

Final Report

**Revised Proposal for a List of Priority Substances in the Context of  
the Water Framework Directive (COMMPS Procedure)**

Declaration ref.: 98/788/3040/DEB/E1

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Umweltchemie und Ökotoxikologie  
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Germany

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# CONTENT

	Page
Executive Summary	1
1 Introduction	5
1.1 Background	5
1.2 Description of the COMMPS procedure, version 2	6
2 Selection of candidate substances	7
3 Monitoring data	8
3.1 Description and assessment of data sets included in the COMMPS database	8
3.2 Check of plausibility of monitored concentrations	9
3.3 Selection of monitored substances with regard to their EU-wide relevance and representativeness	15
3.3.1 Selection of substances monitored in water	16
3.3.2 Selection of substances monitored in sediment	17
3.4 Aggregation of monitoring data	18
4 Exposure scoring	21
4.1 Monitoring-based exposure scoring	21
4.1.1 Organic substances in the aquatic phase	21
4.1.1.1 Comparison of exposure scorings by the arithmetic mean method and by the maximum likelihood method	22
4.1.2 Organic substances in sediment	23
4.1.3 Metal compounds in the aquatic phase	23
4.1.4 Metal compounds in sediment	24
4.2 Modelling-based exposure scoring	24
5 Effects assessment	28
5.1 Effect scoring for organic substances in the aquatic phase	28
5.2 Effect scoring for organic substances monitored in sediments	32
5.3 Effect scoring for metal compounds monitored in the aquatic phase	33
5.4 Effects assessment for metal compounds monitored in sediments	35
6 Results of the risk-based ranking	36
6.1 Monitoring-based ranking of organic substances in the aquatic phase	36
6.1.1 Comparison of the arithmetic mean method with the maximum likelihood method	36
6.2 Modelling-based ranking of organic substances in the aquatic phase	37
6.3 Monitoring-based ranking of organic substances in sediments	46
6.4 Monitoring-based ranking of metal compounds in the aquatic phase	49

6.5	Monitoring-based ranking of metal compounds in sediments	50
7	Processing and combination of ranked lists	56
7.1	Monitoring-based lists, aquatic phase, organic micropollutants	59
7.2	Modelling-based list, aquatic phase, organic micropollutants	66
7.3	Monitoring-based lists, sediment, organic micropollutants	73
7.4	Monitoring-based lists, metals and metal compounds	80
8	References	81
Annex 1		A 1
Table A1:	Candidate substances compiled from the official lists and completed by monitored substances	A 2
Table A2:	Basic candidate list for the monitoring-based ranking (water)	A 29
Table A3:	Candidate substances selected for the monitoring-based ranking of substances in the aquatic phase	A 39
Table A4:	Substances excluded from the monitoring-based ranking of substances in the aquatic phase	A 42
Table A5:	Basic candidate list for the monitoring-based ranking of substances found in sediments	A 48
Table A6:	Candidates selected for the monitoring-based ranking of substances found in sediments	A 54
Table A7:	Substances excluded from the monitoring-based ranking of substances found in sediments	A 56
Table A8a:	Numerical information on exclusion of sampling stations and measurements upon the application of the 10/20%-criterion for measurements required to be above the corresponding determination limit at sampling station level - substances monitored in the aquatic phase	A 60
Table A8b:	Numerical information on exclusion of sampling stations and measurements upon the application of the 10/20%-criterion for measurements required to be above the corresponding determination limit at sampling station level - substances monitored in sediments	A 65
Table A9:	Results of the aggregation of monitoring data (organic substances in the aquatic phase)	A 68
Table A10:	Results of the aggregation of monitoring data (organic substances in sediment)	A 70
Table A11:	Results of the aggregation of monitoring data (total and dissolved concentrations of metal compounds in the aquatic phase)	A 72
Table A12:	Results of the aggregation of monitoring data (metal compounds in sediment)	A 73
Table A13:	Results of the aggregation of monitoring data (maximum likelihood method; organic substances in the aquatic phase)	A 74

Table A14: Monitoring based exposure indices of organic substances in the aquatic phase	A 76
Table A15: Maximum likelihood - exposure scoring for organic substances in the aquatic phase	A 78
Table A16: Comparison of exposure indices obtained by the COMMPS and the maximum likelihood method	A 80
Table A17: Monitoring based exposure indices of organic substances in the sediment	A 82
Table A18: Ratio factors "dissolved fraction : total concentration" used to derive calculated exposure concentrations for the dissolved fraction from figures referring to the total concentration	A 84
Table A19: Monitoring based exposure indices of metal compounds in the aquatic phase	A 85
Table A20: Monitoring based exposure indices of metal compounds in the sediment	A 86
Table A21: EURAM exposure indices and exposure related information for those chemicals on the COMMPS candidate list for which information was available at the European Chemicals Bureau	A 87
Table A22: Effect scoring for organic substances in the aquatic phase	A 99
Table A23: Effect scoring for organic substances in sediments	A 111
Table A24: Background concentrations of the dissolved and total (diss. & particle bound) fractions of metal compounds in surface freshwaters of Germany, The Netherlands, and Finland	A 115
Table A25: Effect scoring for the dissolved fraction of metal compounds in the aquatic phase - without consideration of background concentrations	A 116
Table A26: Effect scoring for the dissolved fraction of metal compounds in the aquatic phase - with consideration of background concentrations	A 117
Table A27: Effect scoring for the total metal levels in the aquatic phase - without consideration of background concentrations	A 118
Table A28: Effect scoring for the total metal levels in the aquatic phase - with consideration of background concentrations	A 119
Table A29: Maximum likelihood - Monitoring-based ranking of organic substances in the aquatic phase	A 120
Table A30: Comparison of priority ranks obtained by the COMMPS and the maximum likelihood method	A 123
Table A31: Comparison of exposure indices for monitored and modelled substances	A 125
Annex 2	A126
Form sheet "Effects Data" (addition/replacement of effects data)	A127

## Executive Summary

In March 1999 the European Council adopted the Common Position on the *Council Directive establishing a framework for Community Action in the field of Water Policy*), based on a proposal and two amended proposals of the European Commission. Article 21 requires the Commission to establish a list of substances prioritised on the basis of their risk to the aquatic environment and to human health via the aquatic environment.

In order to establish a list of priority substances in accordance with the given provisions, a combined monitoring-based and modelling-based priority setting scheme (COMMPS) has been elaborated.

In February 1998, a working paper outlining the COMMPS procedure was presented and discussed with experts from Member States, CSTE, industry and NGOs. In response to the comments which the Commission received, the working document was modified and redrafted. It comprised the basis for the elaboration of a first run of COMMPS. The results were presented and discussed at the expert meeting of 2 and 3 July 1998.

Following the meeting of 2 and 3 July 1998 and taking into account the comments which were made in the expert consultation, both the COMMPS procedure and the databases were revised. The following modifications were introduced:

⇒ for the COMMPS procedure:

- A modified assessment of monitoring raw data including the introduction of a plausibility test and a comparison of different statistical approaches to handle the heterogeneous monitoring data base.
- The replacing of the “ZIP” mechanism by a more flexible approach which includes the use of additional information of monitoring data to verify the likeliness of the rank of substances on the modelling-based list.

⇒ for the monitoring database:

- A complete update of the database. New raw data were included and some data sets were replaced or modified after re-evaluation by Member States. In addition, monitoring data provided by water suppliers (EUREAU) were included.

⇒ for the effects database:

- The re-evaluation of all effect data, accounting for information from ongoing risk assessments and comments of experts.

⇒ for metals:

- Several exposure variants were explored based on the information of Member States on the dissolved and total metal concentrations.

## Description of the COMMPS procedure

The COMMPS procedure is based on an approach to combine an automated relative risk-based ranking and a subsequent expert judgement (simplified risk assessment).

The automated relative risk-based ranking results in two independent ranking lists for the aquatic environment. Another ranking list is obtained on the basis of sediment monitoring data. For metals, a number of different lists are established using various scenarios for the exposure and effects scoring.

The COMMPS procedure comprises the following steps:

**Step A:** Selection of candidate substances subject to the ranking procedure:

The candidate substances are selected from various official substance lists and monitoring programmes ("list-based approach").

**Step B:** Calculation of exposure scores.

Two ranking lists are established for organic substances in the aquatic compartment, one based on surface water monitoring data and one based on modelling data, using the Mackay I distribution model. Further exposure lists - based exclusively on monitoring data - are established for pollutants adsorbed by sediments and for metals (several scenarios).

**Step C:** Calculation of effects scores.

Effect scores are established on the basis of test data. One list is established for organic pollutants in the aquatic compartment, one for sediments and several lists based on various scenarios for metals.

**Step D:** Computation of the risk-based score.

Ranked lists are calculated by multiplying the exposure and the corresponding effects score for each substance. Finally two lists are obtained for organic substances based on aquatic monitoring data and on modelling data, respectively, one list is obtained based on sediment monitoring data and several lists are obtained for metals (various scenarios).

**Step E:** Recommendation of priority substances.

A selection of priority substances is made on the basis of these risk-based ranking lists by a substance by substance judgement. For this purpose a two step procedure is applied. In the first step, the obtained lists are screened and a subset of candidate priority substances is selected from each of the lists. In the second step, recommendations are given for the inclusion/exclusion of these candidate substances into the priority list.

## Recommendation for the selection of priority substances

Following the above mentioned steps A - D, several ranking lists were obtained: a monitoring-based list for the water phase, a modelling-based list, a monitoring-based list for the sediment phase, several monitoring-based list for metals and metal compounds. In step E, priority substances were selected from these lists in a two-step process. In the first step, a number of the top-ranked substances from the lists were selected as candidate priority substances. For this purpose, the high-ranked substances on each of the ranked lists were screened and reorganised on the basis of the of following criteria:

- Grouping of substances which occur normally as mixtures
- Elimination of candidate substances if their marketing and use is already severely restricted or prohibited at European level (“historic“ pollution)

In the second step, a substance by substance judgement was applied to decide whether a candidate priority substance should be included or excluded from the final list. As a general principle, candidate substances selected based on the monitoring exposure data are accepted for inclusion in the priority list unless there is strong evidence against their high relative rank. On the other hand, substances taken from the modelling list are only accepted if there is additional information available (e.g. additional monitoring data) which support the high relative rank of the substance. For the purpose of this judgement, additional information was used as described in this report.

The following substances were finally selected and recommended for inclusion in the first priority list:

### Priority organic micropollutants in the aquatic phase, monitoring-based list

Number	Compound
1	PAHs
2	pentachlorophenol
3	heptachlor
4	chlorpyrifos
5	hexachlorobenzene
6	monochloronitrobenzenes
7	trichlorobenzenes
8	chlorfenvinphos
9	diuron
10	trifluralin
11	trichloromethane
12	dichloromethane
13	1,2-dichloroethane
14	isoproturon
15	endosulfan
16	alachlor
17	hexachlorobutadiene
18	HCHs
19	atrazine
20	simazine



**Priority organic micropollutants in the aquatic phase, modelling-based list**

<b>Number</b>	<b>Compound</b>
1	chloroalkanes, C10-13
2	benzene
3	nitrobenzene
4	di(2-ethylhexyl)phthalate (DEHP)
5	octylphenols -nonylphenols

**Priority organic micropollutants in the sediment, monitoring-based list**

<b>Number</b>	<b>Compound</b>
1	pentachlorobenzene
2	brominated diphenylethers

**Priority metals**

<b>Number</b>	<b>Compound</b>
1	nickel
2	lead
3	cadmium
4	copper
5	arsenic

# 1 Introduction

## 1.1 Background

In March 1999 the European Council adopted the Common Position on the *Council Directive establishing a framework for Community Action in the field of Water Policy*. Article 21 of this document (hereinafter referred to simply as “Article 21”) requires the Commission to propose by the end of 1998 a list of substances prioritised on the basis of their risk to the aquatic environment and to human health via the aquatic environment. Article 21, paragraph 2 of the WFD proposal sets out the principal strategy which shall be applied to establish priority substances. The following three optional routes are foreseen:

**Route A:** Risk assessments carried out under Council Regulation (EEC) No. 793/93<sup>[1]</sup>, Council Directive 91/414/EEC<sup>[7]</sup> and Council Directive 98/8<sup>[57]</sup>; or

**Route B:** Targeted risk-based assessment (following the methodology of Council Regulation (EEC) No. 793/93) focusing solely on aquatic ecotoxicity and on human toxicity via the aquatic environment; or where this proves impracticable within the time scale; or

**Route C:** A simplified risk-based assessment procedure based on scientific principles taking particular account of:

- evidence regarding the intrinsic hazard of the substance concerned, and in particular its aquatic ecotoxicity and human toxicity via aquatic exposure routes; and
- evidence from monitoring of widespread environmental contamination; and
- other proven factors which may indicate the possibility of widespread environmental contamination, such as production or use volume of the substance concerned as well as use pattern.

In order to establish a list of priority substances in accordance with these provisions, a combined monitoring-based and modelling-based priority setting scheme (COMMPS) has been elaborated on the basis of previous approaches for priority setting of hazardous substances.

In February 1998, a working paper outlining the COMMPS procedure was presented and discussed with experts from Member States, CSTEE, industry and NGOs. In response to the comments which the Commission received, the working document was modified and redrafted. It finally comprised the basis (COMMPS procedure, version 1, COMMPS\_1) upon which the Fraunhofer Institute elaborated a first draft report<sup>[31]</sup> and presented it at the expert meeting of 2 and 3 July 1998.

Following the meeting of 2 and 3 July 1998 and accounting for all comments received, the COMMPS procedure as well as the monitoring and effects databases were completely revised or updated, respectively.

The revision comprised

⇒ with respect to the COMMPS procedure:

- A modified evaluation of monitoring raw data including the introduction of a further plausibility check for monitoring sites.
- The comparison of different statistical approaches to handling the heterogeneous monitoring database.
- Replacing of the ZIP-mechanism applied in COMMPS\_1 for the final selection of priority substances from the ranking lists by the more flexible approach described in this study.

⇒ with respect to the monitoring database:

- A complete update of the database. New raw data were included and some data sets already in the database were replaced or modified after re-evaluation by Member States.

⇒ with respect to the effects database:

- The re-evaluation of all effect data, accounting for comments of experts and recently provided information.

## 1.2 Description of the COMMPS procedure, version 2

Version 2 of the COMMPS procedure (COMMPS\_2) is based on an approach to combine an automated risk based ranking and a subsequent expert judgement (simplified risk assessment).

The automated risk based assessment results in two different types of risk-based ranking lists, one type is based on monitored exposure levels and the other on modelled exposure estimates based on production volumes, use pattern, environmental distribution (Mackay Level I), and biodegradation as input parameters.

