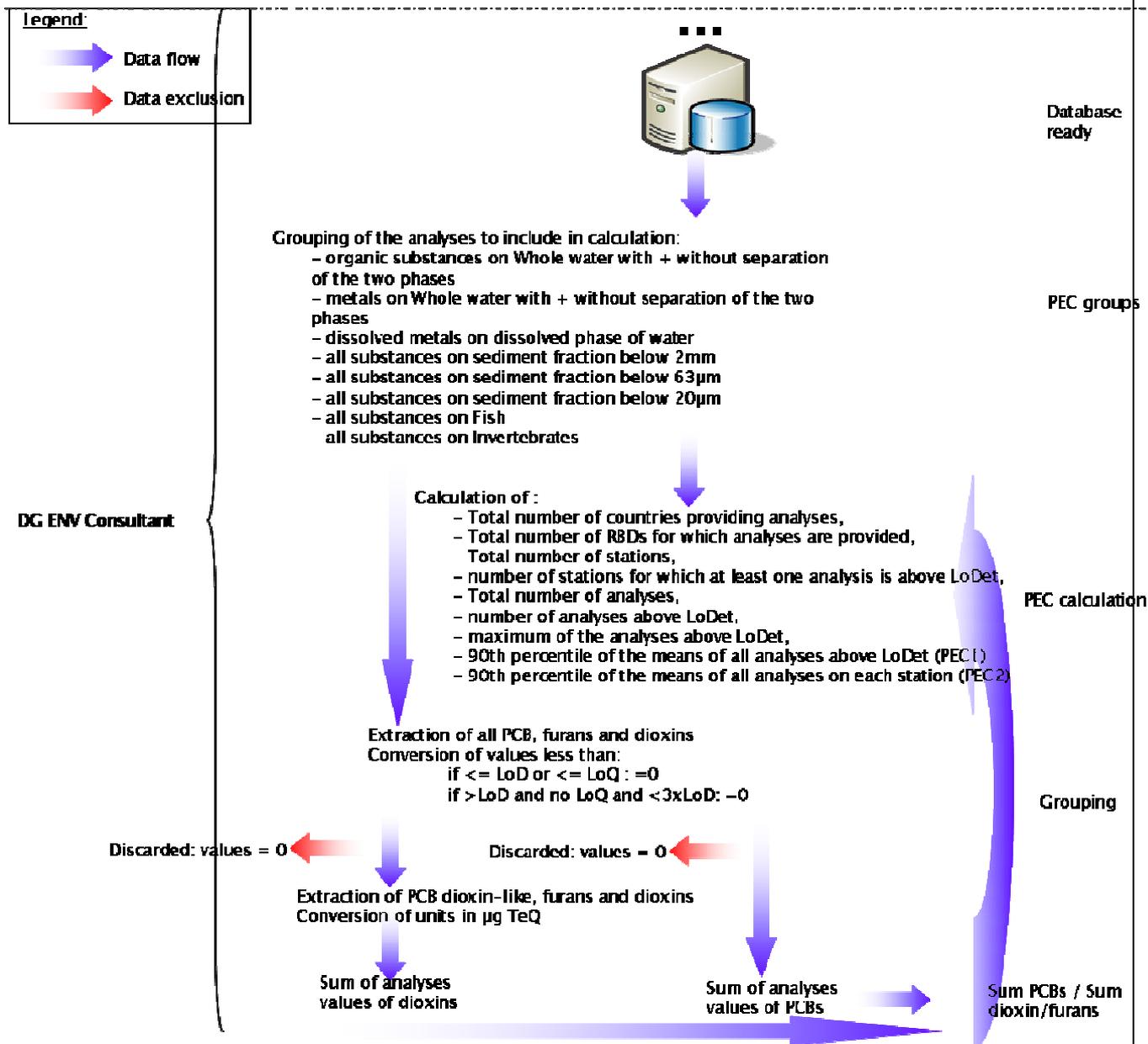


Figure 4: Calculation of PECs

III.4.1 The calculation of PECs for all substances but PCBs and dioxins

Monitoring data from the Member States were collected as raw, non-aggregated data, which means that several, and sometimes numerous, measurements (i.e. chemical analyses) could be available for a given substance and a given station.





Raw, non-aggregated data and associated metadata¹⁴ are essential for refined temporal trend analysis or/and spatial analysis. But for this prioritisation exercise the purpose is to compare, substance by substance, a single concentration, representing the general European contamination, to the substance's predicted no-effect concentration (i.e. PNEC).

For each substance, predicted environmental concentrations (PECs) have therefore been calculated. In practice, for each substance, distinct PECs were calculated for each analytical fraction (i.e. whole water, dissolved in water, sediment 2 mm, sediment 20 µm, sediment 63 µm).

Basically, PECs are calculated in two steps:

- The 1st step is about calculating the arithmetic mean¹⁵ on all analytical measurements for a given substance, a given station, and a given analytical fraction. This represents, for the given analytical fraction, the average contamination level by the substance at a given geographical point¹⁶.
- The 2nd step consists in calculating the 90th percentile of all the arithmetic means resulting from the 1st step, for a given substance and a given analytical fraction. This represents the PEC for the substance and the considered analytical fraction.

In theory, the PEC thus means that on a European scale, the average contamination level for 90% of the stations is expected to be below the PEC. In term of risk assessment, this implies that if the PEC is below the PNEC, 90% of the stations' sites are, on average, expected to be safe¹⁷.

In practice, difficulties are introduced by measurements that are below the analytical determination limit¹⁸. Two PEC calculation rules were consequently proposed:

For the calculation of PECs, two scenarios are considered and all values are calculated at the same time :

- "PEC1" stands for PEC calculated according to the 2 steps described above, but using only measurements that are above the analytical determination limit. Measurements that are below the analytical determination limit (<DL) were discarded.
PEC (scenario 1) = the 90th percentile of the mean per station of values above DL
- "PEC2": In this option, for the 1st step of the PEC calculation, the arithmetic means on analytical measurements that comprise "less-than values", were calculated according to the general rules introduced by article 5 of the "*Proposal for a Commission Directive adopting technical specifications for chemical monitoring and quality of analytical results*

¹⁴ See Dulio, V. and Fribourg-Blanc, B. (2006). Implementation of requirements for priority substances within the context of the Water Framework Directive. Task 05/01b/01 - Data processing: preparation for data collection. Under DG ENV contract No 07-010401/2005/4001371/MAR/D2.

¹⁵ See Background Document (Bonnomet and Dulio, 2007), section IV.2.e, for a discussion on the aggregation of monitoring data.

¹⁶ Provided that the sampling rate is representative!

¹⁷ Provided that the station locations are representative!

¹⁸ i.e. measurements provided as "less-than values". For further details see Section IV.2.d of Bonnomet and Dulio 2007





in accordance with WFD requirements". That is, in most cases¹⁹, analyses labelled as being below the determination limit (<DL) were replaced by DL/2.

PEC (scenario 2) = the 90th percentile of the mean per station of all values

PEC1 and PEC2 values for all the substances of the candidate list are presented in Annex VI of this report.

As a matter of fact, data were provided by MS for different types of fractions (e.g. for sediment: the grain fraction <2mm; <20µm, <63µm). However, the additional complementary information requested in the template that should allow an improved comparability and a more appropriate aggregation of the results (e.g. for water: SPM concentration, hardness, ionic concentration, pH, or for sediments: TOC%; grain size distribution; information on whether the data have been normalised or not for grain size distribution) was very seldom provided. This makes comparability of data for different fraction analysed not possible. It is therefore necessary to select the most appropriate / representative set of data (fraction analysed) for the calculation of the ratio PEC/PNEC.

A simplified procedure is thus applied:

Each substance is affected to a group, either organic substances or metals. Combined with the fractions reported, this allows the definition of the following 8 groups:

- PEC water for organic substances, that includes fractions: Whole water with + without separation of the two phases
- PEC water for metals for whole water, that includes fractions: Whole water with + without separation of the two phases
- PEC water for metals dissolved in water, that includes only the dissolved fraction of metals in water
- PEC sediment for all substances for fraction below 2mm
- PEC sediment for all substances for fraction below 63µm
- PEC sediment for all substances for fraction below 20µm
- PEC biota for all substances for fish
- PEC biota for all substances for invertebrates

For each group and by substance, the following elements are calculated:

- Total number of countries providing analyses,
- Total number of RBDs for which analyses are provided,
- Total number of stations,
- Number of stations for which at least one analysis is above LoDet,
- Total number of analyses,
- Number of analyses above LoDet,
- Maximum of the analyses above LoDet,
- 90th percentile of the means of all analyses on each station (PEC2)
- 90th percentile of the means of all analyses above LoDet (PEC1)

The selection criteria are designed to take into account both, the level of contamination and the level of representativity of the different fractions / species groups analysed.

¹⁹ See Annexes IX and X for distinct treatments in cases of PCBs and dioxins/furans





Other difficulties arise when data with heterogeneous quality are aggregated. Different quality checks have therefore been applied. Details of all applied procedures for data aggregation and processing were explained in a dedicated report (Fribourg-Blanc, 2008).

Still, remaining problems were noticed that should be taken into account when interpreting the results:

- There are large variations in the number of analyses, of stations, or of substances, per country. Quite every possible combination can occur: (high number of analyses but low number of stations, low number of analyses but high number of stations, high number of stations but low number of substances, etc.). Thus the representation of each country greatly differs, and this may be exacerbated by the way PECs are calculated. Indeed, when determining the 90th percentile during the second step of the PEC calculation, countries that have provided few analyses per station but for lots of stations will weight more than countries that have provided lots of analyses but for few stations.
- There are large variations in the measurement values between different countries. Apparently some Member States have mainly provided data from stations near point source releases and therefore tend to have highest measured values than other countries.
- There are notable differences in the monitoring practices between the countries. For instance, for a given matrix, measurements from different analytical fractions have been reported. For this prioritisation exercise, distinct PECs have been calculated and therefore distinct priorities have been assigned for these different analytical fractions. But at the end this may confuse the interpretation of the results. A stunning example can be cited regarding measurements for metals. Indeed, recent recommendations specify that metal should preferably be monitored as dissolved in water. But traditionally, most of the countries still continue to monitor metals in whole water. Coincidentally, countries that have provided measurements for metals as dissolved in water tend to have few analyses, but high measurement values (measurements in the vicinity of point source releases?) and for lots of stations. At the end, for several metals, PEC values for dissolved are higher than PEC values for whole water.

III.4.2 The specific case of PCBs and Dioxins

For PCBs and dioxins/furans, the same treatment as detailed in section III.4.1 are applied for each individual substance.

However, many of these substances are analysed on the same sample and can thus be aggregated to groups called:

- "Sum PCBs", representing the sum of concentrations of all PCBs monitored at a same location and at a same time, and expressed as µg/l for water, µg/kg dw for sediment or µg/kg ww for biota,
- "Sum dioxin/furans", representing the sum of concentrations of all dioxins, furans and PCB dioxin-like and expressed as µg TEQ/l for water, µg TEQ/kg dw for sediment or µg TEQ/kg ww for biota.

In order to calculate PECs on these substance groups, it is first necessary to keep only quantified values. Data are first corrected as follows:





Table 7: Calculation applied for individual substances part to a substance group

	<=LoQ	LoQ not available	>LoQ
<=LoD	0	0	-
>LoD	0	0 or measured value if >3xLoD	Measured value
LoD not available	0	Measured value	Measured value

Once this is done, two separate treatments are applied to calculate for each sample the resulting PEC values:

- all PCBs are summed on the one hand;
- for each dioxin, furan and PCB dioxin-like, the TEF is applied on the analysis value to have the result in TEQ then all individual substances are summed.

Then the PEC calculations detailed in section III.4.1 are applied.

III.5. Central database content

III.5.1 Data sources

The monitoring data used in this test run are those provided by the Member States during the two data collection exercises, from March 2007 until April 2008 and from October 2008 until January 2009.

At the end of March 2009, the situation regarding the data collection exercise is as follows: 28 countries (including NO and CH) of which 26 Member States of the European Union had provided a dataset. And although it was initially planned to include also datasets from other stakeholders, only one dataset was received from Vewin in the Netherlands.

Table 8 : Countries which provided monitoring data between March 2007 and January 2009.

AT	BE	BG	CH	CY	CZ	DE	DK	EE	EL	ES	FI	FR	HU	IE
☺	☺	☺	☺	☺	☺	☺	☺	☺	☺	☺	☺	☺	☺	☺
IT	LT	LU	LV	MT	NL	NO	PL	PT	RO	SE	SI	SK	UK	
☺	☺	☺	☺	☹	☺	☺	☺	☺	☺	☺	☺	☺	☺	

☹	no file provided
☺	file provided

III.5.2 Summary statistics

Overall, the data provided are as follows:

- 19 946 stations on 4 water body types,
- 547 269 samplings on the three matrixes,
- 14 603 049 analysis on 1151 substances of which 316 reported by more than 4 countries





a. Information geographically localised

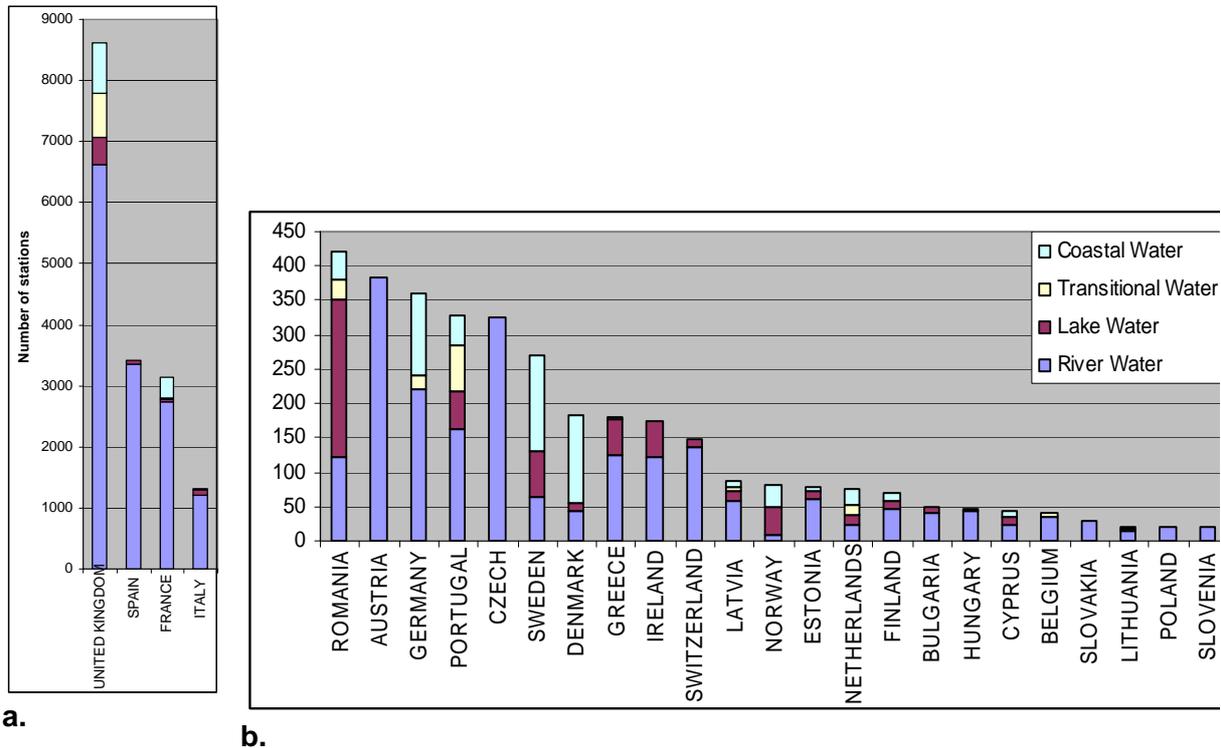
The 19 946 stations are provided mostly on rivers (81%) but all the four water body types are represented with the following distribution:

- 16066 stations on river;
- 1232 stations on lake;
- 864 stations on transitional waters
- and 1784 stations on coastal waters.