In detail, COMMPS\_2 comprises the following steps:

**Step A:** Selection of candidate substances for the ranking procedure. This step is described in chapter 2.

**Step B:** Calculation of exposure indices. Two ranking lists are established for organic substances in the aquatic compartment, one based on surface water monitoring data and one based on modelling data, using the Mackay I distribution model. Further exposure lists are established for pollutants adsorbed by sediments and for metals (several scenarios) based only on monitoring data. The details are described in chapter 4.

**Step C:** Calculation of effect indices. These are established on the basis of test data as described in chapter 5. Along with a list for organic pollutants in the aquatic compartment and one for sediments, several lists based on various scenarios for metals are established.

**Step D:** Computation of the risk-based priority index. Ranked lists are calculated by multiplying the exposure and the corresponding effects index for each substance. Finally two lists are obtained for organic substances based on aquatic monitoring data and on modelling data, respectively, one list is obtained based on sediment monitoring data and several lists are obtained for metals (various scenarios). The details are described in chapter 6.

**Step E:** These risk-based ranking lists must be combined by expert judgement. For this purpose a two step procedure is applied. In the first step, the obtained lists are screened and a subset of candidate priority substances is selected from each of the lists. In this step certain substances are grouped and "historic pollutants" are eliminated. In the second step, recommendation is made for the inclusion/exclusion of these candidate substances into the priority list. The details are described in chapter 7.

## 2 Selection of candidate substances

For the selection of candidate substances a "list-based" approach was followed according to which the candidates were selected from official lists and monitoring programmes. In accordance with agreements reached during the consultations, the candidate substances for the present priority setting were taken from the following lists:

- List I and II of Council Directive 76/464/EEC<sup>[2]</sup>
- Annex 1A and 1D of the Third North Sea Conference (3. NSC)<sup>[3]</sup>
- Priority lists 1-3 identified under Council Regulation No 793/93<sup>[4]</sup>
- OSPAR list of individual candidate substances<sup>[5]</sup>
- HELCOM lists of priority substances<sup>[6]</sup>
- Pesticides prioritised under Council Directive 91/414/EEC<sup>[7]</sup> (and specified under Council Regulation 3600/92<sup>[8]</sup>)
- Monitored substances not mentioned on any of the lists above (based on the monitoring data obtained from Member States)

In summary, 658 substances were compiled. Table A1 of annex 1 summarises these compounds.

### **3 Monitoring data**

#### **3.1 Description and assessment of data sets included in the COMMPS database**

For the second run of COMMPS the monitoring database was completely updated. This update comprised the addition of new monitoring data as well as the replacement of data identified as defective.

Following the expert meeting in July 1998, Member States and all other interested parties were invited by the Commission to submit additional monitoring data and/or to re-examine the data already provided. Following this invitation, many new monitoring data sets were provided to the consultants, including data from Member States which had not yet submitted their monitoring results (for details see table 1). Thus, the new monitoring database includes contributions from all 15 Member States. Besides the Member States, the "European Union of National Associations of Water Suppliers and Waste Water Services" (EUREAU) provided monitoring data for chemicals in surface waters close to drinking water abstraction points via its members BGW and VEWIN ("Bundesverband der deutschen Gas- und Wasserwirtschaft" and "Vereniging van Exploitanten van Waterleidingbedrijven in Nederland", respectively).

During the consultation of 2/3 July 1998 it was agreed that only unaggregated data should be used to allow for a statistical assessment of data at sampling station level. Consequently, all Member States that had provided aggregated data for the first version of COMMPS<sup>[31]</sup> (AU, FIN, I) replaced this data by the individual measurements on which the aggregation was based.

The update of the monitoring database also comprised the replacement or deletion of all data identified as defective or inappropriate for COMMPS. For example, one Member State, following the request to re-examine the monitoring data, noticed that the previously provided data set comprised doublets and monitoring sites not matching the requirements agreed for COMMPS (e.g. marine or groundwater monitoring, point sources, etc.) and consequently provided a revised data set. For the data set of another Member State it was noticed that many of the previously used concentration units were incorrect. The defective units were replaced after consultation with the authority that provided the data. Beside the revision of entire data sets, the cleaning of the database comprised the deletion of individual measurements identified as inconsistent (e.g. deletion of those entries for which zero was given as monitored level and no determination limit was provided or deletion of all entries which could not be assigned to a catchment area since the relevant information on river name and sampling site was missing).

With respect to the geographical significance of provided monitoring data and their quality, it was the main idea to collect as much information about sampling, chemical analysis and supplementary information about the sampling location, catchment area, population in the catchment, annual water flow, annual loads of pollutants, monitoring frequency as available and to process these data posterior on the basis of the mentioned parameters.

For this purpose, Member States were asked in February 1998 and again following the expert meeting of 2/3 July 1998 to provide the Fraunhofer Institute not only with monitoring data but also with supplementary information as described above. However, only the following minimum of supplementary information was made available for all samples:

- Name of the monitoring station
- River basin where the sampling took place
- Year of sampling
- Determination limits of the applied analytical method

Consequently, an extensive assessment of monitoring data quality and relevance as initially intended and described in <sup>[31]</sup> was not feasible.

One of the most crucial points, however, the question as to whether monitored levels of metal compounds refer to the total amount (dissolved and particle bound fraction) or merely to the dissolved fraction, could be clarified satisfactorily. All Member States except one submitted a definite statement with respect to the nature of their metal monitoring data (for details see table 1). The metal data set provided by the Member State from which a statement is not available is very small (every 2 measurements for 3 different metals), the provided levels were considered as referring to the total amount (best case assumption). Thus, given the total number of provided metal monitoring data, the chance that even an erroneous assignment of the 6 individual measurements to the total fractions of the respective metals could cause biased results can be ruled out.

On the basis of the above sketched situation regarding data availability and quality the following assessment steps were carried out:

- Check of plausibility of monitored concentrations at sampling station level
- Selection of substances considered as relevant on the EU-level
- Statistical assessment

### 3.2 Check of plausibility of monitored concentrations

In order to improve the reliability of the monitoring database to the extent possible, it was decided to introduce a plausibility check. The purpose of this check was to identify and eliminate implausibly high concentrations of a substance at the sampling station level (e.g. due to point source monitoring, dimension errors or errors in analyses). Initially it was intended to base this check on an algorithm suggested by a consulted expert in statistics <sup>[32]</sup>. The algorithm is based on nonparametric summary statistics. Each monitoring station arithmetic mean for the substance of concern is selected that exceeds the following threshold:

$$\text{threshold} = dz75 + 2 * (dz75 - \text{median})$$

with:

threshold a sampling station arithmetic mean higher than this threshold level may be implausible

dz75 75 percentile of sampling station arith. means for substance of concern

median median of sampling station arith. means for substance of concern

However, in practice this approach did not work satisfactorily since in many cases sampling station means were selected as presumably implausible whereas the available information (description of location, distance of sampling station mean to the next lower means of other sampling points) demonstrated that these sampling station means could not unequivocally be considered as implausible.

In order to avoid the exclusion of valid data sets it was therefore decided to use a very simple, straightforward check based on the sampling station level arithmetic means of positive findings (measurements > determination limit). All respective sampling station means exceeding a level of 100 µg/l for substances monitored in water were selected and checked with the available supplementary information on location and EU-level mean and EU-level 90-percentile concentration of the respective substance. Based on this check 41 sampling station means of 9 different substances were excluded from the monitoring database. For substances sorbed by sediment a similar check was performed. However, since the concentration levels in sediment are considerably higher than in the water phase and extreme outliers could not be detected for organic substances, only one monitoring station with extreme levels for sediment-bound copper and zinc was excluded.

The sizes of the national monitoring data sets after the above described checks and exclusions are listed in table 2. The size is defined as the number of records which is the total sum of measurements recorded for any substance at any monitoring station.

The database (in Microsoft Access 97) comprising the monitoring data (except the data provided by Austria and Finland) can be retrieved via the Internet at the following URL:

<http://www.iuct.fhg.de/commps/>

Table 1: Monitoring data and supplementary information provided by the Member States

Country, Source	Description of Monitoring Data Sets	Information on Sample Preparation, Methods and Determination Limits	Supplementary Information
<p><b>Austria</b> Bundesministerium für Land- und Forstwirtschaft, Sektion Wasserwirtschaft und Wasserbau</p>	<p>Water and sediment data from 1994 until present. All data from "general screening sites". For the current report the aggregated data provided for the first COMMPS report issued on 13 August 1998 was replaced by unaggregated raw data.</p>	<p>Information on analytical methods, sample preparation and determination limits. Concentrations of metal compounds in water were monitored for both the dissolved and the total (dissolved + particle bound) fraction. For the estimation of dissolved concentrations samples were filtered through a 0.45 µm membrane.</p>	<p>Information on local levels of contaminants in sewage sludge and effluents from sewage treatment plants, power plants and industrial installations. Information on levels of plant protection products in groundwater and rivers. Information on levels of heavy metals in sediments. Maps: Localisation of sampling sites, watersheds and catchment areas, population density and water flow.</p>
<p><b>Belgium</b> Vlaamse Milieumaatschappij</p>	<p>Data referring to water and suspended sediment samples collected in the Flemish region. Plant protection products, organic chemicals and metals (1995 - 97). For the current report the data referring to suspended sediment was added to the COMMPS sediment data base. This data was not considered for the first COMMPS report issued on 13 August 1998.</p>	<p>Information on detection limits. The provided monitoring data of metal compounds refer to total (dissolved + particle bound) concentrations.</p>	
<p><b>Denmark</b> Danish Environmental Protection Agency, Marine Division</p>	<p>Monitoring data on organic substances in river water and river and lake sediments from different sites in the county of Aarhus (1997). Nation wide monitoring data not yet available. For the current report the sediment data was revised (deletion of marine data).</p>	<p>Information on sample preparation, analytical methods, and detection limits. No metal monitoring data was provided.</p>	<p>Monitoring data on contaminants in marine sediments . Information on water quality criteria for surface waters in DK.</p>
<p><b>Finland</b> Finnish Environment Institute</p>	<p>a) National monitoring data for 30 rivers flowing to the Baltic Sea, mostly heavy metals. Data characterise the average and partly upper range of heavy metal concentrations in various watercourses in Finland, being still not in the immediate influence of individual polluters. The aggregated data provided for the previous COMMPS report (13 Aug. 98) were replaced by the unaggregated raw data. b) UN/ECE Convention on long range transboundary air pollutants (LRTAP) Integrated Monitoring Sites (3 small forested catchments): Heavy metal data from 94-96. Data characterise background areas, forest lakes with only slight atmospheric influence. c) Raw data on sediment pollution by chlorophenols and resin acids in pulp and paper mill effluent recipients (lakes).</p>	<p>Information on analytical methods and detection limits for metals. The monitoring data provided for metal compounds refer to total (dissolved + particle bound) concentrations.</p>	<p>Background levels for metals. Data on organic pollutants in indicator species. Recent publications on aquatic monitoring and research in Finland: Heavy metals (HM) in deposition and run-off HM in headwaters (water, sediment, biota) HM surveys in headwater lakes and streams Human intake of mercury Persistent organic pollutants (POP) in deposition and surface waters POP in sedimenting material and sediments POP in biota Map with localised river monitoring sampling sites</p>



Table 1: (continued) Monitoring data and supplementary information provided by the Member States

Country, Source	Description of Monitoring Data Sets	Information on Sample Preparation, Methods and Determination Limits	Supplementary Information
<b>France</b> Office International de l'Eau	Raw data on organic micropollutants and metals in water, sediment, suspended sediment and bryophytes (1995 & 96) from the 6 French water agencies. For the 2 <sup>nd</sup> run of COMMPS units of monitoring data were re-checked and corrected, if necessary.	Information on detection limits and analytical methods. The provided monitoring data of metal compounds refer to total (dissolved + particle bound) concentrations.	
<b>Germany</b> Umweltbundesamt; Bundesanstalt für Gewässerkunde  Bundesverband der Deutschen Gas- u. Wasserwirtschaft	Raw data for water and suspended sediment (1994 - 98). For the current report the monitoring data set was updated by addition of further data from various monitoring programmes. Monitoring data referring to suspended sediments were considered as sediment data. For the previous report data referring to <u>suspended</u> sediment was not considered.  Monitoring data for organic micropollutants in surface waters close to inlets of drinking water preparation facilities. The BGW data was provided after publication of the first COMMPS-report.	Information on determination limits. Metal concentrations in surface water are reported for the dissolved fraction, the suspended sediment and the total amount (dissolved + particle bound) as well.  Information on determination limits.	Reports on background levels and quality objectives for metals and quality objectives for organic substances. Rhine action programme of the International Commission for the Protection of the Rhine (e.g. quality objectives for water and sediment). Information on levels of heavy metals and organic contaminants in sewage sludge and agricultural soils. Reports of the German environmental specimen bank (1994/95 & 1997). Information on population density, size and water flow of river basins.
<b>Greece</b> Ministry of the Environment Physical Planning and Public Works / Water Section; Aegean University, Thessaloniki	Surface water (rivers and lakes) monitoring data for metal compounds and organic micropollutants. (1996 - 98)	Information on analytical methods and detection limits.  Provided levels for metal compounds in water refer to the dissolved fraction (filtration through 0.45 µm membrane).	
<b>Ireland</b> Environmental Protection Agency, Regional Inspectorate, Dun Laoghaire, Co. Dublin Marine Institute Fisheries Research Centre, Dublin	Raw data on metal levels in surface waters in Ireland arising from monitoring programmes currently in operation (1994-96). All stations except one can be regarded as general screening sites. One station is located 1 km downstream a nitrogen fertiliser plant and is additionally affected by drainage from defunct copper mines further up the river Avoca.	Information on analytical methods, sample preparation, and detection limits. Monitoring data for metal compounds refer to total (dissolved + particle bound) concentrations.	At present, there is no monitoring of organic substances. No emission inventories available. However, a survey of the levels of the 17 substances covered by the daughter directives made under 76/464 and the current monitoring of the metals indicate that these substances are not present in significant amounts in Irish waters. The main exceptions to this are the metal concentrations in the river Avoca. Data on metals and organochlorine contaminants in marine sediments.

Table 1: (continued) Monitoring data and supplementary information provided by the Member States

Country, Source	Description of Monitoring Data Sets	Information on Sample Preparation, Methods and Determination Limits	Supplementary Information
<b>Italy</b> Agenzia Nazionale per la Protezione dell' Ambiente (ANPA)	Reported data represent regions with significant impact in Italy and have been collected according to routine monitoring programs in 1995, 1996 and 1997. Aggregated data provided previously was for the current report replaced by unaggregated raw data .	Information on analytical methods and detection limits for organic substances and metals. Monitoring data for metal compounds refer to the dissolved fraction (samples filtered through a 0.45 µm membrane).	Groundwater analyses in the Emilia Romagna. No data available about sediments and emission inventories.
<b>Luxembourg</b> Administration de l'Environnement, Division des Eaux	Raw data on organic substances in river water (Mosel; 1994-96).	Information on detection limits. No metal monitoring data was provided.	
<b>Netherlands</b> Rijksinstituut voor Integraal Zoetwaterbeheer en Afvalwaterbehandeling (RIZA)	Raw data on organic substances and metal levels in water and sediment (1996-97). Additional monitoring data referring to concentrations of the dissolved fraction of metals compounds in water was provided for the current report.	Information on detection limits. Concentrations of metal compounds in water were provided for both the dissolved and the total (dissolved + particle bound) fraction..	Background levels for metals. Qualitative judgement on relevance of "Candidate List"-substances in The Netherlands. Report "Emission Data for The Netherlands" (1997). Various reports on maximum permissible concentrations of organic and metal compounds and the methods used to derive these MPCs.
<b>Portugal</b> Ministerio do Ambiente, Instituto da Água	Surface water monitoring data for predominantly metal compounds (1997).	Information on detection limits.	
<b>Spain</b> Ministerio de Medio Ambiente; Cuenca Hidrográfica del Ebro	Raw data for organic micropollutants and metal compounds in surface waters and sediment (1996-97).	Information on analytical methods and determination limits. Provided concentrations for metal compounds in water refer to the dissolved fraction (filtration through 0.45µm membrane).	
<b>Sweden</b> Natur Vårds Verket (Swedish EPA)	Raw data on metal monitoring in rivers (1995-97). Data on organic contaminant levels in the Gota river sediment.	Monitoring data for metal compounds refer to total (dissolved + particle bound) concentrations.	Map for sampling station locations. Information on size of catchment area. Data on metal transport (loads) in rivers (1995-96). Data on total Hg and methyl-Hg levels in pikes. Pesticide concentrations and transport in a small agricultural catchment. Information on contaminant levels in marine and freshwater sediments, sewage sludge, groundwater, and biota. Information on emissions, mainly metals and PCBs.

Table 1: (continued) Monitoring data and supplementary information provided by the Member States

Country, Source	Description of Monitoring Data Sets	Information on Sample Preparation, Methods and Determination Limits	Supplementary Information
<p><b>United Kingdom</b> Department of the Environment Transport and the Regions Water Quality Division</p>	<p>Raw data for individual sampling sites covering England, Wales, Northern Ireland and Scotland (1994 - 1996). The data was revised for the current report by UK. This revision included deletion of doublets and monitoring sites not matching the requirements agreed for COMMPS (e.g. marine, groundwater, point sources, etc.). Additional data referring to metal compounds was provided.</p>	<p>Information on detection limits. For most metal compounds monitoring data referring to the dissolved and total (diss. + particle bound) fractions were provided. However, for Fe only concentrations for the dissolved fraction and for V and Zn only the total concentrations were reported.</p>	

Table 2: Years for which monitoring data were provided and size (record numbers) of the data sets after initial quality and plausibility check

a) Water																
Member State																
Year	AU	B	D	DK	E	F	FIN	GR	I	IRL	LUX	NL	Pt	S	UK	Σ all MS
unknown								1								1
1994	2397		36674				2700			420	247				178660	221098
1995	1740	2882	40963			8341	2620		4940	652	247			9549	160180	232114
1996	3265	9418	17389		1045	7612	2498	1327	2704	982	132	6997		11179	175991	240539
1997	6999	12371	5729	282	809		1543	3011	50			6866	8	11399	7031	56098
1998	472		94					1628								2194
total	14873	24671	100849	282	1854	15953	9361	5966	7694	2054	626	13863	8	32127	521862	752043

b) Sediment											
Member State											
Year	AU	B	D	DK	E	F	FIN	NL	S	UK	Σ all MS
unknown		5	18			6		29	24	43	125
1994	159	1274	16778							157	18368
1995	122	2800	17993			4497					25412
1996	135		8923		592	4185		4141		167	18143
1997	72		501	583	449		125	5078			6808
1998	24										24
total	512	4079	44213	583	1041	8688	125	9248	24	367	68880

### 3.3 Selection of monitored substances with regard to their EU-wide relevance and representativeness

Prior to the check and selection of substances with regard to their relevance at EU-level, some inorganic compounds and sum parameters as well as all organic sum or group parameters whose properties could not be related to a defined mixture of substances or a key-substance were excluded from the monitoring list. Further, the metals aluminium and iron were excluded also since they were considered as irrelevant with regard to their Community-wide significance as pollutants from direct anthropogenic emissions. This assumption seems to be justified since adverse environmental effects of iron emissions are not reported in the literature. Aluminium toxicity in surface waters, however, is known but is mostly not a result of anthropogenic emissions of aluminium compounds. It is mainly due to the acidification of watercourses, which in turn leads to an increased solubility of naturally present but, under undisturbed conditions, unavailable (insoluble) aluminium compounds. Moreover, salts of both aluminium and iron are used in considerable amounts in sewage treatment plants in order to coagulate and remove fine particles from the effluents. Adverse environmental effects in receiving watercourses due to the use of these metal salts are not known.

Compounds and parameters excluded in this first step are listed in table 3.

Further, certain substances very similar in nature and effect potential have been clustered as described in table 4 (these compounds otherwise had not passed the representativeness checks described in chapters 3.3.1 and 3.3.2).

Table 3: A priori excluded substances and sum-parameters

Inorganic Substances and Parameters	Organic Parameters
Aluminium	AOX (adsorbable organic halogens)
Ammonia-Nitrogen	$\Sigma$ BTX
Bromium	$\Sigma$ DDE
Cl <sub>2</sub> , free ( $\approx$ Cl <sub>2</sub> , total residual)	$\Sigma$ DDT ( $\approx$ DDT, total)
Cyanides (calc. as $\Sigma$ CN)	Detergents
Fluorides	Hydrocarbons, total
Iron	Lignine-sulfonic-acid
Nitrate-Nitrogen	MBAS (methylene blue active subst. = $\Sigma$ param. f. anionic detergents)
Orthophosphate	NID (non-ionic detergents)
Phosphorus, total	PAH (calc. as C)
	Oil
	Phenol-Index
	Phenols
	$\Sigma$ Trichloro-benzenes ( $\approx$ Trichloro-benzene, total)

Table 4: Clustering of compounds before representativeness check

CAS	Compound	CAS	clustered with Compound <sup>*)</sup>
3542-36-7	dioctyltin (dichloride)	15231-44-4	dioctyltin
104-40-5	4-nonylphenol	25154-52-3	nonylphenol
84852-15-3	4-nonylphenol, branched	25154-52-3	nonylphenol
unknownHLFU10	nonylphenol-diethoxylate	9016-45-9	nonylphenoethoxylate
unknownDK1	nonylphenolmonoethoxylate	9016-45-9	nonylphenoethoxylate
unknownHLFU2	iso-octylphenol	1806-26-4	octylphenol
27323-18-8	PCB, total	1336-36-3	PCBs
688-73-3	tributyltin compounds	36643-28-4	tributyltin (cation)

<sup>\*)</sup> also name of cluster

### 3.3.1 Selection of substances monitored in water

After the exclusion of substances and parameters which are considered as irrelevant for the purpose of this study (see Table 3) 314 substances monitored in surface freshwater remained. These chemicals are listed in table A2 (annex 1).

The substances shown in table A2 were subjected to a check of their Community-wide relevance and representativeness as agreed for COMMPS and outlined hereafter.

To meet the relevance and representativeness criteria positive findings (i.e. findings above the determination limit) must be reported

- by at least three Member States

or

- by two Member States if positive findings are detected in each Member State within at least one transboundary river basin and these are not the same river basins.

- Furthermore, any substance must be positively monitored in at least 5 instances.

These criteria were the same as those used in COMMPS\_1 which had been introduced following intense discussions with experts during 1998.

To comply with the selection criteria for the Community-wide representativeness, all substances with findings above the determination limit in 3 or more Member States were selected (n = 84). For all cases in which a substance was positively found in only 2 Member States, it was checked whether the substance was found in each of the Member States in at least one transboundary river basin (11 compounds). Thus, 95 substances passed these two selection criteria. No further substance had to be excluded on the basis of the criterion "less than 5 positive findings EU-wide".

Consequently, 95 substances finally passed the selection criteria for the monitoring-based ranking list (table A3, annex 1). 86 of these substances are organic chemicals and 9 are metals. 219 substances (70% of 314 initial candidate substances) were excluded from the monitoring-based ranking on the basis of the selection criteria (for a summary, see table A4 in annex 1).

### **3.3.2 Selection of substances monitored in sediment**

The selection procedure for the sediment monitoring data was similarly performed as described in chapter 3.3.1 for the water monitoring data. The selection criteria used for EU-wide relevance of substances monitored in sediments were also identical.

According to the data provided by the Member States 221 substances have been monitored in freshwater sediments for the last couple of years from 1994 on. Information regarding these substances is summarised in table A5 (annex 1).

60 substances passed the selection criteria for EU-wide relevance and were included in the list for the ranking of substances monitored in sediments (56 positively found in  $\geq 3$  MS, 4 positively found in only 2 MS but in two independent transboundary river systems, no substance which passed the before mentioned criteria had to be excluded because it was less than 5 times positively found). 52 of these substances are organic chemicals and 8 are metals. 161 substances were excluded from the ranking. Thus, the percentage of excluded substances (73%) is slightly higher than for the substances monitored in water (70%). The substances which were finally selected for the establishment of the sediment-based ranking list are summarised in table A6, those excluded are summarised in table A7.

### 3.4 Aggregation of monitoring data

In the consultation of experts in 1998 one Member State criticised the applied aggregation procedure. Therefore, a comprehensive assessment of different options for the statistical treatment and evaluation of monitoring data was carried out on behalf of the European Commission <sup>[33]</sup>.

As a result of the examination of the aggregation procedure it was concluded that the tiered procedure

- calculation of monitoring station arithmetic means with an assumed relative level for measurements below the corresponding determination limits<sup>1</sup> in a 1<sup>st</sup> step
- calculation of 90-percentiles from the monitoring station arith. means in a 2<sup>nd</sup> step

is an acceptable approach. A more sophisticated approach for the aggregation of data at sampling station level such as the maximum likelihood method may produce extremely biased results if the percentage of negative findings becomes very high and the data-sets are very wide-spread (e.g. showing a standard deviation of the log-normal transformed distribution of  $\sigma=1.5$  or larger). In about 4.5% of the COMMPS data sets the estimate of  $\sigma$  exceeds  $\sigma=1.5$ , and the percentage of negative findings exceeds 80% of the measurements). In this case, the results of the maximum likelihood method will yield less reliable results compared to the simple arithmetic mean method.

Details can be found in reference [33]. The findings of the report support the use of the above mentioned aggregation method. It was therefore applied with some recommended modifications as described below. However, for the purpose of comparison the maximum likelihood method (estimating the arithmetic mean on the basis of the parameters  $\mu$  and  $\sigma$  of the log-normal distribution) was also applied in order to illustrate the possible effects on the ranking.

Based on the findings of the report <sup>[33]</sup>, the aggregation procedure was modified with respect to the treatment of measurements below their corresponding determination limit (DL). For the previous (first) run of COMMPS <sup>[31]</sup> half of the level of the corresponding DL was used as value for a measurement at sampling station level if this measurement resulted in a figure below the DL. In case the corresponding determination limit was more than 10 times higher than the lowest DL of that substance in the selected data set, all measurements at that station below the corresponding DL were excluded and not used for the calculation of the sampling station arithmetic mean of the respective substance. Positive findings (levels above the corresponding determination limit) were in any case used for the calculation of sampling station means, irrespective of the level of the corresponding determination limit.

This procedure may result in considerably biased arithmetic mean values since a part of the available data is discarded. In order to reduce the bias it was recommended to introduce as a general requirement that a certain percentage of the measurements at a sampling station must be higher than the determination limit. If this is not the case, the data set should be entirely excluded.

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<sup>1</sup> It was recommended <sup>[33]</sup> that the convention "set measurements < Determination\_Limit to 0.5\*DL" is the most appropriate

Given the heterogeneous data and the varying data quality, while no sound statistical theory for the required minimum percentage of positive findings is applicable, an exclusion of data sets with more than 90% negative findings seems to be a practical approach (reference<sup>[33]</sup>). Since the bias would be even more enhanced if data with very high determination limits were aggregated, it was also recommended<sup>[33]</sup> to exclude data sets with very high determination limits if more than 80% of the measurements fall below DL.

The trigger for switching from 10% to 20% positive findings was defined as follows:

If arithmetic Mean of  $DL_{MS_i} < \text{Threshold}$   $\Rightarrow$  at least 10% positive findings

If arithmetic Mean of  $DL_{MS_i} > \text{Threshold}$   $\Rightarrow$  at least 20% positive findings

Threshold = Median of aM\_DL + 2 \* MAD

with:

$DL_{MS_i}$  - determination limits of a certain substance at monitoring station (i)

aM\_DL - all sampling station arithmetic means of DL for a certain substance

MAD - median of absolute deviations

= Median of (Median(aM\_DL) - | arith. Mean( $DL_{MS_{i-n}}$ ) |

The application of this 10/20%-rule resulted in the exclusion of considerable numbers of data sets. The respective information is provided in table A8a (aquatic phase) and A8b (sediment) in annex 1.

With respect to the assumed relative level of measurements below the determination limit it was recommended<sup>[33]</sup> that the convention (i) "set measurements < DL to 0.5\*DL" is the most appropriate (other tested options: (ii) "measurement < DL = 0"; (iii) "measurement < DL = DL"). It was therefore decided to use convention (i) for the aggregation of monitoring data.

In summary, monitoring data were aggregated as follows:

1. The aggregation was applied to those data-sets which passed the check for representativeness of substances at EU-level (chap. 3.3)
2. All measurements for a specific substance at a monitoring station were excluded from further aggregation if less than 10% (or 20%, depending on the level of the determination limit) of the measurements of that substance, resulted in positive findings.
3. The arithmetic means at sampling station level were calculated.
4. The EU-level 90-percentile for each substance was derived from its sampling station arithmetic mean levels<sup>2</sup>. Thus, the EU-level 90 percentile of concentration for a substance is the exposure level on which the exposure scoring (chap. 4) is based.

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<sup>2</sup> In case less than 10 sampling station arithmetic means were available for the derivation of the EU-level 90-percentile the highest arithmetic mean was instead used for the exposure scoring.