Overall this is summarised in the following Table 9 and associated figures (**Error! Reference source not found.a** and **Error! Reference source not found.b**). Please, note that for better visibility, 2 scales were used, one for the four countries that provide more than 7000 stations (**Error! Reference source not found.a**) and one for the others (**Error! Reference source not found.b**).

Table 9: Number of station by country and water body type

Country	RW	LW	TW	CW	Total
AUSTRIA	383				383
BELGIUM	35		6		41
BULGARIA	40	8		2	50
CYPRUS	24	10		10	44
CZECH REPUBLIC	326				326
DENMARK	44	12		128	184
ESTONIA	61	11		5	77
FINLAND	46	12		12	70
FRANCE	2742	49	2	354	3147
GERMANY	221	1	19	119	360
GREECE	125	51		4	180
HUNGARY	44	3			47
IRELAND	123	50			173
ITALY	1220	72		16	1308
LATVIA	57	15	7	8	87
LITHUANIA	14		4	3	21
LUXEMBOURG	7				7
NETHERLANDS	24	15	13	23	75
NORWAY	9	40		33	82
POLAND	20				20
PORTUGAL	163	56	65	45	329
ROMANIA	122	230	28	40	420
SLOVAKIA	29				29
SLOVENIA	19				19
SPAIN	3350	70	2		3422
SWEDEN	64	67		140	271
SWITZERLAND	136	11			147
UNITED KINGDOM	6618	449	718	842	8627
Total	16066	1232	864	1784	19946



a. b. **Figure 5: Number of stations by country and water body type (update 26/06/2008)**

The stations are mostly representative, surveillance and operational stations thus appropriate for the prioritisation exercise.

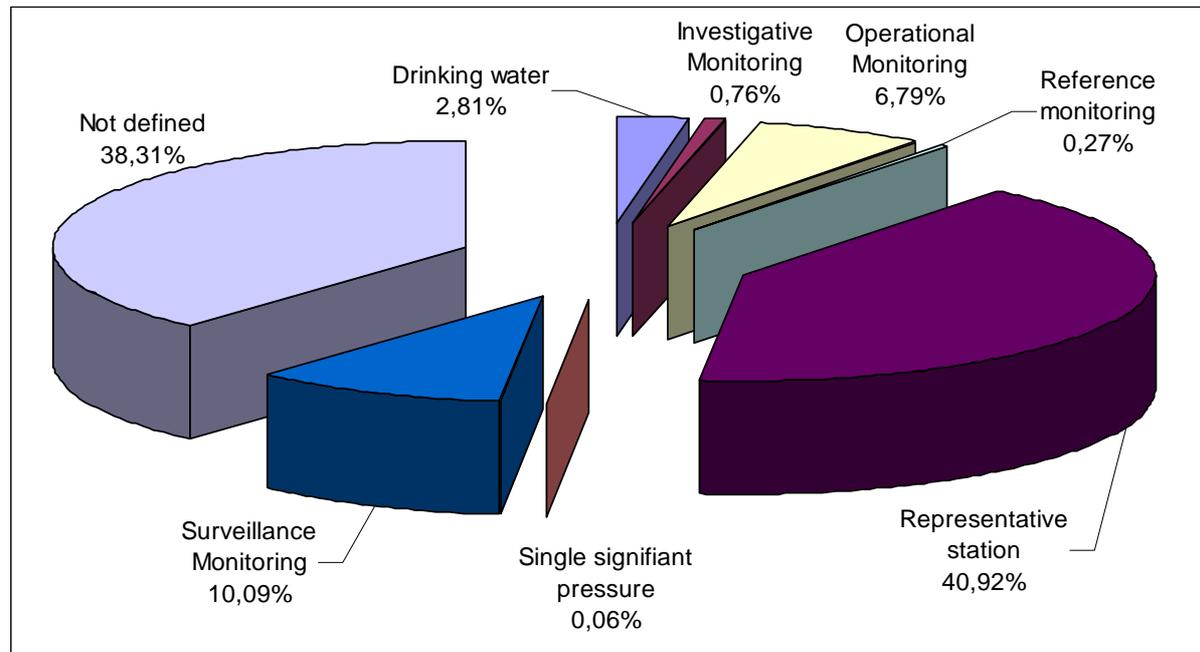
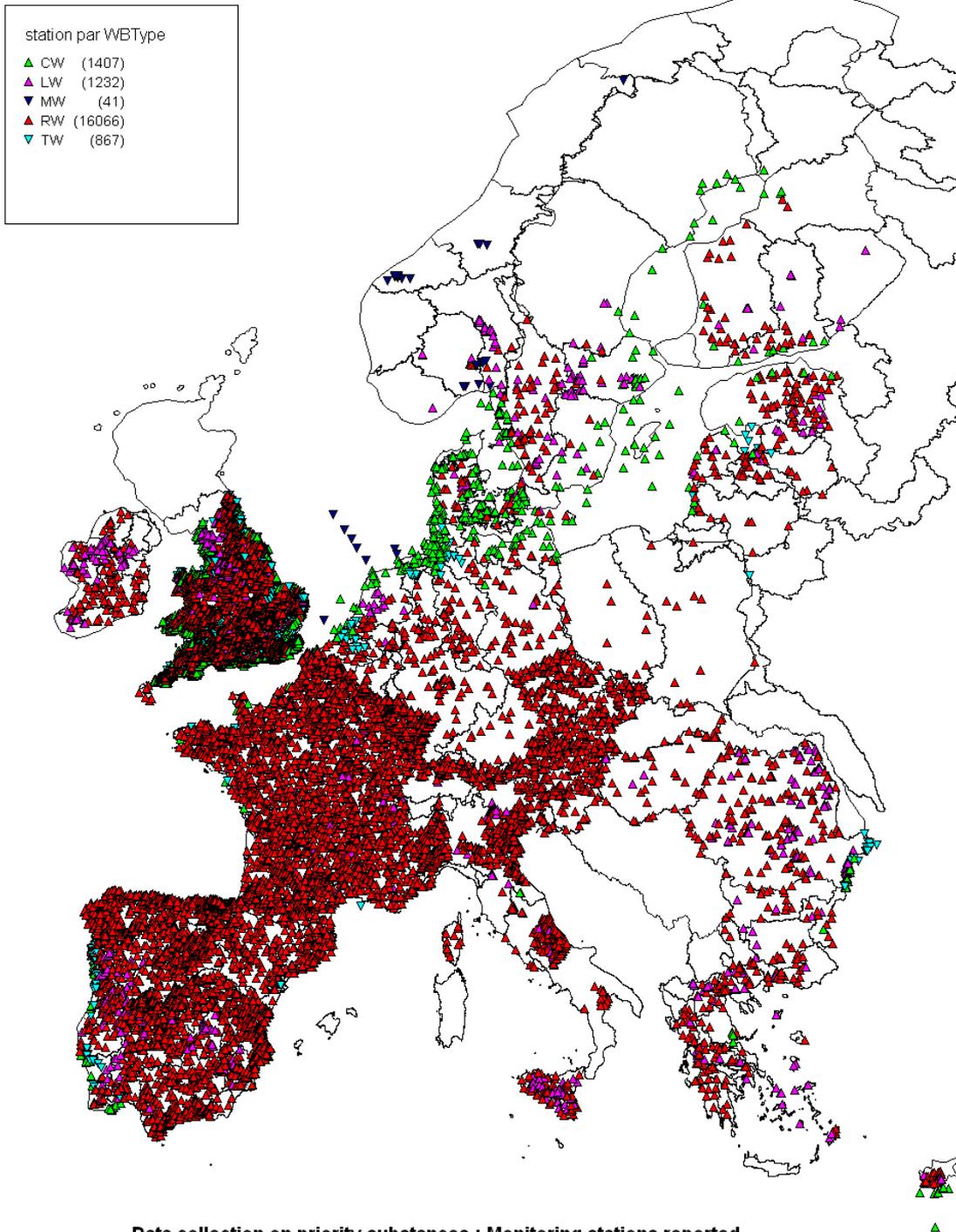


Figure 6: Number of stations by station type (update 03/06/2009)





And the geographical distribution is illustrated in the following maps:

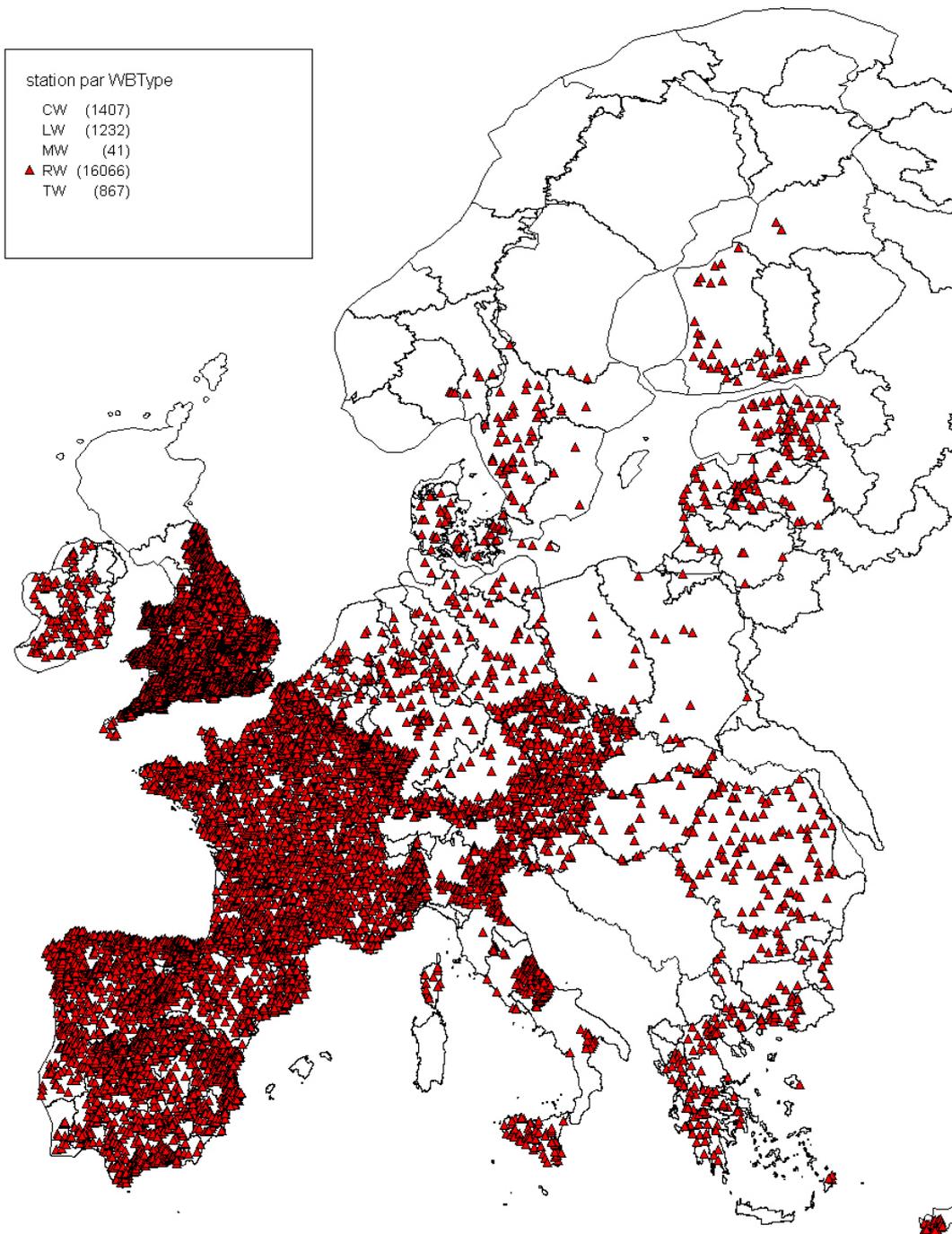


Data collection on priority substances : Monitoring stations reported

Source : Central database, version of 31/03/2009, IOW treatment

Figure 7: Map of localisation of all monitoring stations provided (update 31/03/2009)