In the above described screening, selection, and aggregation steps (collection of data and initial quality screening, check for EU-wide representativeness, application of the 10/20%-rule) the amount of monitoring data sets and substances was reduced as follows:

	Step	No. of records	%	No. of substances	%
<b>Aquatic phase</b>	Collection after quality screening	752043	100	314	100
	Representativeness check	635543	84.5	95	30.3
	10/20%-rule	246651	32.8	94	29.9
<b>Sediment</b>	Collection after quality screening	68880	100	221	100
	Representativeness check	61540	89.4	60	27.1
	10/20%-rule	51162	74.3	60	27.1

The obtained exposure concentrations, together with summary statistics for the data used to calculate these concentrations, are provided in tables A9 (organic substances in the aquatic phase), A10 (organic substances in sediments), A11 (metal compounds in the aquatic phase), and A12 (metal compounds in sediments).

The exposure concentrations calculated with the "maximum likelihood" method<sup>[33]</sup> are listed in table A13 (organic substances in the aquatic phase only). Data selection and aggregation was performed as described in the summary above except that in step 3 the maximum likelihood method was applied in order to calculate the sampling station concentration levels.

## 4 Exposure scoring

### 4.1 Monitoring-based exposure scoring

#### 4.1.1 Organic substances in the aquatic phase

The exposure scores were calculated on the basis of the arithmetic means obtained at each sampling station (for the maximum likelihood method the arithmetic mean was calculated on the basis of the parameters of the log-normal distribution as described in reference <sup>[33]</sup>). The 90 percentile  $C_i$  of these sampling station values was taken for the calculation of the exposure score at EU level. The aggregated levels were scored with a maximum score of 10. For this purpose, a logarithmically scaled exposure index was calculated for each substance as follows:

$$I\_EXP (\text{substance } i) = \frac{\log(C_i / (C_{\min} * 10^{-1}))}{\log(C_{\max} / (C_{\min} * 10^{-1}))} * 10$$

The exposure index was scaled by defining an upper and a lower limit (minimum and maximum concentration). The chosen limits are listed in the table 5. Both the figures for the lower and upper limits were set close to the lowest and highest EU-level 90-percentile of substance concentrations in the data set in order to allow for the use of the full range of the scale and thus for an optimal differentiation of the chemicals with respect to their quantitative occurrence in the aquatic environment. The multiplication of the lower limit ( $C_{\min}$ ) by a factor of 0.1 is introduced in order to avoid zero as a value of the exposure index for the substance with the highest concentration ( $C_i = C_{\max}$ ) because this would result in a priority index of zero ( $\Rightarrow$  the priority index is obtained by multiplication of the exposure index with the effect index).

Table 5: Minimum ( $C_{\min}$ ) and maximum ( $C_{\max}$ ) concentrations used for the calculation of the exposure scores:

	$C_{\max}$	$C_{\min}$	Unit
Organic substances in the water phase	100	0.0001	$\mu\text{g/l}$
Organic substances in the water phase (maximum likelihood)	100	0.0001	$\mu\text{g/l}$
Metal compounds in the water phase	200	0.2	$\mu\text{g/l}$
Organic substances in the sediment	10000	0.01	$\mu\text{g/kg}$
Metal compounds in the sediment	2000	6	$\text{mg/kg}$

Table A14 shows the result of the monitoring-based exposure scoring for organic substances in the aquatic phase. The corresponding exposure indices obtained for the maximum likelihood method are listed in table A15.

#### 4.1.1.1 Comparison of exposure scorings by the arithmetic mean method and by the maximum likelihood method

As can be seen in figure 1 and from table A16, the results of the exposure scoring obtained by both methods correlate well. From the distribution of data points not on the (virtual) regression line in figure 1 it can be concluded that the ranking based on arithmetic means (AM) in comparison with the ML-method results for some substances in lower exposure indices.

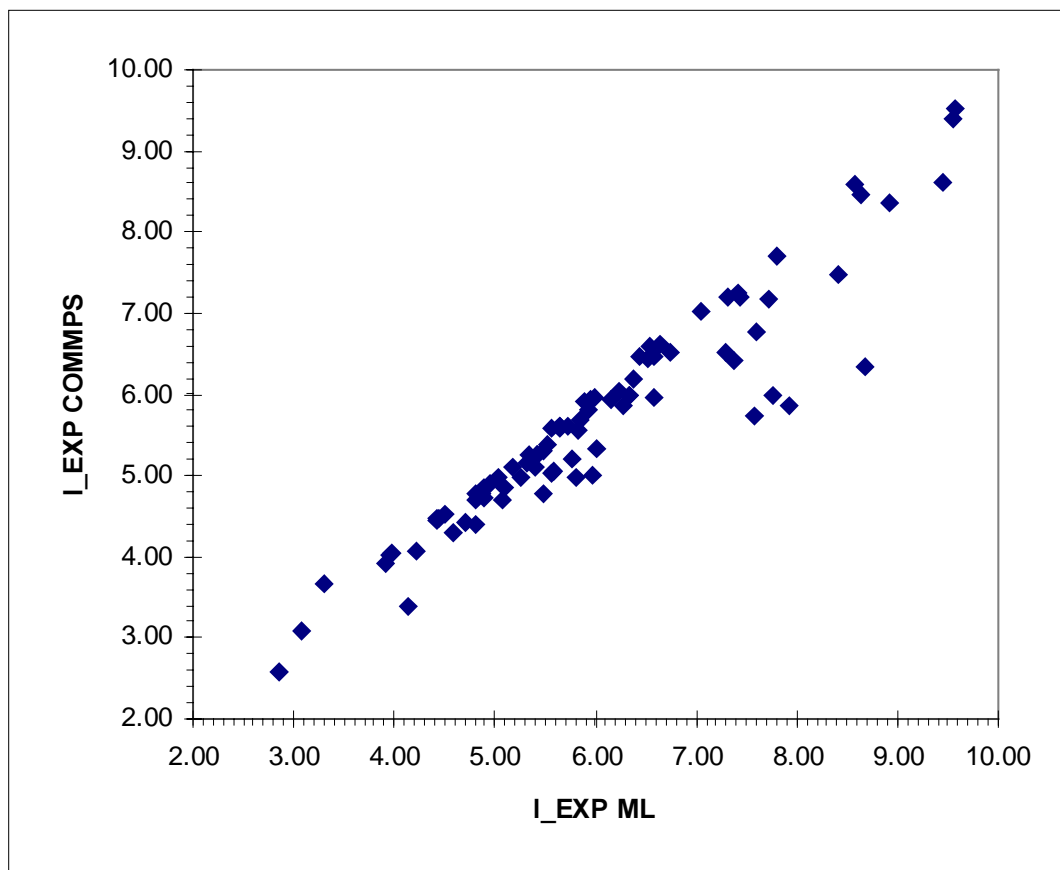


Figure 1: Correlation of exposure scores obtained with the maximum likelihood and the COMMPS method

One reason for the relatively good correlation of the AM and the ML based exposure scoring may be the identical selection of monitoring data as described in chapters 3.2 to 3.4 (plausibility check, selection with respect to EU-wide relevance and representativeness, exclusion of sampling stations at which not at least 10% - or 20%, depending on the level of the determination limit - of the measurements of a substance resulted in positive findings). Another reason is the use of the 90-percentile of monitoring station means as EU-level exposure concentration. This ensures that large discrepancies between the monitoring station means obtained by the two methods are disregarded as long as the percentage of those discrepancies is less than 10%. Thus, it cannot be generally concluded that the AM and ML method perform similarly in any case.

#### 4.1.2 Organic substances in sediment

As for the substances in the aquatic phase, the EU-level 90-percentiles of the concentrations were used as input for the exposure scoring and ranking of sediment substances. Scores were calculated in the same way as described in chapter 4.1.1 (see table 5 for  $C_{\min}$  and  $C_{\max}$ ).

Table A17 (annex 1) shows the results of the exposure scoring for organic substances.

#### 4.1.3 Metal compounds in the aquatic phase

Metals and inorganic metal compounds occur naturally in very different concentrations depending on the local geological and hydrological preconditions. They speciate in a wide range of possible chemical forms and may be found dissolved in water or adsorbed/bound to organic and inorganic matter in suspended or settled sediment. This is reflected by sometimes huge and locally varying differences in monitored levels of the total (dissolved and particle bound) and the dissolved fraction (filtered sample). Since the bioavailability of metals depends significantly on the speciation, some experts suggested during the consultation to use the dissolved fraction instead of the total concentration as basis for the exposure assessment and scoring.

Even though much metal monitoring data referring to the dissolved fraction and/or referring to the total concentration was provided by the Member States, concomitant analyses of dissolved and total levels were not reported for all monitored metals. However, for many of the monitored metal compounds it was feasible to calculate exposure indices for both the EU-level 90-percentiles of the dissolved fraction and the EU-level 90-percentiles of the total concentration. Moreover, a third variant of exposure scores was calculated on the basis of the EU-level 90-percentiles of the total concentrations multiplied by the ratio factor "dissolved fraction : total concentration". The resulting concentration is the calculated share of the dissolved fraction in the monitored EU-level 90-percentile of the total concentration. This variant was used to render the monitored total concentrations better compatible with the results of the effects scoring based on standard test routines<sup>3</sup>. Furthermore, this variant was used to exploit the full information since more data were provided for the total concentrations than for the dissolved ones.

The **ratio factor** "dissolved fraction : total concentration" was obtained as follows: For each metal under consideration those monitoring stations where dissolved fraction and total concentration had been monitored concomitantly and which had passed the selection criterion "10/20% minimum requirement for positive findings" (for details see chapter 3.4) were selected. In a first step, for each of the stations the station-level ratio factor "dissolved : total" was calculated on the basis of the measurements above the respective determination limits (positive findings). In a second step, the arithmetic mean of the station level ratio factors was calculated and then used as (EU-level) ratio factor "dissolved fraction : total concentration". For ratio factors and supplementary information see table A18 in annex 1.

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3 In these standardised tests the metal compounds are usually added in the form of water soluble salts and the water contains only negligible amounts of suspended sediment. The metal compounds can therefore be considered as entirely bioavailable whereas in natural surface waters a certain fraction of the total concentration of a metal is bound to suspended sediment and/or may occur in water-insoluble form. This fraction may therefore be considered as not directly bioavailable. Consequently, monitoring data based on total concentrations are not directly compatible with effect concentrations obtained in ecotoxicological tests.

In conclusion, the following 3 variants of exposure indices (I\_EXP) were calculated on the basis of the 90-percentiles of:

- Variant 1: The monitored concentrations of the dissolved fraction (this variant reflects the assumption that only the dissolved fraction is bioavailable)
- Variant 2: The monitored concentrations for the total amount (this variant reflects the assumption that the total metal content is bioavailable)
- Variant 3: Calculated concentrations for the dissolved fraction - based on monitored concentrations for the total amount multiplied by the ratio factor "dissolved : total" for the respective metal.

The exposure index for metal compounds was calculated in the same manner as for the organic substances (chap. 4.1.1; see table 5 for  $C_{min}$  and  $C_{max}$ ). Table A19 (annex 1) shows the results of the monitoring-based exposure scoring.

#### 4.1.4 Metal compounds in sediment

The EU-level 90-percentiles of the concentrations monitored in sediment were used as input for the scoring of exposure levels in sediment. Scores were calculated in the same way as described in chapter 4.1.1 (see table 5 for  $C_{min}$  and  $C_{max}$ ).

Table A20 (annex 1) shows the results of the exposure scoring for inorganic metal compounds.

## 4.2 Modelling-based exposure scoring

The modelling-based exposure scoring was performed by the European Chemicals Bureau (ECB) according to the EURAM algorithms<sup>[34]</sup>. The provided EURAM exposure scores refer to the aquatic phase.

In EURAM, the exposure of the aquatic environment to a chemical is approximated by a simple exposure model which includes three factors:

1. emissions, based on the tonnage produced or imported and the use pattern
2. distribution to the aquatic environment, based on a Mackay model (an equilibrium box model)
3. degradation, based on aquatic biodegradation.

The EURAM aquatic exposure score is calculated as follows:

$$I\_EXP = 1.37 (\log(EEXV) + 1.301)$$

$$EEXV = \text{EMISSION} \times \text{DISTRIBUTION} \times \text{DEGRADATION}$$

I\_EXP is normalised such that the range is between 0 and 10.

The three factors of EEXV are obtained as follows:

1. EMISSION:  $0.01 \cdot T_1 + 0.1 \cdot T_2 + 0.2 \cdot T_3 + 1.0 \cdot T_4$ , where T is the tonnage of the respective chemical and the figures 1-4 indicate the main use categories table 6).

Table 6: Main use categories and fractions used to calculate emissions

Main use category	Fraction
1 Used in closed systems	0.01
2 Use resulting in inclusion in matrix	0.10
3 Non-dispersive use	0.20
4 Wide dispersive use	1.00
Default	1.00

2. The factor DISTRIBUTION denotes the fraction of a chemical which partitions at equilibrium into the aquatic compartment.

The environmental distribution of a chemical is calculated with the Mackay level I model using the environmental characteristics given in table 7. The Mackay model allows to calculate fugacity values of a chemical in various environmental compartments. The fugacity  $f$  can be regarded as the tendency of a substance to escape from a compartment. For each compartment a fugacity capacity  $Z$  is calculated for an amount of a chemical (i.e. the volume emitted) distributed in the environment under equilibrium conditions. It relates the fugacity  $f$  to the concentration  $C$  of the substance in the respective compartment:

$$C = Zf$$

$Z$  is calculated for the various compartments according to the following formulae and parameters:

$$\begin{aligned} \text{Air (1)} & \quad Z_1 = 1/RT \\ \text{Water (2)} & \quad Z_2 = C^S / VP^S \\ \text{Soil (3)} & \quad Z_3 = Z_2 \tilde{n}_3 f_{oc3} K_{oc} / 1000 \\ \text{Sediment (4)} & \quad Z_4 = Z_2 \tilde{n}_4 f_{oc4} K_{oc} / 1000 \\ \text{Susp. Solids (5)} & \quad Z_5 = Z_2 \tilde{n}_5 f_{oc5} K_{oc} / 1000 \\ \text{Fish (Biota) (6)} & \quad Z_6 = Z_2 \tilde{n}_6 L K_{ow} / 1000 \end{aligned}$$

R : Gas constant (8.314 J/mol K)

T : Temperature (K)

$C^S$  : Water solubility (mol/m<sup>3</sup>)

$VP^S$  : Vapour pressure (Pa)

$\tilde{n}_i$  : Density of phase  $i$  (Kg/m<sup>3</sup>)

$f_{oci}$  : Mass fraction of organic carbon in phase  $i$

L : Lipid content in fish (0.10)

$K_{oc}$  is derived from  $K_{ow}$  according to Mackay et al.:  $K_{oc} = 0.41 K_{ow}$

Table 7: Environmental characteristics of the Mackay level I model used in EURAM

Compartment	Air	Water	Soil	Sediment	Suspended Solids	Fish (Biota)
Volume (m <sup>3</sup> )	10 <sup>14</sup>	2x10 <sup>11</sup>	9x10 <sup>9</sup>	10 <sup>8</sup>	10 <sup>6</sup>	2x10 <sup>5</sup>
Depth (m)	1000	20	0.1	0.01	-	-
Area (m <sup>2</sup> )	10x10 <sup>10</sup>	10x10 <sup>9</sup>	90x10 <sup>9</sup>	10x10 <sup>9</sup>	-	-
Fraction oc (f <sub>oc</sub> )	-	-	0.02	0.04	0.2	-
Density (kg/m <sup>3</sup> )	1.2	1000	2400	2400	1500	1000

3. The factor DEGRADATION accounts for the biodegradability of the respective substance in the aquatic environment and is calculated according to the following table 8.

Table 8: Factors used in EURAM to account for biodegradability

Biodegradability	Factor
Ready biodegradable	0.1
Inherent biodegradable	0.5
Persistent	1.0
Default	1.0

The European Chemicals Bureau kindly provided exposure scores referring to the aquatic phase and supplementary information on data used to calculate the scores for those chemicals of the candidate list for which information in the EURAM (IUCLID) database is available. The supplementary information consisted of e.g. production volumes, information on defaults used and numbers of "Harmonized Electronic Data Sets" submitted by industry for chemicals produced or imported in amounts exceeding 1000 t per year (table A21 of annex 1). In order to prevent back calculation of production/import volumes of individual firms from the exposure scores and to keep the confidentiality agreed with industry, exposure scores were only provided as integers. Production volumes and exposure scores for chemicals for which only 3 or less HEDSETs are available were not provided and marked as confidential.

The calculation of EURAM-based exposure scores for plant protection products (PPP) and inorganic metal compounds was deemed inappropriate. For inorganic metal compounds some of the parameters needed for the application of the Mackay model are not meaningful, e.g. logPow and the Henry constant. With respect to plant protection products used in agriculture Council Directive 91/414/EEC provides the framework for the assessment of risks and the authorisation. The risk assessment scheme developed under this directive foresees the application of sophisticated local scale scenarios which require an in-depth substance-by-substance analysis including further monitoring, where appropriate. In the experts consultation most parties therefore felt that the application of the Mackay distribution model for the exposure assessment would not be fully appropriate to reflect and model the specific use pattern and environmental pathways of PPP in agriculture and that the IUCLID database did not contain sufficient information about the use of these products. It was therefore

decided to subject PPPs and inorganic metal compounds only to the monitoring based ranking.

For 318 of the 658 chemicals on the COMMPS candidate list, information is available in the IUCLID database at the ECB. Due to the above mentioned confidentiality restrictions as well as the exclusion of plant protection products and inorganic metal compounds from the modelling-based prioritisation, EURAM-based exposure scores were available for only 123 substances (see chap. 6.2 and table 14). For the other COMMPS candidate substances the calculation of exposure scores was not feasible since the required input data on production/import volumes, use pattern and degradability is not available in IUCLID. This is the case in particular for substances with low production/import volumes.



## 5 Effects assessment

The effects assessment in COMMPS essentially follows the EURAM (former IPS) method<sup>[34]</sup>. It was modified insofar as the indirect effects to man via the aquatic environment are included in the effects scoring as described below in chapter 5.1.

### 5.1 Effect scoring for organic substances in the aquatic phase

For both the monitoring and modelling-based ranking of organic substances in the aquatic phase, the effects assessment and scoring are identical.

For the effect scoring, direct and indirect effects on aquatic organisms are considered (toxicity and bioaccumulation potential, respectively) as well as some selected endpoints for effects on humans in order to account for indirect effects on humans via ingestion of contaminated water or food (carcinogenicity, mutagenicity and adverse effects on reproduction as well as chronic effects resulting from oral uptake). All data used for the calculation of the effect indices are listed in table A22 (annex 1).

Effects data were collated from the following sources:

- Risk assessments for Existing Substances according to Council Regulation (EEC) No. 93/793 (recent [draft] reports)
- Risk assessments for Plant Protection Products used in agriculture according to Council Directive 91/414/EEC (recent monographs and ECCO-reports)
- Well founded and documented proposals from competent authorities of Member States
- Well founded and documented proposals from industry or other non-governmental organizations (NGOs)
- Data provided by the European Chemicals Bureau (extracted from the IUCLID database and used for EURAM as well)
- Data retrieved from public databases (e.g. AQUIRE, HSDB, RTECS) and literature by the consultant

Data selection from the above mentioned sources was performed in a hierarchical order. Data used in the risk assessments according to Council Regulation (EEC) No. 93/793 and Council Directive 91/414/EEC were considered to be of highest priority and preferred over data available from any other source (since both documents address different groups of chemicals there was no overlap). Next highest priority was conceded to well founded and documented data provided by Member States or industry and NGOs following the invitation to submit data as extended by the Commission during the consultation on 2<sup>nd</sup>/3<sup>rd</sup> July 1998 (minimum requirements for information were described in a circulated form (see Annex 2) and comprised a conclusive description of e.g. test conditions, tested species, examined endpoint(s), references as well as a justification why the provided data should be used). The data received were pre-selected by the consultant (formal check with regard to basic requirements on documentation and justification first, then pre-selection of data according to the principles for the evaluation of effect data as laid down in the TGDs<sup>[9]</sup>). Data meeting the requirements were then sent to the European Chemicals Bureau (ECB) and accepted or rejected in agreement with the ECB. Next highest priority was conceded to IUCLID data

provided by the ECB. Still remaining data gaps and defaults were replaced, as far as possible, with data retrieved from public databases and literature by the consultant.

The basis for the **direct aquatic effects** scoring are concentrations which are considered not to have any effects on aquatic organisms (herein after called Predicted No Effect Concentrations - PNECs). Under consideration of the above mentioned hierarchy of data sources, these PNECs were extrapolated from chronic or acute data according to the method laid down in the TGDs<sup>[9]</sup>. Since the approach is a conservative one, the lowest acute or chronic toxicity data on the highest hierarchical level was selected from the available ensemble of effect data. The selected concentration was then divided by an assessment factor to result in the PNEC. The assessment factor itself depends on the size of the data ensemble, the test duration and the tested trophic levels (for factors see table 9). In case no effect data was available, 10 ng/l was used as default PNEC. If both acute and chronic data were available, the chronic data was normally preferred for the calculation of PNECs.

For substances for which a PNEC was already calculated in the context of a risk assessment according to Council Regulation (EEC) No. 793/93, this PNEC (including the corresponding toxicity test result and assessment factor) was used without applying the above described procedure. The conceptual approach followed in the risk assessment strategy for plant protection products (PPP) according to Council Directive 91/414/EEC (calculation of toxicity : exposure-ratios which must not fall below 10 or 100 for a defined ensemble of non-target species) differs from the concept described in the TGDs. In order to perform the direct effect scoring on the same basis as for the other organic chemicals, the lowest toxicity datum used for the PPP risk assessment was selected and the PNEC was calculated using the TGD assessment factors and the procedural approach as described above. The PNECs derived for PPPs should be regarded as provisional. They do not prejudice against the risk assessment under Council Directive 91/414/EEC and the setting of quality standards under Article 21 of the Water Framework Directive proposal.

Table 9: Assessment factors used to calculate PNECs

Test duration	Number of taxonomic groups <sup>*)</sup> for which toxicity tests are available	Assessment factor
Acute test	1	1000
	2	1000
	3	1000
Chronic test (result must be the NOEC)	1 (fish or invertebrates)	100
	2 (fish and/or invertebrates and/or algae)	50
	3	10

\*) representatives of the following taxonomic groups are usually tested to assess aquatic toxicity: fish; invertebrates (mostly crustaceans); plants (mostly algae)

In analogy to the exposure assessment the **direct aquatic effect scores** ( $EFS_d$ ) were scaled by defining an upper and a lower limit. The chosen limits are listed in table 10. Both figures for the lower and upper limits were set close to the lowest and highest PNECs in the data set in order to allow for the use of the full range of the scale and thus for an optimal differentiation of the chemicals with respect to their aquatic toxicity. The multiplication of the upper limit ( $PNEC_{max}$ ) by a factor of ten is introduced in order to avoid zero as value for the  $EFS_d$  for the substance with the highest PNEC because this could result in a priority index of zero, too.

Table 10: Minimum and maximum PNECs used for the calculation of effect scores

	$PNEC_{max}$	$PNEC_{min}$	Unit
organic substances in the water phase	1	0.000001	mg/l
organic substances in the sediment (see chap. 5.2)	10	0.000001	mg/kg
metal compounds in the water phase (see chap. 5.3)	0.1	0.000001	mg/l

$EFS_d$  (direct effects score) calculation:

$$EFS_d (\text{substance } i) = \frac{\log(PNEC_i / (10 * PNEC_{max}))}{\log(PNEC_{min} / (10 * PNEC_{max}))} * WF$$

with:

WF Weighting factor for direct effects (5 for organic substances, 8 for metals).

Thus, the range of  $EFS_d$  is between > 0 and 5 for organic chemicals and > 0 and 8 for metal compounds.

Information on the tests used to derive  $EFS_d$ , including the tested taxonomic group (predominantly fish, crustaceans or algae), the test endpoint (expressed as L(E)C50 or NOEC), the effect concentration, the assessment factor used to extrapolate the PNEC and the obtained PNEC itself is summarised in table A22.

The **indirect aquatic effect scores** ( $EFS_i$ ) were calculated from measured bioconcentration factors (BCF) or the  $\log P_{ow}$  as a measure for the bioaccumulation potential. If BCF and  $\log P_{ow}$  values were concomitantly available, the scoring (table 11) was preferably based on the BCF.

Table 11: Scoring of indirect aquatic effects

$\log P_{ow}$		Molecular Weight	Bioconcentration Factor (BCF)	Scores
< 3	or	> 700	< 100	0
3 ≤ $\log P_{ow}$ < 4	and	< 700	100 - < 1000	1
4 ≤ $\log P_{ow}$ < 5	and	< 700	1000 - < 10000	2
≥ 5	and	< 700	> 10000	3
default (no $\log P_{ow}$ )	and	< 700	no BCF	3

Data selection was performed by applying the same hierarchical order as described above. As much as possible, data gaps and defaults which could not be updated with experimental data by the consultant were replaced by calculated  $\log P_{ow}$ s. For this purpose two different programmes based on QSAR were used (KowWin (1995), Version 1.50, Syracuse Research Corp., Syracuse; ClogP for Windows (1995), Version 1.0, Biobyte Corp., Claremont). BCF and  $\log P_{ow}$ -values used for the scoring of the indirect effects are listed in table A22.

For the consideration and scoring of **effects on humans** (EFS<sub>h</sub>) the CMR properties (carcinogenicity, mutagenicity, effects on reproduction) as well as chronic effects (oral uptake but not ingestion by inhalation) were taken into account. Predominantly R-phrases were used as a measure of these properties. The European Chemicals Bureau kindly provided the R-phrases for those substances for which an official European classification is available. In cases where the substance is not officially classified on EU-level but evidence and classifications for the mentioned effects on humans is available from other sources<sup>[10, 11, 12, 13]</sup>, the respective information and classifications have been used. The R-phrases selected for scoring as well as the assigned scores are listed in table 12.

Table 12: R-phrases and assigned scores

Carcinogenicity	Mutagenicity	Effects on Reproduction	Chronic Effects (oral)	Scores
R45	R46	R47, R60 or R61	-	2
R40	R40	R62, R63 or R64	-	1.8
-	no test	no test	R48 in any combination with R23 - R28	1.4
-	-	no test	R48 in any combination with R20 - R22	1.2
-	-	-	R33	1
-	-	-	-	0

The EFS<sub>h</sub> scores and the R-phrases on which they are based are listed in table A22.

The overall **effect index for organic compounds** is calculated as a combined score (sum of the scores for each of the three effect parameters). The relative weights of these 3 effect parameters are given by the ratio of their maximum values. Following the expert consultation in 1998 and based on the findings of the sensitivity analysis carried out for the previous COMMPS report<sup>[31]</sup>, the relative weighting 5 : 3 : 2 for EFS<sub>d</sub> : EFS<sub>i</sub> : EFS<sub>h</sub> was used.

$$I\_EFF = EFS_d (5) + EFS_i (3) + EFS_h (2)$$

The effect indices obtained for organic substances in the water phase as well as the scores of the individual effect parameters are listed in table A22.

## 5.2 Effect scoring for organic substances monitored in sediments

The effects assessment and scoring of organic substances monitored in sediments were carried out similarly as described in chapter 5.1 for the aquatic micropollutants. The calculation of the scores for indirect effects ( $EFS_i$ ) and effects on humans ( $EFS_h$ ) was identical with the procedures described for the aquatic phase. However, since toxicity tests with sediments and sediment dwelling organisms are not comprehensively available for a broad spectrum of substances, the calculation of the direct effects scores ( $EFS_d$ ) was based on the water phase PNECs ( $PNEC_{water}$ ) that had been transformed to sediment phase PNECs ( $PNEC_{sediment}$ ) for this purpose. This transformation was performed using the "equilibrium partitioning method" as outlined in the TGDs<sup>[9]</sup>.