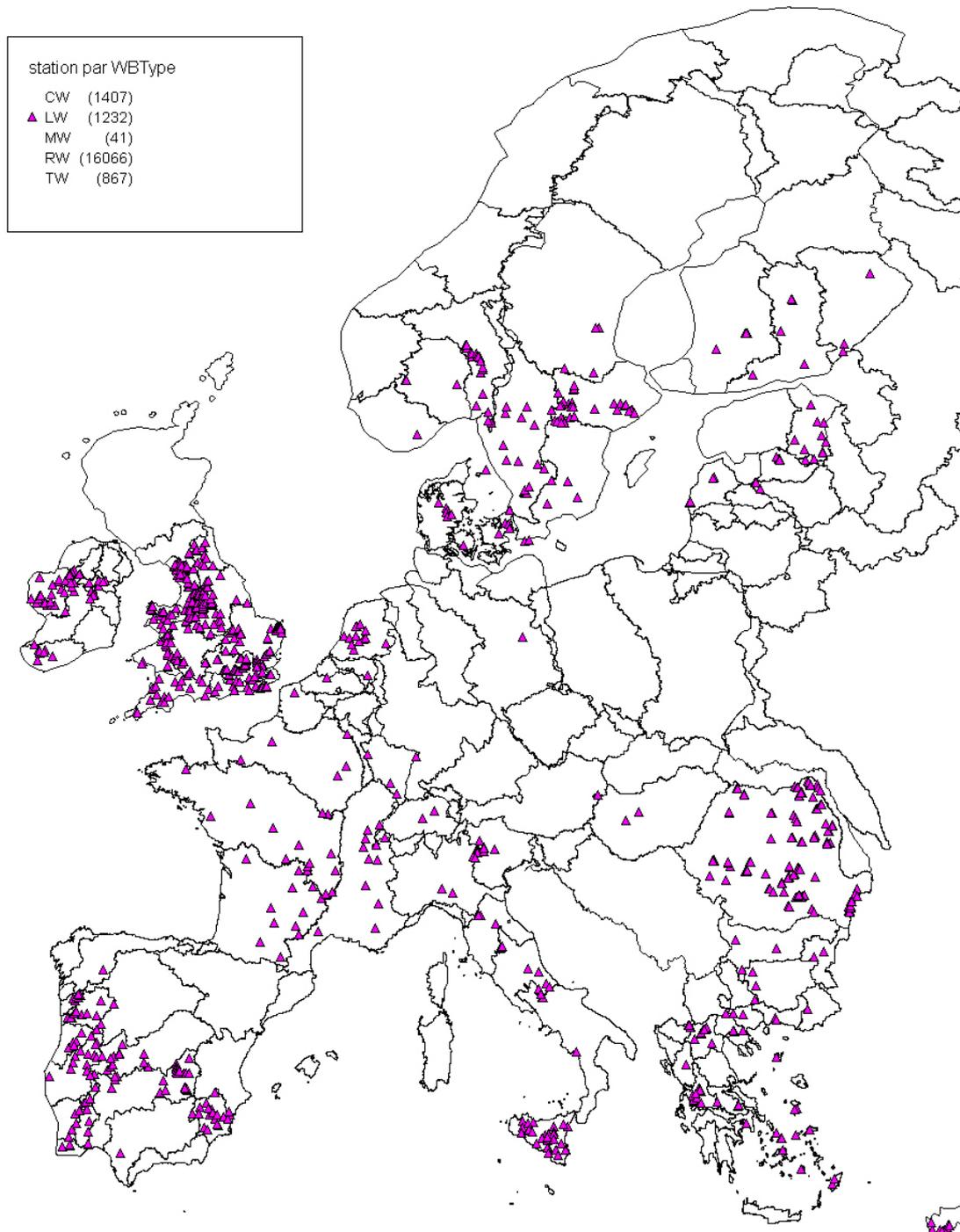




Source : Central database, version of 31/03/2009, IOW treatment

Figure 8: Map of localisation of monitoring stations on rivers provided (update 31/03/2009)





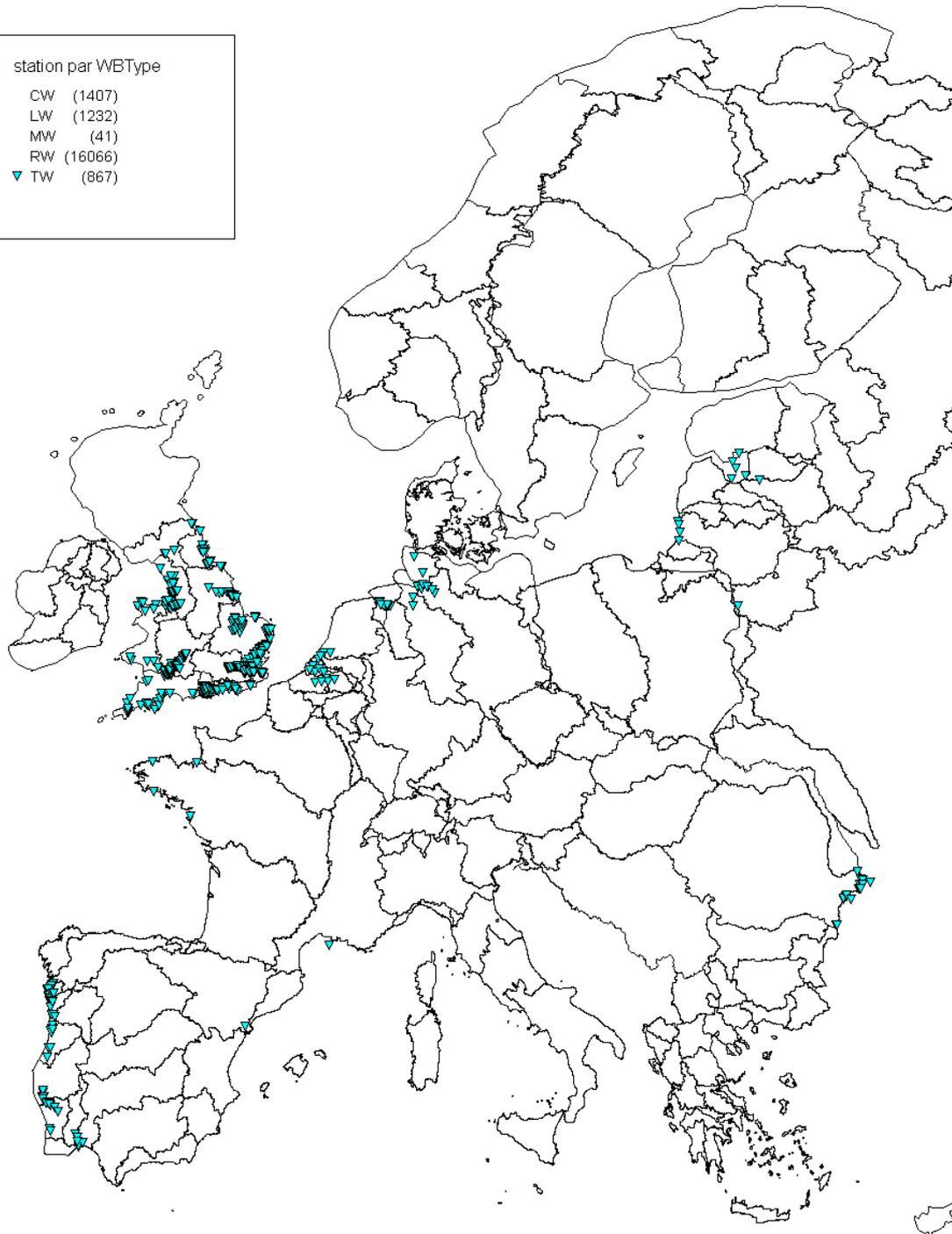
Source : Central database, version of 31/03/2009, IOW treatment

Figure 9: Map of localisation of monitoring stations on lakes provided (update 31/03/2009)





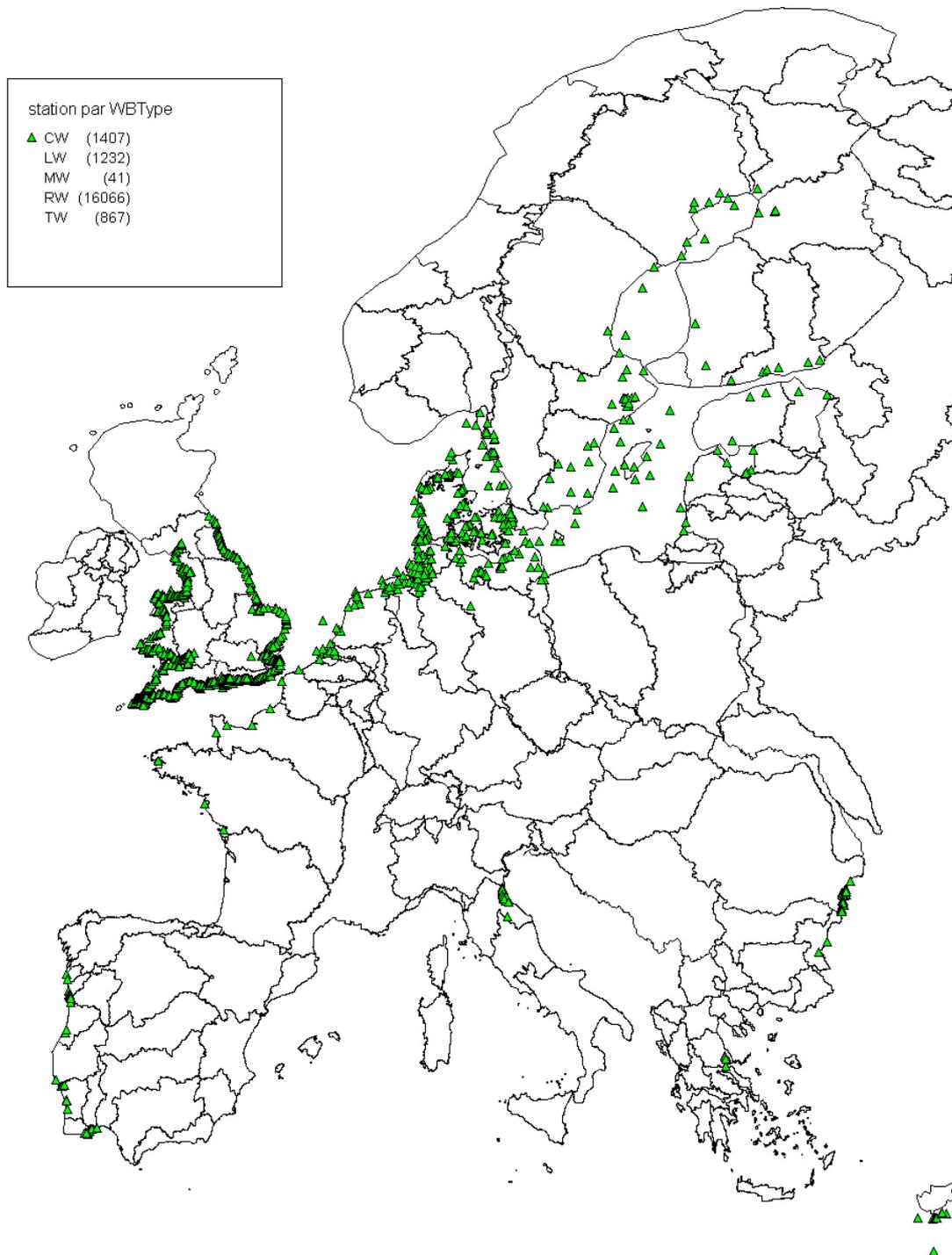
station par WBType	
CW	(1407)
LW	(1232)
MW	(41)
RW	(16066)
▼ TW	(867)



Source : Central database, version of 31/03/2009, IOW treatment

Figure 10: Map of localisation of monitoring stations on transitional waters provided (update 31/03/2009)





Source : Central database, version of 31/03/2009, IOW treatment

Figure 11: Map of localisation of monitoring stations on coastal waters provided (update 31/03/2009)





b. Information with matrix and fraction identified

All data are provided with information on sampling including sampling date, some additional information depending on the matrix (water, sediment or biota), such as pH, hardness, ionic concentration (Ca, Mg, Na, CL, S), and also the matrix sampled. The additional information is rarely provided.

Concerning the matrix, most of the analyses are provided on water, and only a small number is provided on biota.

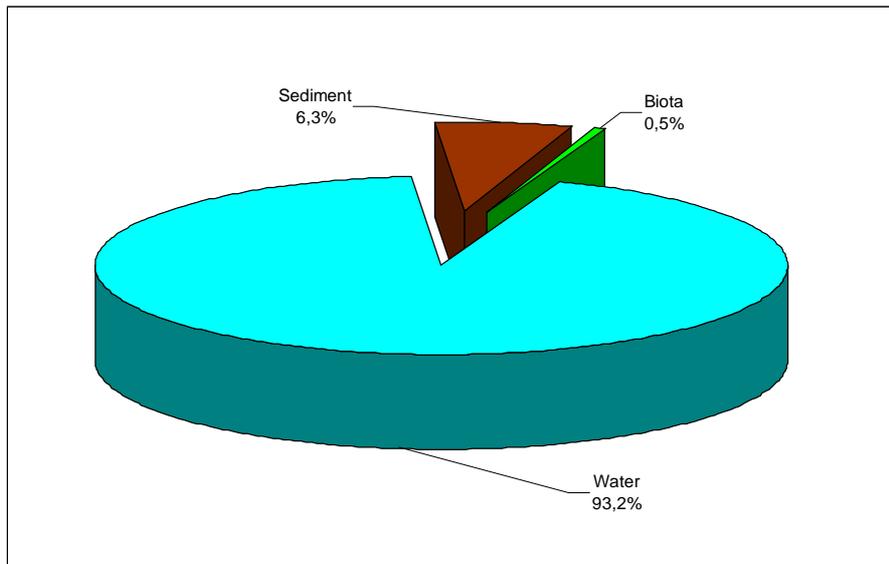


Figure 12: apportionment of analysis by matrix (update 26/06/2009)

A wide variety of fractions are provided for analysis on biota:

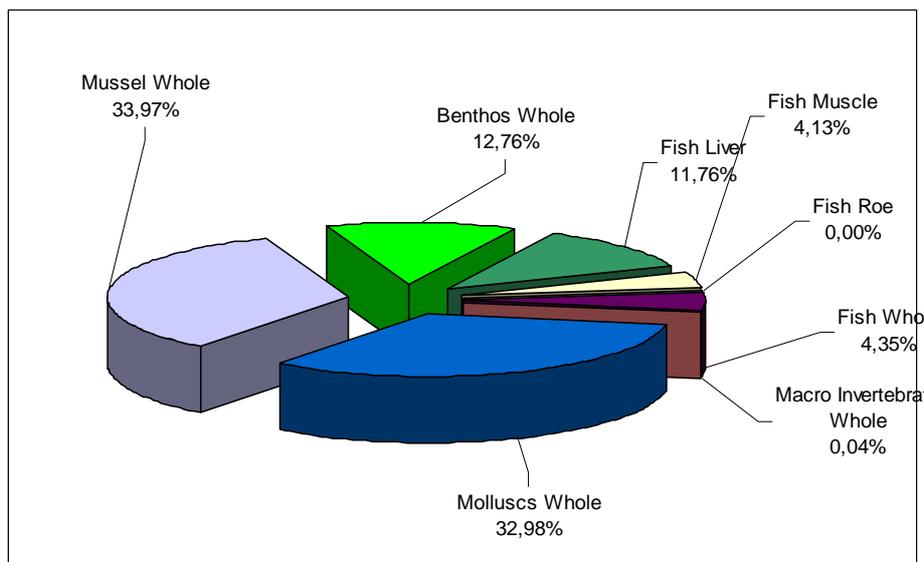


Figure 13: analyses on biota, apportionment by fraction (update 26/06/2009)



On sediment, the main fraction is the biggest (below 2mm), but analysis on the fraction below 20µm also represent a significant part of the results provided:

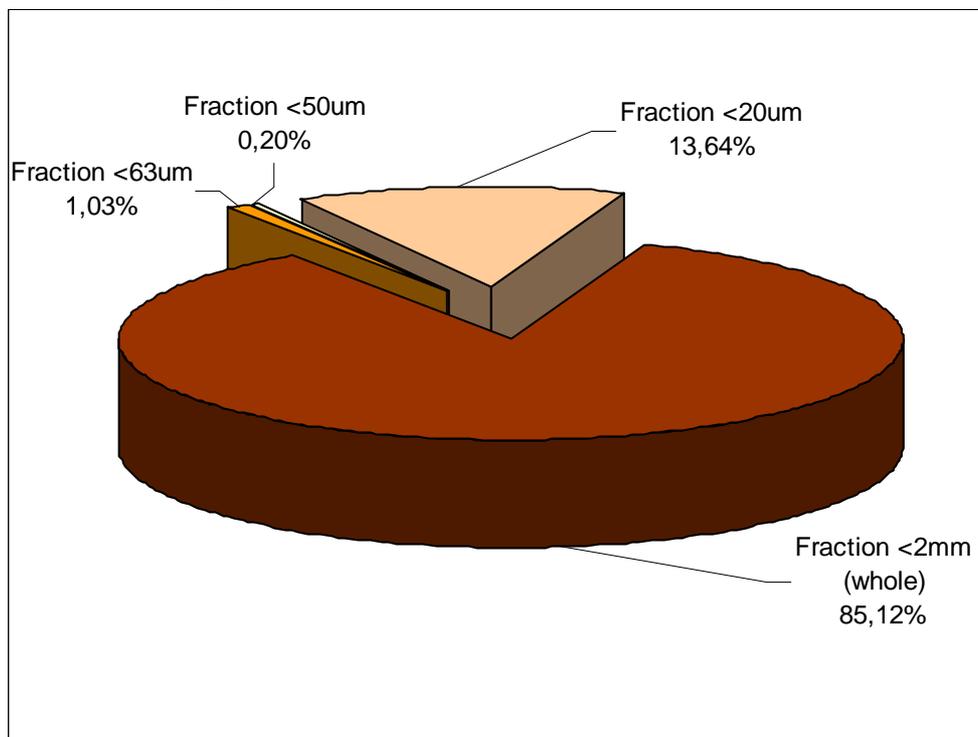


Figure 14: analyses on sediment, apportionment by fraction (update 26/06/2009)

On water, the vast majority of analysis is made on whole water with no separation of liquid and suspended particulate matter (SPM).

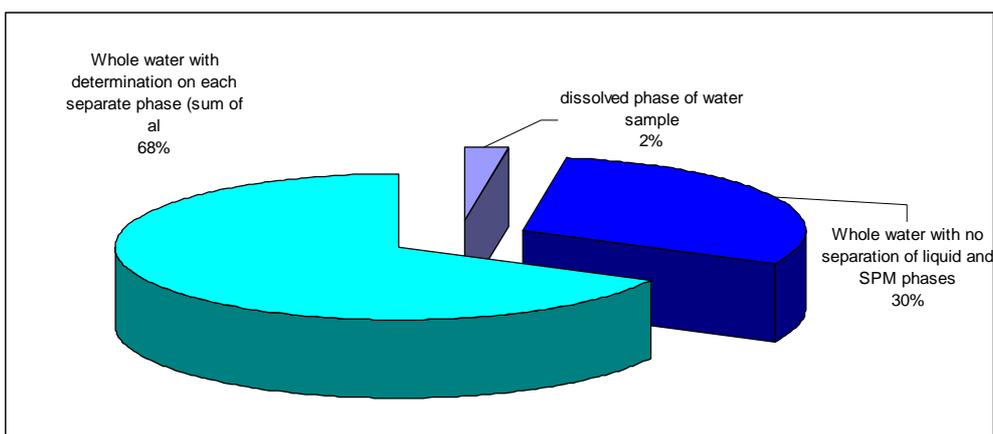


Figure 15: analyses on water, apportionment by fraction (update 26/06/2009)

c. Information on analysis

The number of analysis is highly variable between country, from more than 9 million for France or 2 million for United Kingdom up to 424 for Norway, and with 2 countries representing 79.6% of the analysis provided, and 10 countries 98.3%.





Table 10: Number and overall percentage of analyses by country (update 01/09/2009)

Country	Nb of total analyses	Percentage of analyses
FRANCE	9500916	65.06%
UNITED KINGDOM	2102041	14.39%
CZECH REPUBLIC	721143	4.94%
GERMANY	660455	4.52%
ITALY	352802	2.42%
SPAIN	300097	2.06%
AUSTRIA	251265	1.72%
BELGIUM	210174	1.44%
PORTUGAL	140066	0.96%
DENMARK	102264	0.70%
IRELAND	51198	0.35%
SLOVENIA	41685	0.29%
ROMANIA	24152	0.17%
HUNGARY	24061	0.16%
NETHERLANDS	20526	0.14%
FINLAND	20442	0.14%
GREECE	17322	0.12%
LUXEMBOURG	16519	0.11%
SWITZERLAND	11974	0.08%
SWEDEN	7315	0.05%
SLOVAKIA	7150	0.05%
LITHUANIA	6632	0.05%
CYPRUS	6066	0.04%
ESTONIA	3396	0.02%
POLAND	1451	0.01%
BULGARIA	920	0.01%
LATVIA	593	0.00%
NORWAY	424	0.00%

On the substances provided, from the universe of substances, and with the minimum requirements defined from the beginning on the information associated to these analyses, overall 1151 substances are reported²⁰, of which:

- 53 substances pertaining to substances and/or group of substances of Annex I of Directive 2008/105/EC;
- 9 substances classified as biocides under Directive 98/8/EC;
- 54 substances included in Regulation (EEC) 793/93;
- 313 substances classified as pesticide under the Directive 91/414/EEC;
- 151 substances regulated under Directive 76/464/EEC;
- 89 substances classified under OECD as High Production Volume Chemicals;
- 35 substances classified as metals;
- 24 substances have Persistent, Bioaccumulable and Toxic properties;
- 182 substances considered as endocrine disrupters (*Endocrine Disruption classifications according to the BKH (2000) report²¹, and Grouping of substances according to SEC(2004) 1372²²*)
- and 16 substances are also included in OSPAR List of Substances for Priority Action.

²⁰ Please, note that some substances may be included in more than one list.

²¹ http://ec.europa.eu/environment/endocrine/strategy/substances_en.htm#report3

²² http://ec.europa.eu/environment/endocrine/documents/sec_2004_1372_en.pdf



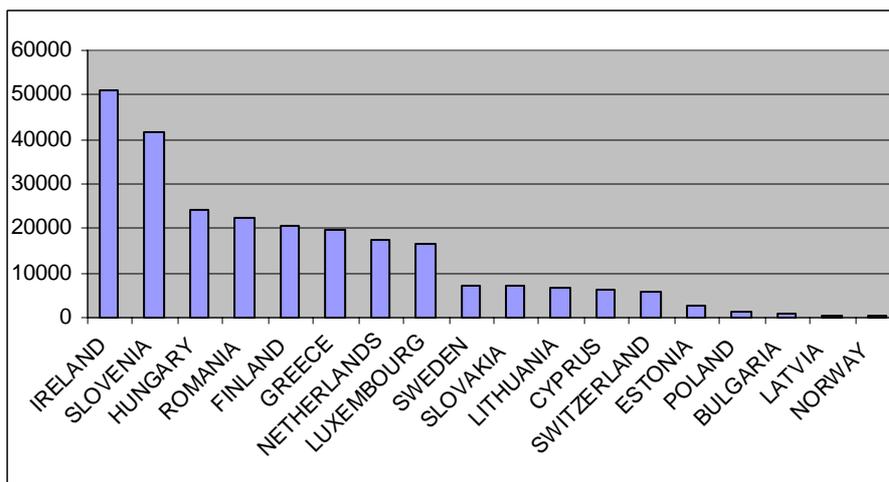
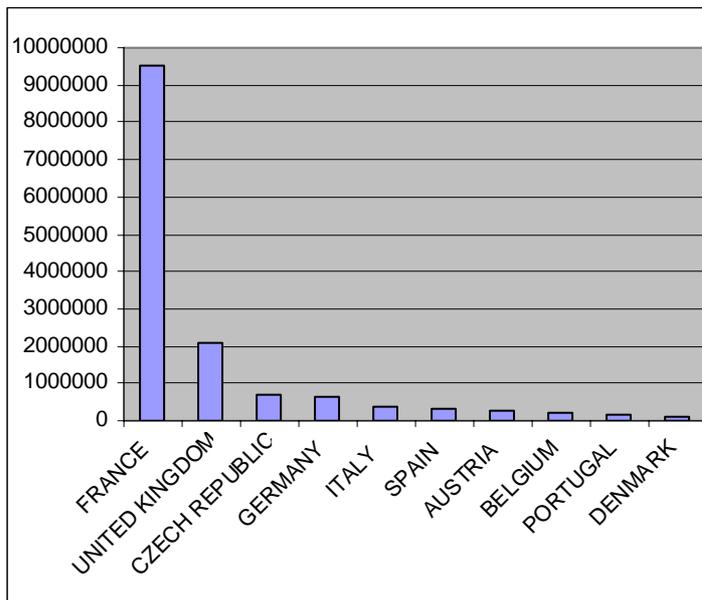


Figure 16: Number of analysis by country (update 03/06/2009)

IV. Step 3 : Relevant parameters for risk evaluation

Parameters were chosen in order to prioritise monitored substances on the basis of risk to or via the aquatic environment, i.e. to the aim of protecting aquatic species, benthic species, predators and humans.

Consequently, effects and exposure data were retrieved for water, sediment, biota and the human health, respectively.

Note that, due to available time and resources, the scientific value of the compiled information has not always been assessed comprehensively by the INERIS/IOW consortium and that the original published data may not have undergone a systematic peer-review process (see section IV.2).





IV.1.Exposure data based on monitoring data

Monitoring data in water, sediment or biota come exclusively from the data provided by the Member States (for more details, see section III.3 Step 2: Data collection, associated data treatments and data processing). No further environmental data were researched in this work, e.g. in the literature, given that a modelling approach is expected to be run in parallel.

Data for water, sediment and biota were provided. For each of these matrices, different fractions were kept separated:

- whole water
- dissolved (only for metals)
- sediment, fraction 2 mm
- sediment, fraction 20 µm
- sediment, fraction 63 µm
- biota, fish
- biota, invertebrates

IV.2.Effects data based on existing (eco)toxicity data

The reader of this report should be aware that, except from values extracted from draft or finalized European Union Risk Assessment Report and Directive 2008/105/EC, PNECs suggested in this document and its annexes have been derived in the only purpose of prioritisation and these values shouldn't be used directly as environmental quality standards without any further review.

IV.2.1 Direct ecotoxicity for water

a. Sources of data and their reliability

Direct ecotoxicity data on aquatic species were retrieved from various sources:

- For the 33 existing priority substances or substances already regulated under List I of Dir. 76/464/EEC, EQS values from the daughter directive 2008/105/EC and supporting datasheets²³ prepared by the Fraunhofer Institute were used.
- For existing substances under Reg. (EEC) 793/93, PNEC values used in risk assessment reports (available online on the ECB²⁴ website) were retrieved.
- For pesticides evaluated under Directive 91/414/EEC, ecotoxicity data can be found in DG-SANCO review reports²⁵, EFSA draft assessment reports²⁶, or EFSA conclusions²⁷.

²³ EQS supporting datasheets of daughter directive 2008/105/EC:
http://circa.europa.eu/Public/irc/env/wfd/library?l=/framework_directive/i-priority_substances/supporting_background/substance_sheets&vm=detailed&sb=Title

²⁴ ECB: <http://ecb.jrc.it/esis/>

²⁵ DG-SANCO review reports: http://ec.europa.eu/food/plant/protection/evaluation/exist_subs_rep_en.htm (existing active substances) and http://ec.europa.eu/food/plant/protection/evaluation/new_subs_rep_en.htm (new active substances)

²⁶ EFSA Drat Assessment Reports: <http://www.efsa.eu.int/DAR/displaySubstance.cfm?provision=1>

²⁷ EFSA conclusions: http://www.efsa.eu.int/science/praper/conclusions/catindex_en.html





- Additional dedicated sources for pesticides were used, in particular the US-EPA's RED (Reregistration Eligibility Decision) reports²⁸ and the US-EPA's OPP (Office of Pesticide Programs Pesticide) Ecotoxicity Database²⁹, and more marginally, data from DEFRA³⁰ (UK's national assessment reports for pesticides), KEMI (ecotoxicological evaluation reports available for some pesticides, from SE), AGRITOX³¹ (database from the French food safety agency providing additional information for pesticides registered in FR).
- Various other sources were considered: the US-EPA's ECOTOX database (formerly ACQUIRE database) which compiles ecotoxicity data from peer-reviewed literature³², the OECD Substances Information Data Set (SIDS) which are prepared in the framework of the OECD High Production Volume Chemical program (SIDS initial assessment reports are available on the UNEP website³³), the ETOX Database for Ecotoxicological Effect Data and Quality Targets³⁴ established by the German Federal Environmental Agency, BUA reports³⁵ edited by the German society of chemical substances, the IUCLID database³⁶, water quality guidelines from the International Commission for the Protection of the Rhine (ICPR)³⁷, US-EPA³⁸, Environment Canada³⁹, British Columbia⁴⁰, PNEC values from the former COMMPS database.