The TGDs suggest the following transformation steps for the calculation of  $PNEC_{sediment}$  from  $PNEC_{water}$ :

$$PNEC_{sediment} = K_{sed/water} / d_{sed} * PNEC_{water} * 1000$$

with:

$PNEC_{sediment}$	PNEC sediment [mg/kg]
$d_{sed}$	density of dry sediment [kg/m <sup>3</sup> ]; (value used: 1500 kg/m <sup>3</sup> )
$PNEC_{water}$	PNEC water [mg/l]
$K_{sed/water}$	partition coefficient of a chemical between sediment and water [m <sup>3</sup> /m <sup>3</sup> ]

$K_{sed/water}$  is defined as:

$$K_{sed/water} = F_{water_{sed}} + F_{solid_{sed}} * K_{p_{sed}} / 1000 * d_{sed}$$

with:

$F_{water_{sed}}$	fraction of water in the sediment [m <sup>3</sup> /m <sup>3</sup> ]; (default value used: 0.8 m <sup>3</sup> /m <sup>3</sup> )
$F_{solid_{sed}}$	fraction of solids in the sediment [m <sup>3</sup> /m <sup>3</sup> ]; (default value used: 0.2 m <sup>3</sup> /m <sup>3</sup> )
$K_{p_{sed}}$	partition coefficient of a chemical between solids and water in the sediment [l/kg]

$K_{p_{sed}}$  is calculated according to:

$$K_{p_{sed}} = F_{oc} * K_{oc}$$

with:

$F_{oc}$	weight fraction of organic carbon in sediment solids; (default value used: 5 % = 0.05)
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$K_{oc}$  partition coefficient of a chemical between organic carbon and water [l/kg]

Since  $K_{oc}$  data were not available, a QSAR estimation of the  $K_{oc}$  using the  $\log P_{ow}$  was performed as suggested in the TGDs. For this purpose the equation given in the TGDs for predominantly hydrophobic chemicals was applied:

$$\log K_{oc} = 0.81 * \log P_{ow} + 0.10$$

The combination of all formulas results in:

$$PNEC_{sediment} = (F_{water_{sed}} / d_{sed} * 1000 + F_{solid_{sed}} * F_{oc} * K_{oc}) * PNEC_{water}$$

The TGDs recommend to include an additional factor in the calculation of  $PNEC_{sediment}$  for chemicals showing  $\log P_{ow}$  values above 5 (and corresponding  $K_{oc}$ -values). For those chemicals it is suggested to divide the  $PNEC_{sediment}$  by a factor of 10 in order to account for the uptake of chemicals by organisms via ingestion of sediment. Consequently, this factor was used in the  $PNEC_{sediment}$  calculation for all chemicals with  $\log P_{ow} > 5$ .

The finally obtained effect scores for sediment-borne organic chemicals are listed in table A23 (annex 1).

### 5.3 Effect scoring for metal compounds monitored in the aquatic phase

For metal compounds the same hierarchical data selection rules were applied as described for organic substances in chapter 5.1.

Since metals are naturally occurring and many of them are essential elements, organisms have adjusted to certain naturally occurring metal concentrations (i.e. many have developed active mechanisms for the intake and excretion of metals by which they may adapt to local natural background levels). Deficient, optimum or toxic concentrations may therefore vary for different species, habitat types and regions. Theoretically, the effect testing design should account for essentiality and the species' adaptation to a certain background. However, available effects data are normally based on internationally agreed test guidelines (e.g. of OECD, EU, etc.) and these do not take account of the peculiarities of specific ecosystems. Further, in these tests the metal compounds are added in the form of water-soluble salts and the water usually contains only negligible amounts of suspended sediment or complexing substances. The metal compounds can therefore be considered as entirely bioavailable.

In natural surface waters a certain fraction of the total concentration of a metal is bound to complexing agents, adsorbed by suspended sediment and/or may occur in water-insoluble form. This fraction can therefore be considered as not directly bioavailable. Consequently, monitoring data based on total concentrations are not directly compatible with effect concentrations found in ecotoxicological standard tests because the fraction relevant for toxicity can be considerably lower than the monitored total concentration.

In order to account for both the reported naturally occurring background concentrations (table A24) and the limited bioavailability of monitored metal concentrations referring to the total amount (dissolved and particle bound fraction), it was decided to calculate different variants for the **direct effects** score ( $EFS_d$ ) as follows:

- Var. 1 Calculation of PNEC and  $EFS_d$  on the basis of effect concentrations obtained by toxicity testing (equivalent to the dissolved fraction) and use of criteria and assessment factors as laid down in the TGDs (see chap. 5.1).
- ⇒ The resulting PNECs and  $EFS_d$ s refer to the dissolved fraction of a metal and are therefore compatible with the monitored dissolved concentration. Background concentrations are not taken into account (table A25).
- Var. 2 Derivation of PNECs not lower than the highest background concentration reported by the Member States for the dissolved fraction of the respective metals (table A24). PNECs were calculated as described for variant 1. Then, each PNEC lower than the highest background concentration was replaced by that background concentration.
- ⇒ The resulting PNECs and  $EFS_d$ s refer to the dissolved fraction and account for background concentrations as well. They are compatible with the monitored dissolved concentration (table A26).
- Var. 3 Calculation of PNECs referring to total metal concentrations. PNECs derived according to variant 1 were divided by the ratio-factor "dissolved : total" for the respective metal. This ratio-factor was obtained from the metal monitoring data referring to the dissolved and total fractions as described in chapter 4.1.3.
- ⇒ The resulting PNECs and  $EFS_d$ s refer to the total amount and are therefore compatible with the monitored total concentration. Background concentrations are not taken into account (table A27).
- Var. 4 Derivation of PNECs referring to total metal concentrations not lower than the highest background concentration reported by the Member States for the respective metals. PNECs were calculated as described for variant 3. Then, each PNEC lower than the highest background concentration was replaced by that background concentration (total fraction).
- ⇒ The resulting PNECs and  $EFS_d$ s are compatible with the total concentrations and account for background concentrations (table A28).

**Indirect effects** which were scored for organic substances by use of BCF or  $\log P_{ow}$  values were not calculated for metals because of various reasons such as the ability of many organisms to actively accumulate or excrete metals, the essentiality of various metals for different groups of organisms, and the diversity and concurrent presence of different species of a metal under natural conditions.

**Effects to humans** were calculated in the same way as described for organic compounds (cf. chap. 5.1). The  $EFS_h$ -scoring for metals is solely based on compounds being soluble in

water. Effects which might occur after inhalation of - e.g. - metal particles are therefore not taken into account.

Since the indirect effects were not determined for metal compounds, the respective weighing of the individual effect parameters had to be modified. The weighing of direct aquatic effects in relation to the effects to humans was chosen to be 8 : 2.

$$I\_EFF \text{ (metals)} = EFS_d \text{ (max. score 8)} + EFS_h \text{ (max. score 2)} \quad (I\_EFF_{\max} = 10)$$

A summary of all relevant data for the calculation of the effect scores for metal compounds in the water phase can be found in annex 1, tables A24 (reported background concentrations) and A25 -A28 (effect data and effect scores).

#### **5.4 Effects assessment for metal compounds monitored in sediments**

For metal compounds sorbed to the sediment, a transformation of  $PNEC_{\text{water}}$  to  $PNEC_{\text{sediment}}$  as conducted for the organic substances is not feasible since the calculation of a unique  $K_{\text{sed/water}}$  is not appropriate for a metal and the different inorganic compounds which may occur in the aquatic environment.

As for organic substances, since toxicity tests for metal compounds with sediments and sediment dwelling organisms are hardly available, the direct effects assessment was replaced by a comparison of exposure concentrations with the quality objectives for metal concentrations in sediment as set by the International Commission for the Protection of the Rhine<sup>[35]</sup> and the maximum permissible limits of metal concentrations in soil according to Annex A1 of Council Directive 86/278/EEC (protection of the environment when sewage sludge is used in agriculture)<sup>[36]</sup>. Effects on human health are accounted for by R-phrases as described in chap. 5.1.



## 6 Results of the risk-based ranking

The ranking of substances is based on **priority indices** obtained by multiplication of a substance's exposure index (chapter 4) with the corresponding effect index (chapter 5):

Priority index:  $I\_PRIO = I\_EXP * I\_EFF$

### 6.1 Monitoring-based ranking of organic substances in the aquatic phase

The results of the monitoring-based ranking for organic micropollutants in the water phase are summarised in tables 13 (COMMPS method) and A29 (maximum likelihood method).

In both tables the CONC./PNEC-ratios are listed beside the priority scores. Several high-ranking substances such as pentachlorophenol etc. show low CONC./PNEC-ratios. However, the CONC./PNEC-approach exclusively predicts risk by direct effects on the aquatic community. In addition to the direct effects, the effect index as calculated in the COMMPS procedure considers indirect effects and effects to humans via the aquatic environment resulting in high ranks despite low CONC./PNEC-ratios. In order to enable a better interpretation and to achieve a higher transparency of results, the contributions of the various effect-types to the effect indices as well as statistical information referring to the calculation of the exposure indices are also included.

Approximately half of the organic compounds ranked in table 13 are plant protection products. This is not surprising since plant protection products are biologically active substances and, thus, are likely to affect aquatic organisms. Furthermore, they are widely used and therefore introduced into parts of the environment in many European regions.

#### 6.1.1 Comparison of the arithmetic mean method with the maximum likelihood method

As can be seen in figure 2 and from table A30, the ranking results obtained by both methods do not differ dramatically, in particular not for the relevant sector with the high ranks from e.g. rank 1 - 30. For further details see chap 4.1.1.1 and reference [33]).

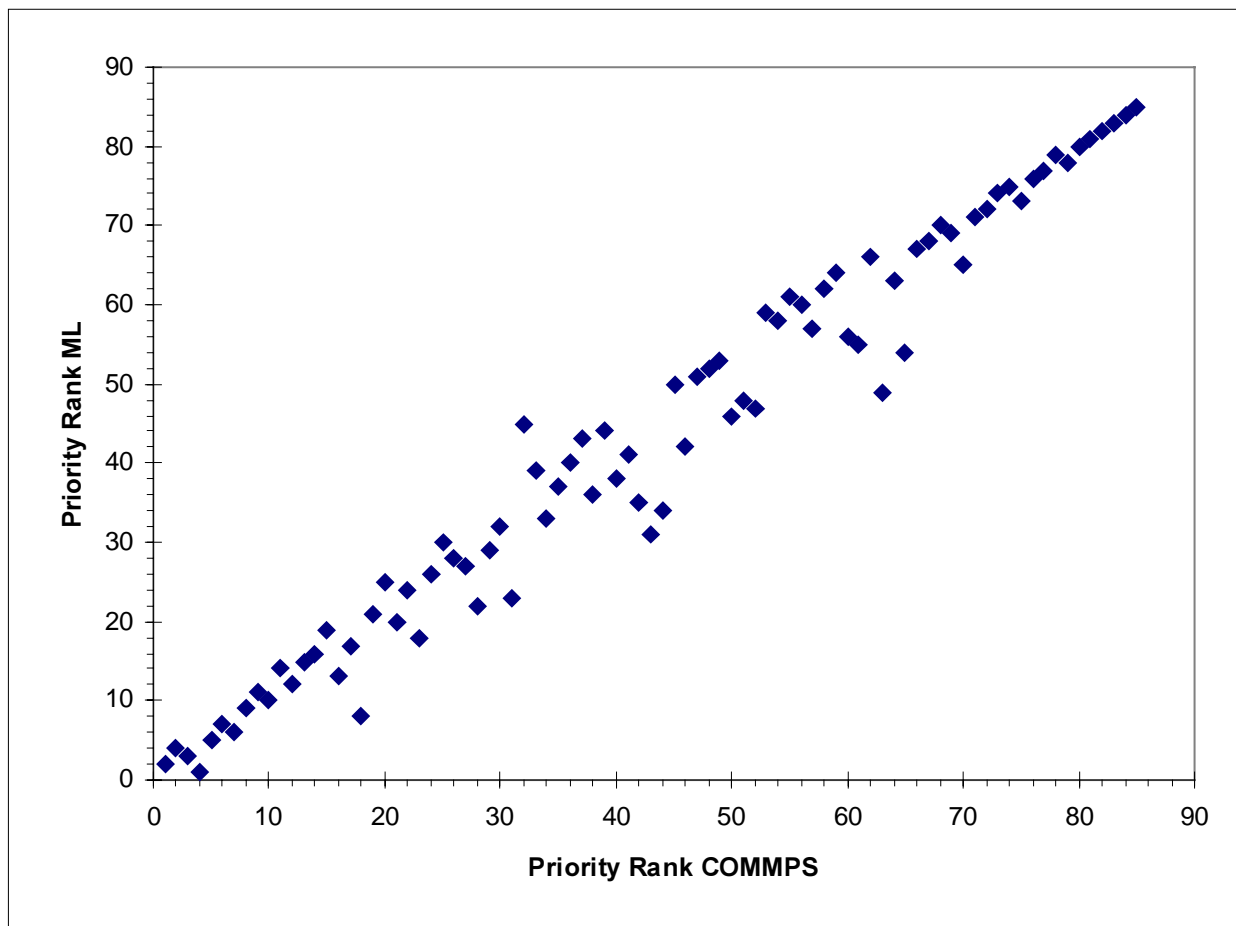


Figure 2: Correlation of priority ranks obtained with the maximum likelihood and the COMMPS method

## 6.2 Modelling-based ranking of organic substances in the aquatic phase

The modelling-based ranking is based on the multiplication of EURAM exposure indices (chap. 4.2) with the same effect indices as used for the monitoring based ranking (chap. 5.1).

As explained in chapter 4.2, no modelling-based ranking was carried out for plant protection products used in agriculture and for inorganic metal compounds.

The results of the modelling-based ranking are summarised in table 14.

Table 13: Monitoring-based ranking of organic substances in the aquatic phase (arithmetic mean method).