It should be underlined that quality and relevancy of the data was not assessed when data were extracted directly from the databases and the reporting data have been “*peer-reviewed*”, “*reviewed by an Agency scientist as well as a second supervisory biologist*” or when data were directly retrieved from sources known as valid at the international or European level (e.g. OECD SIDS and SIARs, finalised European Union Risk Assessment Reports). On the other hand, it should be underlined that quality and relevancy of ecotoxicological data used for the derivation of PNEC was assessed, to the extent possible with available resources, when values were directly retrieved from databases where no peer-review had been done for their use in the context of risk assessment (e.g. US-EPA ECOTOX database, public literature including articles and reports).

Ecotoxicological data extracted from the websites indicated in the Table 11 has been considered valid without restrictions and any further review process.

PNEC for pesticides have been derived from finalised risk assessments if those are available. However, in case the substance has other uses than pesticides, other available data may be relevant (for more details, see Annex XIV).

²⁸ US-EPA's RED reports: <http://cfpub.epa.gov/oppref/rereg/status.cfm?show=rereg>

²⁹ US-EPA's OPP Ecotoxicity Database: <http://www.ipmcenters.org/Ecotox/index.cfm>

³⁰ DEFRA reports: http://www.pesticides.gov.uk/psd_evaluation_all.asp

³¹ AGRITOX: <http://www.dive.afssa.fr/agritox/index.php>

³² US-EPA's ECOTOX database: <http://www.epa.gov/ecotox/>

³³ UNEP: <http://www.chem.unep.ch/irptc/sids/OECD/SIDS/sidspub.html>

³⁴ ETOX database: <http://mars.liwa.de/webETOX/index.do>

³⁵ BUA reports: <http://www.gdch.de/fowi/archiv/bua/berichte.htm>

³⁶ IUCLID database: <http://ecb.jrc.it/esis/>

³⁷ cited in the ETOX database: <http://mars.liwa.de/webETOX/index.do>

³⁸ US-EPA: <http://www.epa.gov/waterscience/criteria/wqtable/index.html>

³⁹ Environment Canada: <http://documents.ccme.ca/download/en/222/>

⁴⁰ British Columbia guidelines for chlorophenols:
http://www.llbc.leg.bc.ca/public/PubDocs/bcdocs/409645/approved_wq_guide.pdf





Table 11: Sources of ecotoxicological data which have been considered valid without further review

ECB website	http://ecb.jrc.ec.europa.eu/
CIRCA website	http://circa.europa.eu/Public/irc/env/wfd/library?!=/framework_directive/i-priority_substances/supporting_background/substance_sheets&vm=detail&d&sb=Title
DEFRA website	http://www.pesticides.gov.uk/psd_evaluation_all.asp
DG SANCO website	http://ec.europa.eu/food/plant/protection/evaluation/exist_subs_rep_en.htm
	http://ec.europa.eu/food/plant/protection/evaluation/new_subs_rep_en.htm
EFSA Website	http://www.efsa.europa.eu/EFSA/ScientificPanels/PRAPER/efsa_locale-1178620753812_Conclusions494.htm
	http://dar.efsa.europa.eu/dar-web/provision
OECD HPV website	http://cs3-hq.oecd.org/scripts/hpv/
Pesticide Ecotoxicity Database of the United States Environmental Protection Agency (US-EPA)	http://www.ipmcenters.org/Ecotox/DataAccess.cfm
Reregistration Eligibility Decisions (RED) of the United States Environmental Protection Agency (US-EPA)	http://www.epa.gov/pesticides/reregistration/status.htm

b. PNECwater derivation

From these ecotoxicity results, Predicted No Effect Concentrations (PNEC) were calculated according to the principles described in the EU technical guidance document on risk assessment (TGD)⁴¹. For deriving the PNEC, the lowest ecotoxicity concentration is divided by an adequate assessment factor. Assessment factors are chosen in order to cover the panel of variations and uncertainties associated with, *inter alia* interspecies variability, extrapolation from short-term to long-term effects, extrapolation from lab to field conditions, etc. The more there are uncertainties associated with the available ecotoxicity results, the more the assessment factor should be high. Practically, the factor value (ranging from 10 to 1000 according to the TGD recommendations⁴²) depends on the quantity (number of trophic levels represented) and the quality (acute or chronic effects) of the available ecotoxicity data.

PNECwater with basic information on the source of keystone and associated assessment factor are provided in Annex VII. PNECwater were proposed for all of the candidate substances for which monitoring data in water were provided by the Member States, except for 13 substances for which this was not possible (insufficient or non-relevant data) : 1,2-Dibromoethane (EDB), 2-Chloro-4-methylaniline, 1,1,2-Tri-chloro-tri-fluoro-ethane, 3-Chlorotoluene, Benzo[e]pyrene, Chlorbromuron, Decabromodiphenylether, Decabromodiphenyl oxide, Dichloro-di-isopropyl ether, Fenchlorvos, Perfluorooctane sulfonate (PFOS), Propoxur, Tecnazene and Total PAHs.

⁴¹ E.C. (2003). Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) N° 1488/94 on Risk Assessment for existing substances, Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market. Office for Official Publications of the European Communities, Luxembourg.

⁴² See TGD Table 16, page 101





IV.2.2 Ecotoxicity for sediment

a. *PNEC sediment derivation based on Equilibrium partitioning approach*

Natural sediments may exhibit a high heterogeneity in composition, granulometry, physico-chemical conditions, etc. These sources of variability may drastically affect their capacity to fix contaminants and therefore their toxicity.

Harmonised bioassays on benthic organisms have been developed. But procedures for spiking sediments, establishing equilibration periods and all the other experimental factors that have an impact on the bioavailability of the substances may not be representative of specific *in-situ* conditions for natural sediments. Furthermore it should be noted that these bioassays are quite expensive and far less abundant in the scientific literature than aquatic bioassays. Retrieving experimental results from bioassays in sediment would therefore be time demanding and would anyway not be possible for most of the substances that are in the candidate list.

In practice, risk assessments for sediment (including EU risk assessment) are commonly based on the equilibrium partitioning approach (EqP approach). This approach assumes that the ecotoxicity of sediment living organisms can be deduced from ecotoxicity results from aquatic tests. This relies on the hypothesis that the intrinsic sensitivities of aquatic and sediment living organisms to contaminants are comparable, but that the availability of the contaminants in sediment is reduced due to their sorption to the sediment solid particles. The EqP approach estimates which proportion of substance is adsorbed on the solid phase of the sediment and which proportion is dissolved in the pore water under equilibrium conditions. Adsorption is generally predicted from the Koc parameter (i.e. organic carbon / water partition coefficient). It is acknowledged that this approach represents a very oversimplified model of the actual phenomenon. In particular, the statement of equilibrium can hardly be seen as realistic for natural sediments. Also, the Koc parameter may not properly capture the adsorption properties for all types of substances. But, with this approach it is possible to estimate, easily and rapidly, benthic toxicity for almost all the substances in the candidate list.

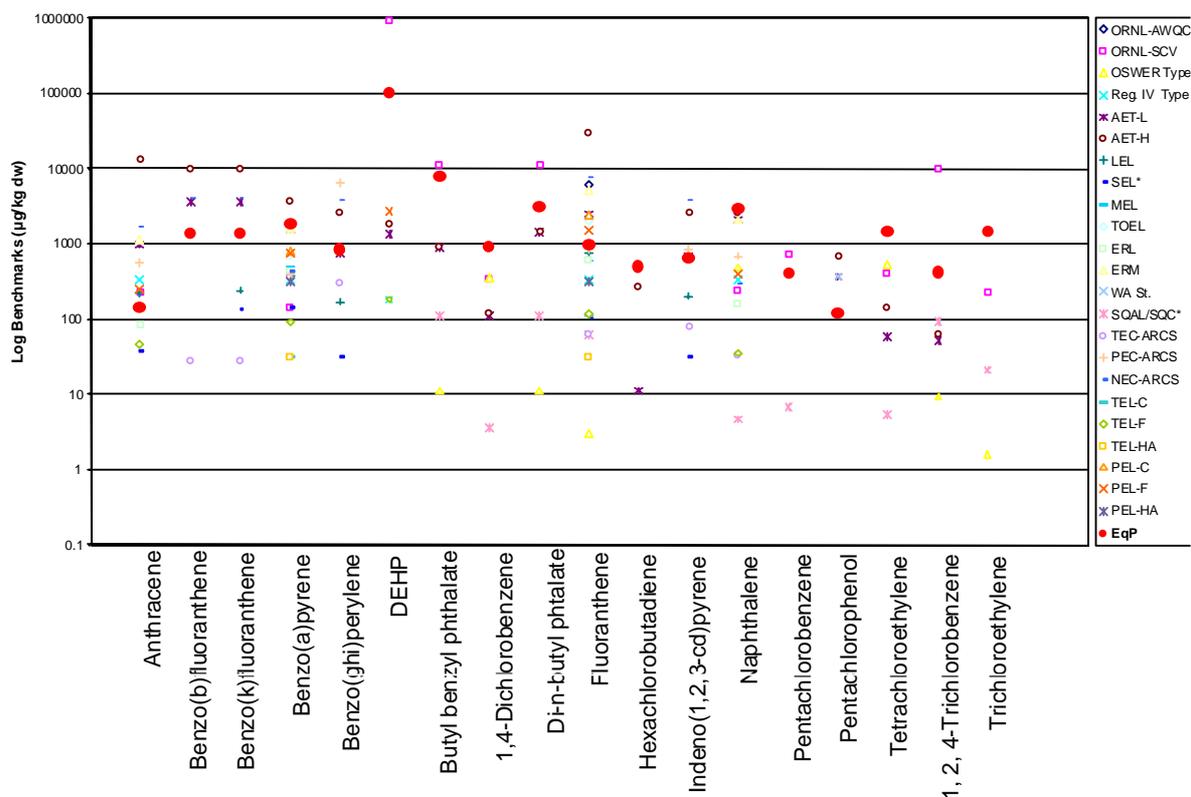
Alternatively, the possibility of using sediment quality benchmark values from third countries (mainly from North-America) was investigated. Numerous benchmark values have been developed by these countries, implying differences in input data and calculation methods⁴³. Most of these benchmarks rely on chemical and biological data collected from numerous individual sites. These data are processed using various statistical treatments that attempt to address a relationship between the concentration of contaminants measured in polluted sediments and the various adverse biological effects that could be observed in the field or in the lab. Benchmark concentrations are then established for each substance, though an unambiguous causal link between the effect endpoint and a specific substance can hardly be guaranteed when complex mixtures of contaminants are encountered in the sediments.

Several of these benchmark values⁴⁴ were compared to each other and to the predictions of the EqP approach. The results are reported on the figure below:

⁴³ See <http://www.sediments.org/ecotox.html>

⁴⁴ Benchmark values were retrieved from: <http://www.sediments.org/ecotox.html>





This example for a limited number of substances still clearly shows huge variations between the different benchmark values. No benchmark appears to be systematically the most protective. In principle and in practice, there is no best method. The method to be used for this prioritisation exercise should therefore be chosen according to other considerations.

A key point is the applicability of the final method to a maximum of substances of the candidate list. Benchmark values established from bioassays on benthic species or from field data are simply too scarce and would be missing for most of the substances of the candidate list. On the contrary, predictions from the EqP approach can be calculated in an automatic way for virtually every substance (though this are not always relevant). On the preceding figure, EqP predictions generally lie in the middle part of the variation intervals. Thus, the EqP approach appears to be a reasonable and convenient compromise for assessing ecotoxicity for sediments.

For this prioritisation exercise, the general EqP formula was therefore applied:

$$C_{sed} = \frac{C_{water} \cdot (F_{water_{sed}} \cdot 1000) + (F_{solid_{sed}} \cdot Kp_{sed} \cdot \rho_{solid})}{\rho_{sed}}$$

C_{water} is the concentration of the substance in the aqueous phase in $\left[\frac{\mu g}{L} \right]$,

C_{sed} is the concentration of the substance in the whole sediment (wet weight) in $\left[\frac{\mu g}{kg_{sed}} \right]$,





Kp_{sed} is the partitioning coefficient of the substance between the aqueous phase and the solid phase, in $\left[\frac{L}{kg_{solid}} \right]$. It can be estimated by $Kp_{sed} = Foc_{sed} \cdot Koc$, with Koc in $\left[\frac{L}{kg_{oc}} \right]$ and Foc_{sed} that is the weight fraction of organic carbon in the solid phase (by default, the EU guidance documents recommend to use 0.1),

ρ_{sed} is the bulk density of wet sediment $\left[\frac{kg_{sed}}{m^3_{sed}} \right]$ (by default, the EU guidance documents recommend to use 1150 kg/m³)

ρ_{solid} is the bulk density of the solid phase $\left[\frac{kg_{solid}}{m^3_{solid}} \right]$ (by default, the EU guidance documents recommend to use 2500 kg/m³)

$Fwater_{sed}$ is the volume fraction of water in whole (wet) sediment (by default, the EU guidance documents recommend to use 0.9)

$Fsolid_{sed}$ is the volume fraction of solids in whole (wet) sediment (by default, the EU guidance documents recommend to use 0.1)

Applying default values recommended by the EU guidance documents for all the parameters, this leads to:

$$C_{sed} = EqP(C_{water}) = C_{water} \cdot (0.783 + 0.0217 \cdot Koc)$$

and

$$C_{water} = EqP^{-1}(C_{sed}) = C_{sed} \cdot \frac{1150}{900 + 25 \cdot Koc}$$

To express concentrations in dry sediment, a generic wet weight to dry weight ratio of 4.6 was used.

Koc values were retrieved from the PCKOC of EPISUITE v1.66 software⁴⁵.

Thus, applying the EqP using PNECwater and Koc as input parameters, PNEC values for sediments were calculated and could be compared to available monitoring results in sediments. Note that the inverse approach is also possible, i.e. by comparing PNECwater values to concentrations in pore water estimated by the EqP method using monitoring results in sediment and Koc as input parameters.

PNEC values for sediment and associated Koc are presented in Annex VII.

⁴⁵ EPISUITE v1.66 software: <http://www.epa.gov/oppt/exposure/pubs/episuite.htm>





Note that the EqP approach was not applied for metals. Indeed, the prediction of solid/water partitioning for metals is deemed to be problematic since the adsorption of metals onto solid particles depends not only on the content of organic matter of the sediment, but also on many other parameters, such as pH, redox conditions, content of clay of the particles, water chemistry, etc., which are generally not known for the monitoring data submitted by the Member States. Therefore, benthic ecotoxicity was not investigated for metals.

b. A posteriori checking for PNEC_{sediment}

If a substance would be highly prioritised on the basis of sediment ecotoxicity, an a posteriori checking will permit to state on the degree of reliability of PNEC_{sediment} and, if deemed necessary and relevant, sediment dwelling ecotoxicity data may be used at this stage to confirm or not the prioritisation of the substance.

IV.2.3 (Eco)toxicity via biota

a. Sources of data and their reliability

Risk of secondary poisoning for predators and risk to human via consumption of contaminated aquatic living biota were assessed concomitantly. Indeed, they both use toxicity results on mammals (mainly rodents). Assessment of secondary poisoning can also rely on toxicity tests on birds.

Toxicity results were mainly retrieved from the ITER (International Toxicity Estimates for Risk) database⁴⁶. It is compiled by the Toxicology Excellence for Risk Assessment (TERA) and contains over 650 chemical records with key data from the Agency for Toxic Substances & Disease Registry (ATSDR), Health Canada, National Institute of Public Health & the Environment (RIVM) - The Netherlands, U.S. Environmental Protection Agency (EPA), the International Agency for Research on Cancer (IARC), NSF International, and independent parties whose risk values have undergone peer review. ITER data, focusing on hazard identification and dose-response assessment, are extracted from each agency's assessment and contains links to the source documentation. Data retrieved from these databases were deemed relevant and it was considered that there was no need for a systematic peer-review.

Alternative sources that were used include: datasheets prepared by the Fraunhofer Institute for the 33 existing priority substances, risk assessment reports for Reg. (EEC) 793/93 or Dir. 91/414/EEC, AGRITOX, INCHEM⁴⁷, HSDB⁴⁸, US-EPA's ECOTOX (formerly TERRETOX database)⁴⁹. Data retrieved from these databases were reviewed if deemed necessary on the basis of expert judgement.

b. PNEC_{oral} derivation

Key data for the oral route were researched, including both non cancer and cancer data. PNEC based on secondary poisoning for predators (PNEC_{sec.pois.}) and PNEC based on risk for human health from consumption of fish and shellfish (PNEC_{hh}) can then be derived. PNEC_{sec.pois.} or PNEC_{hh} are globally calculated by dividing the lowest toxicity result by an assessment factor. The rationale for choosing the appropriate assessment factor is detailed in the EU TGD.

⁴⁶ ITER: <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?iter>

⁴⁷ INCHEM: <http://www.inchem.org/>

⁴⁸ HSDB: <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>

⁴⁹ US-EPA's ECOTOX: <http://www.epa.gov/ecotox/>





For assessment of secondary poisoning of predators, daily doses expressed as $\text{mg}_{\text{tox}}/(\text{kg}_{\text{body weight}} \cdot \text{day})$ are converted into food concentration (i.e. $\text{mg}_{\text{tox}}/\text{kg}_{\text{food}}$) using generic conversion factors (i.e. body weight per daily food intake in $(\text{kg}_{\text{body weight}} \cdot \text{day})/\text{kg}_{\text{food}}$) as recommended by the TGD⁵⁰. For example, for >6 week rats, the conversion factor is 20 $(\text{kg}_{\text{body weight}} \cdot \text{day})/\text{kg}_{\text{food}}$; for mouse it is 8.3 $(\text{kg}_{\text{body weight}} \cdot \text{day})/\text{kg}_{\text{food}}$.

Note that in databases or literature, oral toxicity results are commonly expressed in terms of daily doses, i.e. $\text{mg}_{\text{tox}}/(\text{kg}_{\text{body weight}} \cdot \text{day})$.

For secondary poisoning, $\text{PNEC}_{\text{sec.pois.}}$ is currently calculated (EU TGD) as :

$$\text{PNEC}_{\text{sec.pois.}} (\text{mg} / \text{kg}) = \frac{\text{NOEC}_{\text{oral}}}{\text{Conversionfactor (TGD)}}$$

For human health, the associated acceptable concentration in food is calculated according to the generic scenario presented in Lepper (2005)⁵¹. It assumes:

- an average consumption of fishery products of 0.115 $\text{kg}_{\text{food}}/\text{day}$;
- an average body weight of 70 $\text{kg}_{\text{body weight}}$;
- that the contamination *via* consumption of food originating from aquatic sources represents only 10% of all the possible contamination sources. So, the acceptable contaminant intake from fishery products should not exceed 10% of the total acceptable contaminant intake.

The PNEC_{hh} in terms of concentration in food is therefore calculated as:

$$\text{PNEC}_{\text{hh}} (\text{mg} / \text{kg}) = \frac{0.1\text{ADI} (\text{mg} / \text{kg} / \text{day}) \times 70 (\text{kg})}{0.115 (\text{kg} / \text{day})}$$

For assessment of genotoxic carcinogens (non threshold effects), all the presented PNEC_{hh} correspond to a cancer risk of 10^{-6}

The most stringent of the $\text{PNEC}_{\text{sec.pois.}}$ or PNEC_{hh} was chosen for assessing hazard *via* biota ($\text{PNEC}_{\text{oral}}$). $\text{PNEC}_{\text{oral}}$ values with basic information on the source of keystone are provided in Annex VII. Values were proposed for all of the candidate substances for which monitoring data in biota were provided by the Member States (i.e. 91 substances, more precisely 89 individual substances/grouped substances + sum PCBs + sum dioxins/furans), except for 10 substances for which this was not possible (insufficient or non-relevant data) : 2-Methylnaphthalene, Benzo[e]pyrene, Chromium, Endosulfan, Metolachlor, Monobutyl tin, Perfluorooctane sulfonate (PFOS), Propanil, Terbutylazine and Tetrachloroethylene.

⁵⁰ see TGD, Table 22, page 129

⁵¹ Lepper, P. (2005). Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC). Fraunhofer-Institute Molecular Biology and Applied Ecology, Schmallenberg, Germany.





IV.3. Water intended for human consumption

Existing standards or recommendations for drinking water were retrieved for the candidate substances in the manageable list.

Of course, raw water in the environment is not supposed to comply with drinking water standards. Indeed, raw water intended for human consumption is treated before being distributed, and some part of the pollutants are therefore removed. The purpose of presenting drinking water standards is to identify those substances for which the ratio between the PEC and the drinking water standards is high, i.e. to identify substances for which high treatment removal efficiency would be necessary. Still, the removal efficiency varies with substances and treatment technology, and so every case where the ratio between the PEC and the drinking water standards is exceeded should be investigated further on a case by case basis. For example, persistent polar pollutants require advanced and expensive techniques to be removed from the raw water, whereas pollutants that are hydrophobic or volatile are expected to be quite easily eliminated.

Drinking water standards were retrieved from Dir. 98/83/EC or drinking water guidelines from WHO⁵² and are presented in Annex VII. When both standards were available, the most stringent was selected for the prioritisation exercise, as a conservative approach.

IV.4. Metals

⇒ Background concentrations

Given that a certain amount of metals found in the environment can be attributed to natural sources, available information on background concentrations of most metals in water and sediment was retrieved from the FOREGS database⁵³ and presented in the "First stage ranking report". The purpose of retrieving this information was to compare actual environmental concentrations (as revealed by the monitoring data provided by the Member States) with background concentration, and then to point out those metals with the largest anthropogenic "enrichments" but this approach, which is not based on risk, was not supported by WG E and was therefore abandoned.

⇒ Hazard info

PNEC_{water} or PNEC_{oral} values for metals in water and biota were also proposed:

- for Cadmium, Lead, Mercury and Nickel, values cited in public substances factsheets provided by CIRCA website⁵⁴ in the context of Directive 2008/105/EC were used;
- for other metals, if available, values from risk assessment reports were used, or alternatively data were retrieved from the literature. When toxicity values in water are known to vary according to different bioavailability conditions (e.g. water hardness, pH), the PNEC values corresponding to the reasonably most protective and EU realistic conditions were selected, i.e. values liable to be protective enough for risk to sensitive water bodies not to be severely underestimated⁵⁵.

⁵² http://www.who.int/water_sanitation_health/dwq/guidelines/en/index.html

⁵³ <http://www.gtk.fi/publ/foregsatlas/article.php?id=15>

⁵⁴ http://circa.europa.eu/Public/irc/env/wfd/library?l=/framework_directive/i-priority_substances/supporting_background/substance_sheets&vm=detailed&sb=Title

⁵⁵ This approach was also followed for Cadmium for which several EQS values are proposed in Directive 2008/105/EC. For this prioritisation exercise, the lowest value (0.08 µg/L) was selected. Note that for Nickel, Directive 2008/105/EC provides only an





Note that added risk approach was not used in this prioritisation process unless recommended in a finalised European Union Risk Assessment Report (e.g. for zinc). A more in depth analysis of such a choice might however be done for a further refinement of PNEC_{water} values, on a case by case basis using reliable background concentrations (e.g. provided in FOREGS database).

Note that use of biota monitoring data for risk ranking of essential metals raises some complexities. Indeed, deriving PNEC or ADI based on large assessment factors can lead to values well below the essentiality dose. For example, for copper in biota, it was proposed to base the assessment using the essentiality dose for humans. It has to be stressed as well that concentrations of essential metal in biota will vary depending on the species (e.g. hemoglobine vs haemocyanin organisms), the life stage and the season and that this should be taken on board to further assess risk for top predators using biota monitoring data. PNEC values for sediment were not proposed. Indeed, adsorption and bioavailability processes of metals in sediment are even more complex than for organics. Benthic ecotoxicity values than can be found in the literature or in EU risk assessments refer to specific conditions which are not necessarily comparable for all the metals considered under this prioritisation exercise.

All PNEC and ADI values are presented in Annex VII.

V. Step 4: Prioritisation algorithms

V.1. Algorithm for organic substances and metals

Different options for the prioritisation algorithm were identified and treated in the "Background document" (Bonnomet and Dulio, 2007)⁵⁶. As result of the consultation process with WG E, it was finally decided to use a ranking procedure based on the calculation of risk ratio.

The chosen prioritisation algorithm is quite straightforward: priority was assigned according to risk ratio values.

Following the risk assessment paradigm, a risk is generally expressed as the ratio between a predicted exposure concentration and a predicted no-effect concentration. Risk ratios were therefore calculated for each PEC which was divided by the associated PNEC (Table 12).

Since 2 scenarii were investigated for the PEC calculation, 2 risk ratios were provided for each of the analytical fractions listed above:

- "Risk1" is based on PEC1, i.e. calculated only from measurements that are above the analytical determination limit.
- "Risk2" is based on PEC2, i.e. calculated from all measurements, replacing censored values (ie. <DL) by DL/2.

unique EQS value of 20 µg/L which is based on the drinking water standard. But according to the draft EU risk assessment report for Nickel, the aquatic toxicity of this metal can be significantly lower under certain water chemistry.

⁵⁶ Bonnomet, V. and Dulio, V. (2007). Prioritisation of Substances: Background document. Version 3 (March 2007).





Table 12 : PEC and PNEC derived for each fraction and each matrix.

	Organics	Metals
Water	PEC for water, as whole water, divided by PNEC _{water}	PEC for water, as dissolved in water, divided by PNEC _{water}
Sediment	PEC for sediment, fraction 2 mm, divided by PNEC _{sed}	Not investigated
	PEC for sediment, fraction 20 µm, divided by PNEC _{sed}	Not investigated
	PEC for sediment, fraction 63 µm, divided by PNEC _{sed}	Not investigated
Biota	PEC for biota, fish, divided by PNEC _{coral} or human health ADI	PEC for biota, fish, divided by PNEC _{coral} or human health ADI
	PEC for biota, invertebrates, divided by PNEC _{coral} or human health ADI	PEC for biota, invertebrates, divided by PNEC _{coral} or human health ADI

Theoretically, PEC₁ overestimates the level of contamination because it only focuses on sites where a contamination is identified and does not account for cases where the contaminant was looked for but not found. However, in practice, cases where PEC₁ < PEC₂ (or even max quantified value < PEC₂) can occur. This may be explained by the sometimes huge heterogeneity in DL values amongst Member States⁵⁷. For a given substance, if the majority of the data originate from analyses with poor DL values (i.e. relatively high DL values), then the PEC₂ value (and therefore the Risk₂ value) will be mainly driven by those high DL values and actual quantified measurements could be occulted by all those censored data that were replaced by DL/2.

For this reason, substances for which Risk₂ > 1 but Risk₁ < 1 are deemed not to show strong evidence for actual risk. This obviously means that the analytical performances behind the measurements provided by the Member States should be improved before arriving at a firm conclusion about the risk.

For the same reason, cases where PEC₁ < PEC₂ (or Risk₁ < Risk₂) should also be regarded as suspect.

This is the reason why another criterion has been investigated: the value, for a given fraction and a given substance, of the ratio between the number of analyses that are actually >DL and the total number of analyses⁵⁸. Empirically, risks calculated from more than 98% measurements that are <DL or for which PEC₁ < PEC₂, could not be seen considered as strong evidences for concluding on priority of the substance.

Risk₁ and Risk₂ ratios, along with corresponding PEC₁, PEC₂, PNEC and information on fraction of analyses >DL, are presented in Annex XI for organics and metals.

⁵⁷ Even after the analyses with the highest DL values, regarded as outliers, were discarded during the quality check procedure (see section III.3.3 and Fribourg-Blanc 2008)

⁵⁸ (nb anal. > DL)/(nb all anal.) in Annex XI.





Substances for which risk ratios⁵⁹ are presented in Annex XI were grouped according to 5 distinct priority categories:

- a "Very high" priority basically represents cases when priority ratios exceed 100;
- a "High" priority basically represents cases when priority ratios exceed 10;
- a "Medium" priority basically represents cases when priority ratios exceed 1;
- the label "Not applicable" points out uncertain cases for which calculated priority ratios exceed 10, but for which number and/or distribution of measurements <DL does not allow to conclude with a reasonable confidence that there is actually a risk; or cases for which PEC1, PEC2 or PNEC is not available;
- a "Low" priority label is attributed to substances for which none of the above conclusions are met.