**I\_PRIO** - priority index; **I\_EXP** - exposure index, **I\_EFF** - effects index; **%\_EFSd**, **%\_EFSi**, **%\_EFSH** - % contribution of the direct, indirect, and human effect scores to I\_EFF; **Sampl. Stat.** - number of sampling stations from which data were used to calculate I\_EXP; **entries used** - number of measurements used to calculate I\_EXP; **entries >DL** - number of used measurements with concentrations higher than the corresponding determination limit; **Defaults I\_EFF** - shows the effect parameter(s) scored on the basis of defaults; **CONC/PNEC** - ratio between averaged EU-level exposure concentration and PNEC

CAS	Compound	Rank	I_PRIO	I_EXP	Sampl. Stat.	entries used	entries >DL	I_EFF	%_EFSd	%_EFSi	%_EFSH	Defaults I_EFF	CONC/PNEC
193-39-5	indeno(1,2,3-cd)pyrene	1	52.65	5.67	11	70	54	9.29	46.2	32.3	21.5	EFSd	9.36E+0
56-55-3	benzo-a-anthracene	2	51.91	5.59	14	116	72	9.29	46.2	32.3	21.5		8.31E+0
191-24-2	benzo-g,h,i-perylene	3	51.35	5.24	29	446	286	9.80	51.0	30.6	18.4		2.35E+2
72-55-9	DDE, 4,4'- isomer	4	50.96	5.20	11	125	38	9.80	51.0	30.6	18.4		7.39E+1
205-99-2	benzo-b-fluoroanthene	5	48.84	5.26	41	768	448	9.29	46.2	32.3	21.5	EFSd	4.84E+0
87-86-5	pentachlorophenol	6	48.03	5.90	85	2296	1527	8.14	41.0	36.8	22.1		6.44E-1
207-08-9	benzo-k-fluoroanthene	7	47.89	4.84	29	451	294	9.90	49.5	30.3	20.2		1.77E+1
50-32-8	benzo-a-pyrene	8	46.55	4.90	38	579	388	9.50	47.4	31.6	21.1		5.44E+0
309-00-2	aldrin	9	45.33	4.77	52	1246	1163	9.50	49.5	31.6	18.9		8.53E+0
76-44-8	heptachlor	10	43.32	4.42	3	14	5	9.80	51.0	30.6	18.4		2.50E+1
72-54-8	DDD, 4,4'- isomer	11	42.08	5.26	7	121	48	8.00	62.5	37.5	0.0		7.55E+1
2921-88-2	chlorpyrifos	12	41.02	5.86	6	22	10	7.00	71.4	28.6	0.0		1.16E+3
118-74-1	hexachlorobenzene	13	39.74	4.28	79	2354	1757	9.29	46.2	32.3	21.5		1.00E+0
121-73-3	3-chloronitrobenzene	14	39.21	9.39	2	80	50	4.18	66.5	0.0	33.5		2.88E+1
60-57-1	dieldrin	15	38.19	3.92	106	2861	1844	9.74	50.7	30.8	18.5		4.66E+0
53-19-0	DDD, 2,4'- isomer	16	38.08	4.76	4	87	47	8.00	62.5	37.5	0.0		3.41E+1
120-82-1	1,2,4-trichlorobenzene	17	37.30	5.99	63	1605	1308	6.23	39.0	32.1	28.9		3.93E-2
470-90-6	chlorfenvinphos	18	36.02	5.73	11	51	16	6.29	68.2	31.8	0.0		1.03E+1
330-54-1	diuron	19	35.80	7.18	71	786	535	4.99	75.9	0.0	24.1		2.15E+1
50-29-3	DDT, 4,4'- isomer	20	35.38	4.02	47	1427	1221	8.80	56.8	22.7	20.5		3.66E+1
1582-09-8	trifluralin	21	34.52	4.97	61	874	538	6.94	56.8	43.2	0.0		1.02E+0
67-66-3	trichloromethane	22	34.22	7.24	241	6349	4139	4.73	61.9	0.0	38.1		1.47E+0
91-20-3	naphthalene	23	34.21	7.46	9	95	32	4.59	56.4	43.6	0.0		7.01E-1

120-12-7	anthracene	24	34.08	5.60	10	54	45	6.09	67.1	32.9	0.0		4.39E+0
75-09-2	dichloromethane	25	33.58	8.58	14	284	184	3.91	54.0	0.0	46.0		9.32E-1
107-06-2	1,2-dichloroethane	26	33.19	8.45	64	1557	1362	3.93	49.1	0.0	50.9		4.12E-1

Table 13: (continued) Monitoring-based ranking of organic substances in the aquatic phase (arithmetic mean method).

For explanation of abbreviations see top of table

CAS	Compound	Rank	I_PRIO	I_EXP	Sampl. Stat.	entries used	entries >DL	I_EFF	%_EFSd	%_EFSi	%_EFSH	Defaults I_EFF	CONC/PNEC
34123-59-6	isoproturon	27	32.80	6.52	47	592	311	5.03	64.2	0.0	35.8		1.23E+0
465-73-6	isodrin	28	32.75	4.40	53	1127	1049	7.44	59.7	40.3	0.0		2.03E+0
72-20-8	endrin	29	32.56	4.07	44	1240	1157	8.00	62.5	37.5	0.0		1.18E+2
959-98-8	endosulfan, alpha- isomer	30	32.22	5.37	27	191	93	6.00	83.3	16.7	0.0		3.64E+2
15972-60-8	alachlor	31	32.01	5.96	25	120	39	5.37	66.5	0.0	33.5		1.50E+0
789-02-6	DDT, 2,4'- isomer	32	31.92	3.65	5	36	11	8.74	45.1	34.3	20.6		1.21E-1
87-68-3	hexachlorobutadiene	33	31.72	4.03	68	1391	1154	7.87	39.0	38.1	22.9		1.33E-2
319-84-6	HCH, alpha- isomer	34	30.84	4.84	77	1974	1190	6.37	56.1	15.7	28.3		2.48E-1
319-86-8	HCH, delta- isomer	35	30.66	4.76	18	208	106	6.44	41.0	31.0	27.9		1.09E-2
1912-24-9	atrazine	36	30.61	6.46	573	8667	5759	4.74	62.0	0.0	38.0		4.18E-1
206-44-0	fluoroanthene	37	30.34	5.59	49	832	587	5.43	44.7	55.3	0.0		2.06E-2
319-85-7	HCH, beta- isomer	38	29.77	5.10	44	1226	751	5.84	52.0	17.1	30.8		6.74E-2
122-34-9	simazine	39	29.46	6.19	460	7441	4568	4.76	62.2	0.0	37.8		3.03E-1
56-23-5	tetrachloromethane	40	29.06	7.17	88	2664	2057	4.05	55.6	0.0	44.4		1.50E-1
108-88-3	toluene	41	28.39	8.61	24	506	166	3.30	45.4	0.0	54.6		1.35E-1
7286-69-3	sebutylazine	42	28.23	5.34	7	27	7	5.29	81.1	18.9	0.0	EFSd	5.50E+0
333-41-5	diazinon	43	28.10	5.00	31	242	84	5.62	82.2	17.8	0.0		9.40E+0
51218-45-2	metolachlor	44	27.97	6.42	30	164	79	4.36	77.0	23.0	0.0		1.57E+0
58-89-9	HCH, gamma- isomer (lindane)	45	26.68	5.09	546	11666	8260	5.24	61.8	38.2	0.0		1.27E-1
122-14-5	fenitrothion	46	26.38	4.96	37	447	395	5.32	81.2	18.8	0.0		3.33E+0
62-73-7	dichlorvos	47	26.30	5.26	52	600	493	5.00	100.0	0.0	0.0		8.03E+1
121-75-5	malathion	48	26.06	5.14	33	501	439	5.07	80.3	19.7	0.0		2.00E+0
56-38-2	parathion-ethyl	49	25.96	4.72	40	780	733	5.50	81.8	18.2	0.0		4.07E+0
7287-19-6	prometryn	50	25.51	5.03	21	245	101	5.07	60.6	0.0	39.4		6.69E-2
33213-65-9	endosulfan, beta isomer	51	25.29	4.69	25	180	82	5.39	81.5	18.5	0.0		2.73E+0
72-43-5	methoxychlor	52	25.09	2.56	1	4	1	9.80	51.0	30.6	18.4		8.01E-1

55-38-9	fenthion	53	24.73	4.53	32	404	292	5.46	81.7	18.3	0.0		2.60E+0
79-01-6	trichloroethene	54	24.56	7.71	238	7588	4716	3.19	43.5	0.0	56.5		2.17E-2
83-32-9	acenaphthene	55	23.96	6.60	10	67	40	3.63	72.5	27.5	0.0		2.01E-1

Table 13: (continued) Monitoring-based ranking of organic substances in the aquatic phase (arithmetic mean method).

For explanation of abbreviations see top of table

CAS	Compound	Rank	I_PRIO	I_EXP	Sampl. Stat.	entries used	entries >DL	I_EFF	%_EFSd	%_EFSi	%_EFSH	Defaults I_EFF	CONC/PNEC
1031-07-8	endosulfan-sulfate	56	23.93	4.69	37	246	126	5.10	80.4	19.6	0.0		1.08E+0
541-73-1	1,3-dichlorobenzene	57	23.40	8.35	6	159	53	2.80	64.3	35.7	0.0		2.37E-1
2642-71-9	azinphos-ethyl	58	22.07	4.44	27	387	383	4.97	100.0	0.0	0.0		1.17E+1
95-47-6	xylene, o- isomer	59	20.80	5.95	7	174	52	3.50	71.4	28.6	0.0		4.57E-2
67-72-1	hexachloroethane	60	20.57	3.39	6	59	17	6.07	47.3	33.0	19.8		2.45E-3
60-51-5	dimethoate	61	20.07	5.98	58	701	533	3.36	100.0	0.0	0.0		7.70E-1
139-40-2	propazine	62	19.98	5.30	43	331	153	3.77	52.2	0.0	47.8		2.97E-3
886-50-0	terbutryne	63	19.93	6.34	15	81	19	3.14	68.2	31.8	0.0		2.79E-2
108-70-3	1,3,5-trichlorobenzene	64	19.84	5.05	43	1188	1093	3.93	49.1	50.9	0.0		1.72E-3
21725-46-2	cyanazine	65	19.63	5.85	10	57	19	3.36	100.0	0.0	0.0		6.24E-1
608-93-5	pentachlorobenzene	66	19.51	3.07	7	179	83	6.36	52.8	47.2	0.0		7.10E-3
106-46-7	1,4-dichlorobenzene	67	19.32	6.60	10	321	139	2.93	65.8	34.2	0.0		2.11E-2
71-55-6	1,1,1-trichloroethane	68	18.63	5.92	23	629	340	3.15	42.8	0.0	57.2		1.08E-3
5915-41-3	terbutylazine	69	18.56	6.04	69	611	339	3.07	100.0	0.0	0.0		3.40E-1
95-50-1	1,2-dichlorobenzene	70	18.50	6.76	18	759	412	2.74	63.5	36.5	0.0		1.47E-2
15545-48-9	chlortoluron	71	18.25	5.81	5	119	33	3.14	100.0	0.0	0.0		2.92E-1
298-00-0	parathion-methyl	72	18.16	4.46	30	411	367	4.07	100.0	0.0	0.0		6.67E-1
86-50-0	azinphos-methyl	73	17.96	4.46	28	798	798	4.03	100.0	0.0	0.0		5.78E-1
67129-08-2	metazachlor	74	17.50	5.57	3	59	25	3.14	100.0	0.0	0.0		2.00E-1
6190-65-4	atrazine desethyl	75	17.08	5.56	69	1524	933	3.07	100.0	0.0	0.0		1.56E-1
93-65-2	mecoprop	76	16.53	7.01	212	3408	2321	2.36	100.0	0.0	0.0		1.62E-1
60-00-4	ethylenediamine-tetraacetic acid	77	16.22	9.51	84	1877	1838	1.71	100.0	0.0	0.0		1.11E+0
87-61-6	1,2,3-trichlorobenzene	78	14.84	4.98	44	1296	1165	2.98	66.4	33.6	0.0		1.83E-3
1007-28-9	desisopropylatrazine	79	14.56	5.94	40	282	169	2.45	100.0	0.0	0.0		3.91E-2
93-76-5	2,4,5-trichlorophenoxyacetic acid	80	13.80	6.44	4	102	39	2.14	100.0	0.0	0.0		3.23E-2
94-75-7	2,4-dichlorophenoxyacetic acid	81	11.96	6.52	70	1412	1035	1.83	100.0	0.0	0.0		1.37E-2
127-18-4	tetrachloroethene	82	11.77	7.19	183	4923	3502	1.64	100.0	0.0	0.0		2.14E-2

25057-89-0	bentazon	83	8.40	5.61	57	859	687	1.50	100.0	0.0	0.0		1.07E-3
94-74-6	MCPA	84	7.27	5.99	14	156	62	1.21	100.0	0.0	0.0		7.82E-4
100-41-4	ethylbenzene	85	4.52	6.45	6	123	35	0.70	100.0	0.0	0.0		7.58E-5



Table 14: Modelling-based ranking of organic substances in the aquatic phase.

(**I\_PRIO** - priority index; **I\_EXP** - EURAM exposure index; **DEFAULTS I\_EXP** - kinds of defaults used to calculate the exposure score, **MC** - in Mackay partitioning model, **BD** - for biodegradation, **PV** - for production volume, **UP** - for use pattern; **I\_EFF** - effects score; **%\_EFSd, h, i** - % contribution of the direct, indirect and human toxicity scores to **I\_EFF**; **DEFAULTS I\_EFF** - defaults used to calculate EFSx)

CAS	Compound	RANK	I_PRIO	I_EXP	DEFAULTS I_EXP	I_EFF	%_EFSd	%_EFSi	%_EFSH	DEFAULTS I_EFF
7681-52-9	hypochlorite, sodium salt	1	70.27	10	MC, BD, PV, UP	7.03	57.3	42.7	0.0	EFSi
7782-50-5	chlorine	2	64.26	10	MC, BD, PV, UP	6.43	53.3	46.7	0.0	EFSi
87-68-3	hexachlorobutadiene	3	62.98	8	PV, UP	7.87	39.0	38.1	22.9	
71-43-2	benzene	4	53.80	9	MCPV, UP	5.98	33.1	33.5	33.5	
11138-47-9	perboric acid, sodium salt	5	51.13	10	MC, BD, PV, UP	5.11	41.3	58.7	0.0	EFSi
120-82-1	1,2,4-trichlorobenzene	6	49.82	8	PV, UP	6.23	39.0	32.1	28.9	
85535-84-8	chloroalkanes, C10-13	7	48.58	8	MC, BD, UP	6.07	50.6	49.4	0.0	
98-95-3	nitrobenzene	8	48.34	9	PV, UP	5.37	66.5	0.0	33.5	
77-78-1	dimethyl sulfate	9	47.53	10	BD, PV, UP	4.75	57.9	0.0	42.1	
61790-33-8	amines, tallow-alkyl-	10	46.71	6	MC, UP	7.78	61.5	38.5	0.0	
101-77-9	4,4'-methylenedianiline	11	44.13	8	UP	5.52	45.6	18.1	36.3	
8012-95-1	mineral oil	12	43.71	6	MC, BD, UP	7.29	58.8	41.2	0.0	EFSd, EFSi
78-00-2	tetraethyl-lead	13	43.17	7	BD, UP	6.17	18.9	48.6	32.4	
117-81-7	phthalic acid 2-ethylhexyl-ester (DEHP)	14	43.00	7	PV, UP	6.14	34.9	32.6	32.6	
683-18-1	dibutyltin dichloride	15	42.67	9	PV,	4.74	70.5	0.0	29.5	
106-89-8	epichlorohydrin	16	41.25	10	PV, UP	4.12	51.5	0.0	48.5	
62-53-3	aniline	17	40.60	9	PV, UP	4.51	60.1	0.0	39.9	
10039-54-0	bis(hydroxylammonium)-sulphate	18	40.57	10	MC, BD, PV, UP	4.06	70.4	0.0	29.6	
140-66-9	1,1,3,3-tetramethyl-4-butylphenol (4-tert-octylphenol)	19	40.08	8	PV, UP	5.01	60.1	39.9	0.0	
84-66-2	phthalic acid diethyl-ester (DEP)	20	39.12	9	PV, UP	4.35	31.0	23.0	46.0	
106-93-4	1,2-dibromoethane	21	37.14	8	UP	4.64	56.9	0.0	43.1	
61789-80-8	dimethyl-bis(hydrogenated tallowalkyl) ammonium chloride	22	37.11	8	MC,	4.64	100.0	0.0	0.0	
75-56-9	methyloxirane	23	36.31	10	PV, UP	3.63	44.9	0.0	55.1	
115-86-6	phosphoric acid triphenyl-ester	24	36.27	7	PV, UP	5.18	80.7	19.3	0.0	

25167-70-8	2,4,4-trimethylpentene	25	35.45	10	MCPV, UP	3.54	71.8	28.2	0.0	
85535-85-9	chloroalkanes, C14-17	26	35.36	9	MC, BD, UP	3.93	23.7	76.3	0.0	
27458-94-2	isononanol	27	35.00	10	MC, BD, PV, UP	3.50	71.4	28.6	0.0	

Table 14: (continued) Modelling-based ranking of organic substances in the aquatic phase.