Classification as "Very high", "High" or "Medium" is only possible if the monitoring data meets the quality criteria defined in the previous section related to values lower than DL.

The first 3 categories ("Very high", "High" and "Medium") are quite straightforward for identifying substances with different levels of concern (according to risk). The different matrices and analytical fractions were considered together when establishing these categories, i.e. the overall priority is defined by the maximum priority amongst the calculated priority ratios either for water, sediment or biota.

The fourth category ("Not applicable") spots substances for which no conclusion can be made, because of the overall poor analytical performance for the available measurements or because of insufficient (eco)toxicological dataset to derive the PNEC and/or ADI. So, concerns may exist for these substances and would then be ranked relatively high (calculated priority ratios are >10 for substances in this category) but this cannot be firmly established.

Finally, the fifth category ("Low" priority) stands for substances for which quite strong evidence demonstrate a low probability of risk for the environment and the human health.

Detailed algorithms defining these 5 categories and all the results are provided in Annex XI for organics and for metals.

V.2. Specific cases

V.2.1 Water intended for human consumption

Annex VIII presents the ratios between PEC and drinking water standards or guidelines for organic substances and metals (see Section IV.3). This helps identifying those substances liable to require high treatment removal efficiency. Information is also given as whether the standards have been set according to toxicity criteria or not, as this influences decisively the interpretation of the data.

⁵⁹ so-called "priority ratios"





V.2.2 PCBs

Monitoring practices for PCBs differ amongst Member States: PCBs can be measured as a whole category, namely “total PCBs” (i.e. sum of all the congeners or sum of the 7 standard congeners), or they can be measured separately as individual PCBs.

Besides, hazard data are not available for all the individual congeners, and it is not necessarily straightforward to assess hazard due to a sum of congeners.

Three approaches, which are presented in detail in Annex IX, were tested⁶⁰:

- The first approach assesses the risk due to PCBs only from monitoring results identified as “total PCBs”.
- The second approach is about a tentative estimation of risk due to each individual congener. Unfortunately, the toxicity of each congener is not known, and the risk assessment should then rely on the toxicity for total PCBs and a proper estimation of each congener's proportion in the environment, this later being very uncertain because it is based on congener ratios in common commercial mixtures.
- The third approach consists in summing all the monitoring results provided for PCBs on each sampling record (i.e. summing all the available PCB congeners' concentrations measured at the same sampling point and sampling date) and then to compare with the toxicity for total PCBs. Unfortunately, only a few congeners may have been measured concomitantly at the same sampling point, and so this approach may overlook the toxicity induced by all the other congeners.

V.2.3 Dioxins/Furans

Dioxins (i.e. polychlorinated dibenzo-p-dioxins) and dioxin-like compounds (e.g. polychlorinated dibenzofurans and dioxin-like PCBs) share the same mode of action, i.e. binding to the aryl hydrocarbon receptor (AhR receptor). For this reason, toxicity effects induced by dioxin-like compounds are generally considered as additive.

Furthermore, since such compounds always occur as mixtures in the environment, risk assessment is usually made by adding up toxicity contribution of all dioxin-like compounds.

All dioxin-like substances do not have the same toxicity level and Toxic Equivalency Factors (TEF), expressed as toxicity equivalence to 2,3,7,8-Tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD), have been defined for each of them. The risk assessment is then performed by summing environmental concentrations of each measured dioxin-like substance multiplied by the substance corresponding TEF. The results, expressed as an equivalency 2,3,7,8-TCDD concentration in the environment, is then compared to the toxicity of 2,3,7,8-TCDD.

Dioxin-like compounds considered for this prioritisation exercise include relevant⁶¹ dioxins, furans and PCB congeners.

⁶⁰ It should be noted here that, whatever the approach is chosen, the results show risk from PCB in water, sediment and biota (see Annex IX).





None of the records submitted by the Member States include measurements for all the possible dioxin-like substances for a given sampling point and a given sampling date, thus risk may be underestimated⁶².

V.3. Comparison with COMMPS

The monitoring-based part of the COMMPS algorithm was also applied to organics in order to compare the results with the algorithm presented in this report. The outcomes of the two procedures are compared and presented in Annex XIII (see the discussion of results in section VII.5).

VI. Step 5: Review of the results

VI.1. General approach of the review

After the “First stage ranking report”, the Working Group E on Priority Substances discussed a number of options to carry out *a posteriori* checks on data quality and representativeness for those substances ranking high⁶³.

A number of *a posteriori* checks were performed in a review phase after the application of the algorithm, to evaluate the reliability and relevancy of the results for substances ranked as “Very high” and “High” priority. Two main issues were checked in the review: the EU representativeness and the quality and reliability of the monitoring data.

VI.2. Methodology of the review

VI.2.1 EU representativeness

For each substance classified as “Very high” or “High” (and not included in Directive 2008/105/EC), some statistics were investigated for each fraction (Number of countries monitoring the substance, Number of RBD where the substance is monitored, Number of stations sampled, Number of analysis). Then, it was highlighted whether or not the fraction determinant for the final rank was monitored by at least 3 countries (deemed EU representative at fraction level).

- When the substance is not monitored by at least 3 countries for the determinant fraction, then the substance has been identified as a candidate for de-selection that needs further investigation
- When the substance is monitored by 3 countries or more for the determinant fraction, then the criterion for EU representativeness is deemed satisfied. In this case, the quality/reliability of monitoring data is subsequently investigated

⁶¹ i.e. that are known to bind to the AhR receptor

⁶² Despite that probable underestimation, risk *via* sediment and biota has been identified (see Annex X)

⁶³ See Annex XIV and document WG E(5)-09-06.1a - Testing robustness and limits of the prioritisation methodology applied for 1st stage ranking exercise. Discussion Paper. Version 1. March 2009.





VI.2.2 Quality/reliability of monitoring data

For each substance monitored by 3 countries or more for the determinant fraction, the number and percentage of analysis deemed non reliable from an analytical point of view, i.e. non-quantified analysis for which limit of determination are above 2 times the PNEC, is investigated.

VI.2.3 Recalculation of risk after discarding monitoring data deemed unreliable

This review step consisted in discarding unreliable analysis (non-quantified analysis for which $LOD > 2 * PNEC$) and re-calculating PECs and risk-ratios and this for the fraction determinant of the final rank only. Ranks before and after discarding of unreliable data were compared.

- If discard of data leads to a new rank lower than "Very high" or "High", then the substance is identified as a candidate for de-selection that needs further investigation

Details on the results of the review are available in Annex XII.

VII. Overall results and discussion

VII.1. Results of prioritisation for substances of highest priority

Substances not included in the Environmental Quality Standards Directive (2008/105/EC) but retained in the manageable list and identified according the risk ratio monitoring-based methodology as "Very high" or "High" priority before any review are recalled thereafter (first organics, then metals).

Substances are sorted out by "Overall priority" and then by CAS number, except for PCBs and PAHs, that for the sake of clarity have been grouped at the end of the table.





VII.1.1 Organics

Table 13 : Results of monitoring-based prioritisation for organic chemicals of highest priority.

No.	SubstanceName	CAS	EQSD Annex III subst.	Final Priority WATER	Final Priority SEDIMENT	Final Priority BIOTA	OVERALL Priority
1	Heptachlor epoxide	1024-57-3		Very high	Very high	Very high	Very high
2	Heptachlor	76-44-8		Very high	Very high	Very high	Very high
3	Permethrin	52645-53-1		Very high	High	NA	Very high
4	Cyanides	57-12-5	X	High	Very high	NA	Very high
5	Malathion	121-75-5		Medium	Very high	NA	Very high
6	Methiocarb	2032-65-7		Medium	Very high	NA	Very high
7	Cypermethrin	52315-07-8		Very high	NA	NA	Very high
8	Deltamethrin	52918-63-5		NA	Very high	NA	Very high
9	Parathion	56-38-2		Very high	NA	NA	Very high
10	Dichlorvos	62-73-7		Very high	NA	NA	Very high
11	Dichlorodiphenyldichloroethane - o,p'	53-19-0		High	High	High	High
12	Tetrabutyltin compounds			High	High	NA	High
13	Triphenyltin compounds			NA	High	Medium	High
14	Dicofol	115-32-2	X	Medium	High	NA	High
15	Fenitrothion	122-14-5		Medium	High	NA	High
16	Diazinon	333-41-5		Medium	High	NA	High
17	Omethoate	1113-02-6		High	NA	NA	High
18	Nitrite	14797-65-0		High	NA	NA	High
19	Phoxime	14816-18-3		High	NA	NA	High
20	Chloroxuron	1982-47-4		High	NA	NA	High
21	Azinphos-ethyl	2642-71-9		High	NA	NA	High
22	Pirimiphos-methyl	29232-93-7		High	NA	NA	High
23	Trichlorfon	52-68-6		High	NA	NA	High
24	2,2',4,4'-Tetrabromodiphenyl ether	5436-43-1		NA	High	NA	High
25	Fenthion	55-38-9		High	NA	NA	High
26	Chlorpyrifos-methyl	5598-13-0		High	NA	NA	High
27	Methoxychlor	72-43-5		High	NA	NA	High
28	Mevinphos	7786-34-7		High	NA	NA	High
29	Chloroacetic acid	79-11-8		High	NA	NA	High
30	Methidathion	950-37-8		High	NA	NA	High
31	Monobutyl tin compounds			Low	High	NA	High
32	2,4-Dichlorophenol	120-83-2		Low	High	NA	High
34	Dioxins/Furans						
	Dioxins/Furans/PCB dioxin-like		X	High	Very high	Very high	Very high
	PCBs						
	PCBs - worst case 3 approaches		X	Very high	Very high	Very high	Very high
	2',3,4,4',5'-Pentachlorobiphenyl	31508-00-6	X	Very high	Very high	Very high	Very high
	2,3,3',4,4'-Pentachlorobiphenyl	32598-14-4	X	Very high	Very high	Very high	Very high
	2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1	X	Very high	Very high	Very high	Very high
	2,2',3,4,4',5'-Hexachlorobiphenyl	35065-28-2	X	Very high	Very high	Very high	Very high
	2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3	X	Very high	Very high	Very high	Very high
	2,2',5,5'-Tetrachlorobiphenyl	35693-99-3	X	Very high	Very high	Very high	Very high
	2,3,3',4,4',5'-Hexachlorobiphenyl	38380-08-4	X	Very high	Very high	Very high	Very high
	2,4,4'-Trichlorobiphenyl	7012-37-5	X	Very high	Very high	Very high	Very high
	2,2',4,5,5'-Pentachlorobiphenyl	37680-73-2	X	NA	Very high	Very high	Very high
	3,3',4,4'-Tetrachlorobiphenyl	32598-13-3	X	NA	Very high	High	Very high
	PAHs						
36	Pyrene	129-00-0		Medium	High	NA	High
37	Benzo(a)anthracene	56-55-3		Medium	High	NA	High

The results show a total of 46 organic substances (or groups of substances), 24 ranking "High" and 22 "Very high" (among which 10 individual PCBs, the groups "total PCBs" and dioxins/furans).





VII.1.2 Metals

Table 14 : Results of monitoring-based prioritisation for metals of highest priority

No.	Substance	CAS	Final Priority WATER (dissolved)	Final Priority BIOTA	OVERALL Priority
38	Arsenic (and mineral compounds)	7440-38-2	Medium	Very high	Very high
39	Selenium	7782-49-2	Medium	Very high	Very high
40	Uranium	7440-61-1	High	NA	High
41	Vanadium	7440-62-2	High	NA	High

The results show a total of 4 metals, 2 ranking “High” and 2 “Very high” priority.

VII.2. Results of the review

The substances that have been identified as candidates for de-selection that need further investigation according to the methodology and criteria set out for the review (see section VI.2) are listed in Table 15. The details of the review for each substance are given in Annex XII.

Table 15 : Results of the review for each substance of highest priority.

No.	SubstanceName	CAS	Reason for being candidate for de-selection	
5	Malathion	121-75-5	Monitoring data for the fraction ranking "High" or "Very high" comes from a number of country <3.	
6	Methiocarb	2032-65-7		
8	Deltamethrin	52918-63-5		
14	Dicofol	115-32-2		
15	Fenitrothion	122-14-5		
16	Diazinon	333-41-5		
24	2,2',4,4'-Tetrabromodiphenyl ether	5436-43-1		
32	2,4-Dichlorophenol	120-83-2		
35	3,3',4,4'-Tetrachlorobiphenyl	32598-13-3		
38	Arsenic (and mineral compounds)	7440-38-2		
39	Selenium	7782-49-2		
40	Uranium	7440-61-1	After discarding non-quantified analysis in which LOD>2*PNEC and recalculation of risk ratios, ranking is still "Very high" but data is available from 2 countries only on the determinant fraction (Whole water).	
41	Vanadium	7440-62-2		
3	Permethrin	52645-53-1		
29	Chloroacetic acid	79-11-8		After discarding non-quantified analysis in which LOD>2*PNEC and recalculation of risk ratios, ranking is not "High" anymore but "Low".
13	Triphenyltin compounds	-		After discarding non-quantified analysis in which LOD>2*PNEC and recalculation of risk ratios, ranking is not "High" anymore but "Medium".
22	Pirimiphos-methyl	29232-93-7		
23	Trichlorfon	52-68-6		
30	Methodathion	950-37-8		
12	Tetrabutyltin compounds	-		Following discard of data deemed non reliable, it is demonstrated that the substance is not ranking “High” anymore but “Very high”. However, this is based on monitoring data from 2 countries only

This review has investigated some of the most important issues in relation with EU representativeness and quality/reliability of monitoring data. However, due to the diversity of quantity and quality of the available monitoring data for each of the substances, it is recommended that the results are subject to further in-depth consideration by an expert group, in particular for those substances identified as candidates for de-selection.





In addition, PNECs used for the highly-ranked substances should be subject to expert review⁶⁴. In order to facilitate further review, the PNECs of the highly ranked substances are compiled in Annex XV (extracted from Annex VII).

VII.3. Substances in Annex III of Directive 2008/105/EC

The that likely need high removal efficiencies in the drinking water treatment 16 presents the results of the monitoring-based prioritisation for the substances included in Annex III of the EQSD (Directive 2008/105/EC) which were included in the manageable list (Musk-xylene and Quinoxifen were not included on the manageable list as data is available only from 3 and 2 countries respectively).

that likely need high removal efficiencies in the drinking water treatment 16 : Results of the monitoring-based prioritisation for the substances included in Annex III of the EQSD (Directive 2008/105/EC)

SubstanceName	CAS	EQS Annex III subst.	Final Priority WATER (whole water)	Final Priority SEDIMENT	Final Priority BIOTA	OVERALL Priority
Cyanides	57-12-5	X	High	Very high	NA	Very high
Dicofol	115-32-2	X	Medium	High	NA	High
Perfluorooctane sulfonate	1763-23-1	X	NA	NA	NA	NA
Aminomethylphosphonic acid	1066-51-9	X	Low	NA	NA	NA
Glyphosate	1071-83-6	X	Low	NA	NA	NA
Bentazone	25057-89-0	X	Low	NA	NA	NA
Edetic acid	60-00-4	X	Low	NA	NA	NA
Bisphenol A	80-05-7	X	Low	NA	NA	NA
Mecoprop	93-65-2	X	Low	NA	NA	NA
PCBs						
2',3,4,4',5'-Pentachlorobiphenyl	31508-00-6	X	Very high	Very high	Very high	Very high
2,3,3',4,4'-Pentachlorobiphenyl	32598-14-4	X	Very high	Very high	Very high	Very high
2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1	X	Very high	Very high	Very high	Very high
2,2',3,4,4',5'-Hexachlorobiphenyl	35065-28-2	X	Very high	Very high	Very high	Very high
2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3	X	Very high	Very high	Very high	Very high
2,2',5,5'-Tetrachlorobiphenyl	35693-99-3	X	Very high	Very high	Very high	Very high
2,3,3',4,4',5-Hexachlorobiphenyl	38380-08-4	X	Very high	Very high	Very high	Very high
2,4,4'-Trichlorobiphenyl	7012-37-5	X	Very high	Very high	Very high	Very high
2,2',4,5,5'-Pentachlorobiphenyl	37680-73-2	X	NA	Very high	Very high	Very high
3,3',4,4'-Tetrachlorobiphenyl	32598-13-3	X	NA	Very high	High	Very high

Monitoring data is scarce for some of the Annex III substances. The Table 17 presents the available monitoring data⁶⁵:

⁶⁴ In particular those for sediments (see section IV.2.2b)

⁶⁵ All Annex III substances are presented except dioxins/furans and PCB congeners not included in the manageable list. See Annex V for more information about the monitoring data.





Table 17 : Monitoring data for substances of the Annex III of Directive 2008/105 which present few monitoring data.

CAS	Substance name	Water			Sediment			Biota		
		Nb of countries	Nb of Stations	Nb of analyses	Nb of countries	Nb of Stations	Nb of analyses	Nb of countries	Nb of Stations	Nb of analyses
80-05-7	Bisphenol A	7	132	1370						
57-12-5	Cyanides	12	2245	23029	1	19	19			
25057-89-0	Bentazone	13	2779	39037	1	706	1842			
60-00-4	Edetic acid	6	295	7896						
1071-83-6	Glyphosate	9	1133	21308	1	78	78			
115-32-2	Dicofol	4	1199	22991	1	670	1838			
1066-51-9	Amino Methyl Phosphonic Acid (AMPA)	4	862	17165	1	78	78			
1763-23-1	Perfluorooctane Sulfonate	2	34	81	2	39	62	1	24	24
81-15-2	5-tert-butyl-2,4,6-trinitro-m-xylene (musk-xylene)	1	77	663	1	7	162	1	6	6
93-65-2	Mecoprop	14	2893	43489	1	682	1717			
124495-18-7	Quinoxifen	2	888	13677						
	PCBs									
1336-36-3	Total PCBs	7	386	5689	4	255	666	1	2	2
31508-00-6	2,3',4,4',5-Pentachlorobiphenyl	10	2082	27553	5	2004	6642	8	231	2253
32598-13-3	3,3',4,4'-Tetrachlorobiphenyl	2	644	6172	3	907	1519	2	36	87
32598-14-4	2,3,3',4,4'-Pentachlorobiphenyl	4	907	8583	3	1098	2941	3	178	1468
35065-27-1	2,2',4,4',5,5'-Hexachlorobiphenyl	10	2119	30384	4	2052	7500	7	228	2245
35065-28-2	2,2',3,4,4',5'-Hexachlorobiphenyl	11	2153	30905	5	2057	7729	8	230	2346
35065-29-3	2,2',3,4,4',5,5'-Heptachlorobiphenyl	11	2125	30721	5	2061	7587	8	231	2250
35693-99-3	2,2',5,5'-Tetrachlorobiphenyl	11	2137	30715	5	2058	7653	8	229	2275
37680-73-2	2,2',4,4,5,5'-Pentachlorobiphenyl	5	1089	15389	4	1985	7082	7	202	1565
38380-08-4	2,3,3',4,4',5-Hexachlorobiphenyl	4	610	5375	3	778	998	3	178	1289
7012-37-5	2,4,4'-Trichlorobiphenyl	10	1948	23125	4	2006	7061	7	209	1574





VII.4. Water intended for human consumption

Annex VIII presents the results for the prioritisation considering water intended for human consumption. As referred to in section IV.3, raw water in the environment is not supposed to comply with drinking water standards. Indeed, raw water intended for human consumption is treated before being distributed, and some pollutants are therefore removed. The purpose of presenting drinking water standards is to identify those substances for which the ratio between the PEC and the drinking water standards is high, i.e. to identify substances for which high treatment removal efficiency would be necessary, and thus may cause a failure of the drinking water standard at the tap.

The estimated treatment removal necessary to achieve the drinking water standard is presented in Table 18. The two values have been calculated using PEC1 and PEC2 (see Annex VIII).

Table 18 : Estimated removal efficiency needed for the top ranked substances.

CAS	Substance Name	WFD EQSD PS	EQS Annex III subst.	Estimated removal efficiency needed
7664-41-7	Ammonium compounds			99,96-99,97
91-20-3	Naphthalene	X		17-91
100-00-5	1-Chloro-4-nitrobenzene			80-98
1066-51-9	Aminomethylphosphonic acid		X	89-92
1071-83-6	Glyphosate (incl trimesium aka sulfosate)		X	69-84
1698-60-8	Chloridazon			30-99,7
330-54-1	Diuron	X		46-74
34123-59-6	Isoproturon			49-76
50-32-8	Benzo(a)pyrene	X		60-71
59-50-7	4-Chloro-3-methylphenol			31-60
75-01-4	Chloroethylene			86-99
	Metals			
7440-61-1	Uranium			96-97

These results have to be interpreted with care and it is proposed that they are reviewed in detail by an expert group.

VII.5. Comparison with monitoring-based COMMPS procedure

COMMPS procedure is a combination of a modeling-based prioritisation process and a monitoring-based prioritisation process.





Table 19 : Figures comparing monitoring datasets of COMMPS 1999 and monitoring risk ratio-based approach.

	COMMPS 1999	Monitoring risk ratio-based approach 2009
Nb Countries	15 + Eureau	28 + Vewin
A priori non candidate substances	Al, Br, Fe, NH ₃ , Cyanides, DDT, phenols, etc.	No
Nb candidate substances	314 (water) 221 (sediment)	1 147
Nb substances (manageable list)	95 (water) 60 (sediment)	316
Nb water analysis	752 043	13 581 264
Nb sediment analysis	68 880	918 839
Nb biota analysis	0	78 863

In the comparison, the available monitoring data on some organic substances have been processed using the COMMPS algorithm. This exercise allows highlighting potential differences between the monitoring score-based approach (COMMPS) and the monitoring risk ratio-based approach.

Taking into account the differences between monitoring score-based approach and monitoring risk ratio-based approach (e.g. indirect effects are taken on board differently), the most relevant way to compare the two approaches is to compare overall risks. Annex XIII provides a detail explanation on how the comparison is made.

The results of the comparison can be found in Annex XIII.





VIII. Conclusions and way forward

This document summarises methodology of the monitoring-based prioritisation carried out by the INERIS/IOW consortium to support the review of the WFD priority substances and presents the results.

- 316 substances have been selected as candidates for prioritisation (Annex V). For these 316 substances, monitoring data (in water, sediment and/or biota) were provided by more than 3 countries (out of the 28 countries that have collaborated in this exercise).
- PNEC in water, sediment and/or biota were, when possible, derived for these 316 candidate substances. Information relevant to human health via the aquatic environment were also retrieved (Annex VII).
- PEC for different fractions in water, sediment and/or biota were calculated (Annex VI).
- Priority was then assigned according to risk ratios, i.e. PEC/PNEC, for each fraction in water, sediment and/or biota (Annex XI). For chemical mixtures (e.g. PCB, dioxins) dedicated methodologies were proposed (Annexes IX and X).
- For comparison, outputs from the COMMPS algorithm were also presented (Annex XIII).

Table 20 : Substances ranking highly according to the monitoring-based prioritisation process. The substances marked with an asterisk (*) have been identified as candidates for de-selection in a review of EU representativeness and quality/reliability of monitoring data (see section VII.2 and Annex XII).

No.	SubstanceName	CAS
1	Heptachlor epoxide	1024-57-3
2	Heptachlor	76-44-8
3	Permethrin*	52645-53-1
4	Cyanides	57-12-5
5	Malathion*	121-75-5
6	Methiocarb*	2032-65-7
7	Cypermethrin	52315-07-8
8	Deltamethrin*	52918-63-5
9	Parathion	56-38-2
10	Dichlorvos	62-73-7
11	Dichlorodiphenyldichloroethane - o,p'	53-19-0
12	Tetrabutyltin compounds*	
13	Triphenyltin compounds*	
14	Dicofol*	115-32-2
15	Fenitrothion*	122-14-5
16	Diazinon*	333-41-5
17	Omethoate	1113-02-6
18	Nitrite	14797-65-0
19	Phoxime	14816-18-3
20	Chloroxuron	1982-47-4
21	Azinphos-ethyl	2642-71-9
22	Pirimiphos-methyl*	29232-93-7
23	Trichlorfon*	52-68-6
24	2,2',4,4'-Tetrabromodiphenyl ether*	5436-43-1
25	Fenthion	55-38-9
26	Chlorpyrifos-methyl	5598-13-0
27	Methoxychlor	72-43-5

No.	SubstanceName	CAS
28	Mevinphos	7786-34-7
29	Chloroacetic acid*	79-11-8
30	Methidathion*	950-37-8
31	Monobutyl tin compounds	
32	2,4-Dichlorophenol*	120-83-2
33	Dioxins/Furans	
	Dioxins/Furans/PCB dioxin-like	
34	PCBs	
	PCBs - worst case 3 approaches	
	2',3,4,4',5'-Pentachlorobiphenyl	31508-00-6
	2,3,3',4,4'-Pentachlorobiphenyl	32598-14-4
	2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1
	2,2',3,4,4',5'-Hexachlorobiphenyl	35065-28-2
	2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3
	2,2',5,5'-Tetrachlorobiphenyl	35693-99-3
	2,3,3',4,4',5'-Hexachlorobiphenyl	38380-08-4
	2,4,4'-Trichlorobiphenyl*	7012-37-5
	2,2',4,5,5'-Pentachlorobiphenyl	37680-73-2
	3,3',4,4'-Tetrachlorobiphenyl	32598-13-3
	PAHs	
35	Pyrene	129-00-0
36	Benzo(a)anthracene	56-55-3
	Metals	
37	Arsenic (and mineral compounds)*	7440-38-2
38	Selenium*	7782-49-2
39	Uranium*	7440-61-1
40	Vanadium*	7440-62-2





The monitoring-based prioritisation as regards water, sediment and biota (including protection of top predators and human health) has ranked 36 organic substances including individual PCBs, PCBs and dioxins/furans “groups” as well as 4 metals (Table 20).

As regards water intended for human consumption, substances in Table 21 have been identified as substances that likely need high removal efficiencies in the drinking water treatment, thus potentially responsible for failures in drinking water standards:

Table 21 : Substances likely to need high removal efficiencies in the drinking water treatment.

CAS	Substance Name
7664-41-7	Ammonium compounds
91-20-3	Naphthalene
100-00-5	1-Chloro-4-nitrobenzene
1066-51-9	Aminomethylphosphonic acid
1071-83-6	Glyphosate (incl trimesium aka sulfosate)
1698-60-8	Chloridazon
330-54-1	Diuron
34123-59-6	Isoproturon
50-32-8	Benzo(a)pyrene
59-50-7	4-Chloro-3-methylphenol
75-01-4	Chloroethylene
	Metals
7440-61-1	Uranium

Given the complexities of the exercise, it is recommended that an expert group reviews the results in detail.

This exercise should be seen as part of a global procedure for the review of the WFD priority list. Indeed, it will be combined to a modelling approach (see section I. and Annex I), in which substances that are not (or insufficiently) monitored should be investigated.

PEC values can be severely affected by the number and the level of measurements below the analytical determination limit. For some substances, analytical performances clearly need to be improved, because otherwise no conclusion about risk or absence of risk would be possible. A great heterogeneity in analytical performances and monitoring practices has been noticed between Member States and further efforts for the implementation of harmonised or comparable chemical monitoring methods are needed.

It is recognised that the methodology used may have underestimated the ranking of some pesticides or other organic chemicals with a seasonal emission pattern. Such characteristics could be taken on board for next prioritisation step, for instance by comparing MAC-EQS with peak measurements.

For metals, a refined assessment can be implemented, by assessing risk at the station level (i.e. risk assessed from aggregated data for each station), if not at the analysis level (i.e. risk assessed from non aggregated data), provided that adequate metadata and bioavailability models are available.





The exercise led to the identification of 183 substances labelled “Not applicable”. For those substances there is insufficient data to derive a PEC and/or a PNEC or the quality of data is too poor to be used for the calculation of a reliable risk ratio. These substances need further investigation.

Finally, as detailed in the present document, the data preparation was a very long and complex process, including many questions sent back to the data providers. If the data collection exercise is to be conducted on a regular basis, stricter rules will need to be applied to limit the post-processing to the minimum possible. It will then be necessary to complete the End user tool toolbox with additional tools such as a unit transformation tool, a short summary of the dataset provided and of possible problems identified for the data providers to check themselves the main points. The development of the data dictionary of the EEA and more widely of REPORTNET tools will also help the improvement, especially in relation to the exact definition of terms and of reference lists.