For explanation of abbreviations see top of table

CAS	Compound	RANK	I_PRIO	I_EXP	DEFAULTS I_EXP	I_EFF	%_EFSd	%_EFSi	%_EFSH	DEFAULTS I_EFF
103-23-1	di(2-ethylhexyl)adipat	28	34.85	6	PV, UP	5.81	34.6	34.4	31.0	
97-00-7	1-chloro-2,4-dinitrobenzene	29	33.58	10	PV, UP	3.36	70.2	0.0	29.8	
95-76-1	3,4-dichloroaniline	30	33.29	7	UP	4.76	70.6	0.0	29.4	
67-66-3	trichloromethane	31	33.08	7		4.73	61.9	0.0	38.1	
122-39-4	n,n-diphenylamine	32	32.98	7	BD, UP	4.71	57.5	21.2	21.2	
25339-17-7	isodecanol	33	32.12	8	PV, UP	4.02	75.1	24.9	0.0	
91-20-3	naphthalene	34	32.10	7	PV, UP	4.59	56.4	43.6	0.0	
110-82-7	cyclohexane	35	31.76	10	MC, BD, PV, UP	3.18	68.5	31.5	0.0	
95-47-6	xylene, o- isomer	36	31.47	9	PV, UP	3.50	71.4	28.6	0.0	
107-06-2	1,2-dichloroethane	37	31.42	8	PV, UP	3.93	49.1	0.0	50.9	
25154-52-3	nonylphenol	38	31.21	6	BD, UP	5.20	61.5	38.5	0.0	
84852-15-3	4-nonylphenol, branched	39	31.21	6	BD, UP	5.20	61.5	38.5	0.0	
107-13-1	acrylonitrile	40	30.11	8	PV, UP	3.76	46.9	0.0	53.1	
98-54-4	butylphenol	41	29.69	8	PV, UP	3.71	73.1	26.9	0.0	
78-87-5	1,2-dichloropropane	42	29.65	8	PV, UP	3.71	46.0	0.0	54.0	
98-51-1	4-tert.-butyltoluene	43	28.87	8	PV, UP	3.61	44.6	55.4	0.0	
115-96-8	tris(2-chloroethyl)phosphate	44	28.23	8		3.53	49.0	0.0	51.0	
112-30-1	decanol	45	28.11	7	PV, UP	4.02	75.1	24.9	0.0	
111-15-9	2-ethoxyethyl acetate	46	27.79	9	PV, UP	3.09	35.2	0.0	64.8	
84-74-2	phthalic acid dibutyl-ester (DBP)	47	27.60	7	PV, UP	3.94	54.3	0.0	45.7	
98-82-8	isopropylbenzene	48	27.53	10	MC, UP	2.75	100.0	0.0	0.0	
79-06-1	acrylamide	49	27.49	7	UP	3.93	49.1	0.0	50.9	
100-44-7	benzylchloride	50	27.45	6	BD, UP	4.58	60.7	0.0	39.3	
75-09-2	dichloromethane	51	27.39	7	UP	3.91	54.0	0.0	46.0	
75-35-4	1,1-dichloroethene	52	27.28	7	PV, UP	3.90	53.8	0.0	46.2	
106-99-0	buta-1,3-diene	53	27.03	7	BD, UP	3.86	48.2	0.0	51.8	

65996-93-2	pitch, coal tar, high-temp.	54	27.00	10	MC, UP	2.70	25.9	0.0	74.1	
7722-84-1	hydrogen peroxide	55	26.42	10	MC, BD, PV, UP	2.64	100.0	0.0	0.0	
88-12-0	1-vinyl-2-pyrrolidone	56	25.73	7	PV, UP	3.68	45.6	0.0	54.4	

Table 14: (continued) Modelling-based ranking of organic substances in the aquatic phase.

For explanation of abbreviations see top of table

CAS	Compound	RANK	I_PRIO	I_EXP	DEFAULTS I_EXP	I_EFF	%_EFSd	%_EFSi	%_EFSH	DEFAULTS I_EFF
100-00-5	4-chloronitrobenzene	57	25.21	7	MC, UP	3.60	50.0	0.0	50.0	
121-73-3	3-chloronitrobenzene	58	25.05	6		4.18	66.5	0.0	33.5	
80-05-7	bisphenol A (2,2-(4,4-dihydroxydiphenyl)propane)	59	25.04	9	PV, UP	2.78	64.1	35.9	0.0	
123-91-1	1,4-dioxane	60	25.00	10	PV, UP	2.50	28.0	0.0	72.0	
56-23-5	tetrachloromethane	61	24.32	6		4.05	55.6	0.0	44.4	
1330-20-7	xylene, (m-, o-, p-)	62	24.09	6	PV, UP	4.02	75.1	24.9	0.0	
79-10-7	acrylic acid	63	23.98	7	PV, UP	3.43	100.0	0.0	0.0	
88-73-3	2-chloronitrobenzene	64	23.78	7	UP	3.40	47.0	0.0	53.0	
103-11-7	2-ethylhexyl acrylate	65	23.76	8	BD, PV, UP	2.97	66.3	33.7	0.0	
1163-19-5	bis(pentabromophenyl)-ether	66	23.49	7	PV, UP	3.36	100.0	0.0	0.0	
79-00-5	1,1,2-trichloroethane	67	23.10	8	PV, UP	2.89	37.7	0.0	62.3	
108-95-2	phenol	68	22.47	9	UP	2.50	100.0	0.0	0.0	
75-01-4	vinylchloride	69	22.39	7	BD, PV, UP	3.20	37.5	0.0	62.5	
71-55-6	1,1,1-trichloroethane	70	22.03	7	UP	3.15	42.8	0.0	57.2	
90-04-0	o-anisidin	71	21.64	5	UP	4.33	53.8	0.0	46.2	
542-75-6	1,3-dichloropropene	72	21.62	6	UP	3.60	100.0	0.0	0.0	
95-48-7	2-methylphenol	73	21.14	8	BD, UP	2.64	100.0	0.0	0.0	
95-33-0	n-cyclohexylbenzothiazole-2-sulphenamide	74	20.72	7	MC, UP	2.96	66.2	33.8	0.0	
85-68-7	phthalic acid benzylbutyl-ester (BBP)	75	20.71	5	UP	4.14	51.7	0.0	48.3	
67774-74-7	benzene; C10-13 -alkyl derivatives	76	20.62	7	MC, UP	2.95	100.0	0.0	0.0	
79-41-4	methacrylic acid	77	20.05	9	PV, UP	2.23	100.0	0.0	0.0	
75-91-2	tert.-butyl hydroperoxide	78	19.97	8	MC, UP	2.50	100.0	0.0	0.0	
108-88-3	toluene	79	19.79	6	PV, UP	3.30	45.4	0.0	54.6	
3327-22-8	(3-chloro 2-hydroxypropyl) trimethylammonium chloride	80	19.78	7	MC,	2.83	36.3	0.0	63.7	
76-13-1	1,1,2-trichlorotrifluoroethane	81	19.52	6		3.25	69.3	30.7	0.0	
109-66-0	pentane	82	19.36	9	MC, BD, UP	2.15	100.0	0.0	0.0	

79-01-6	trichloroethene	83	19.11	6		3.19	43.5	0.0	56.5	
104-76-7	2-ethyl-1-hexanol	84	18.90	9	PV, UP	2.10	100.0	0.0	0.0	
100-42-5	styrol	85	18.00	6	PV, UP	3.00	100.0	0.0	0.0	

Table 14: (continued) Modelling-based ranking of organic substances in the aquatic phase.

For explanation of abbreviations see top of table

CAS	Compound	RANK	I_PRIO	I_EXP	DEFAULTS I_EXP	I_EFF	%_EFSd	%_EFSi	%_EFSH	DEFAULTS I_EFF
99-54-7	1,2-dichloro-4-nitrobenzene	86	17.61	7	UP	2.52	100.0	0.0	0.0	
111-77-3	2-(methoxyethoxy)ethanol	87	17.57	7	PV, UP	2.51	28.3	0.0	71.7	
106-46-7	1,4-dichlorobenzene	88	17.57	6		2.93	65.8	34.2	0.0	
108-90-7	chlorobenzene	89	17.47	7	PV, UP	2.50	100.0	0.0	0.0	
60-00-4	ethylenediamine-tetraacetic acid	90	17.05	10	PV, UP	1.71	100.0	0.0	0.0	
64-02-8	ethylenediaminetetraacetic acid, tetrasodium salt	91	17.05	10	MCPV, UP	1.71	100.0	0.0	0.0	
110-65-6	2-butyne-1,4-diol	92	16.53	9	PV, UP	1.84	100.0	0.0	0.0	
1570-64-5	4-chloro-o-cresol	93	16.44	10	PV, UP	1.64	100.0	0.0	0.0	
110-80-5	2-ethoxyethanol	94	16.29	6	PV, UP	2.71	26.3	0.0	73.7	
106-42-3	xylene, p- isomer	95	15.85	6	UP	2.64	100.0	0.0	0.0	
108-05-4	vinylacetate	96	15.00	7	PV, UP	2.14	100.0	0.0	0.0	
81-15-2	musk xylene	97	14.47	3	UP	4.82	58.5	41.5	0.0	
7664-39-3	hydrogen fluoride	98	14.06	10	MC, BD, PV, UP	1.41	100.0	0.0	0.0	
106-43-4	4-chlorotoluene	99	13.85	4	UP	3.46	71.1	28.9	0.0	
68515-49-1	1,2-benzenedicarboxylic acid, di-C7-11-branched alkyl esters, C10-rich	100	13.15	8	MC, UP	1.64	100.0	0.0	0.0	
81-14-1	4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone	101	12.87	3	UP	4.29	53.4	46.6	0.0	
26447-40-5	methylenediphenyl diisocyanate	102	12.86	9	MC,	1.43	100.0	0.0	0.0	
28553-12-0	di-'isononyl'phthalate	103	12.47	7	PV, UP	1.78	100.0	0.0	0.0	
5064-31-3	nitritotriacetic acid, trisodium salt	104	12.36	10	MC, BD, PV, UP	1.24	100.0	0.0	0.0	
108-91-8	cyclohexylamine	105	11.78	7	PV, UP	1.68	100.0	0.0	0.0	
101-84-8	diphenylether	106	11.08	3		3.69	72.9	27.1	0.0	
95-50-1	1,2-dichlorobenzene	107	10.95	4	UP	2.74	63.5	36.5	0.0	
26761-40-0	di-'isodecyl'phthalate	108	9.86	6	PV, UP	1.64	100.0	0.0	0.0	
127-18-4	tetrachloroethene	109	9.82	6	UP	1.64	100.0	0.0	0.0	
106-44-5	4-methylphenol	110	9.79	7	MCPV, UP	1.40	100.0	0.0	0.0	

71-23-8	propan-1-ol	111	8.53	10	MCPV, UP	0.85	100.0	0.0	0.0	
107-05-1	allylchloride	112	7.86	5		1.57	100.0	0.0	0.0	
124-40-3	dimethylamine	113	7.28	6	PV, UP	1.21	100.0	0.0	0.0	



Table 14: (continued) Modelling-based ranking of organic substances in the aquatic phase.

For explanation of abbreviations see top of table

CAS	Compound	RANK	I_PRIO	I_EXP	DEFAULTS I_EXP	I_EFF	%_EFSd	%_EFSi	%_EFSH	DEFAULTS I_EFF
141-97-9	ethylacetoacetate	114	6.69	6	UP	1.11	100.0	0.0	0.0	
112-34-5	2-(2-butoxyethoxy)ethanol	115	6.43	9	PV, UP	0.71	100.0	0.0	0.0	
79-20-9	methylacetate	116	6.41	6	UP	1.07	100.0	0.0	0.0	
80-62-6	ethylmethacrylate	117	5.71	8	PV, UP	0.71	100.0	0.0	0.0	
100-97-0	methenamine	118	5.60	8	UP	0.70	100.0	0.0	0.0	
1634-04-4	tert.-butyl methyl ether	119	5.60	8	PV, UP	0.70	100.0	0.0	0.0	
100-41-4	ethylbenzene	120	4.90	7	PV, UP	0.70	100.0	0.0	0.0	
75-05-8	acetonitrile	121	4.90	7	PV, UP	0.70	100.0	0.0	0.0	
109-89-7	diethylamine	122	4.83	3		1.61	100.0	0.0	0.0	
75-45-6	chlorodifluoromethane (CFC 22)	123	4.20	6		0.70	100.0	0.0	0.0	

### **6.3 Monitoring-based ranking of organic substances in sediments**

As it had been done for the aquatic ranking list, the ranking of compounds monitored in sediments was carried out by multiplication of the (sediment) exposure indices (chap. 4.1.2) with the corresponding (sediment) effect indices (chap. 5.2). The sediment compounds were ranked separately from those in the aquatic phase, since a common scoring for different reference systems, e.g. mg/l for the water phase and mg/kg for sediment, was not possible (a transformation of one reference system to the other, e.g. by using partitioning factors, is not precise and undebated enough to provide a basis for the prioritisation of substances). Moreover, it was expected that compounds which were highly sorbed to the sediment would not occur in significant concentrations in the water column and vice versa (top ranked substances on the water or sediment priority lists may therefore presumably not occupy the top ranks of a common list).

The result of the sediment phase priority ranking for organic micropollutants is summarised in table 15. As can be seen in the table, mainly PAHs, chlorinated pesticides, PCBs, chlorobenzenes, chlorophenols, brominated flame retardants and phthalates are frequently monitored and found in sediments. Some of the mentioned substances are probably "historic pollutants" indicating the introduction into the environment over the past few years.

Table 15: Monitoring-based ranking of organic compounds sorbed to sediments

**I\_PRIO** - priority index; **I\_EXP** - exposure index, **I\_EFF** - effects index; **%\_EFSd**, **%\_EFSi**, **%\_EFSH** - % contribution of the direct, indirect, and human effect scores to I\_EFF; **Sampl. Stat.** - number of sampling stations from which data were used to calculate I\_EXP; **entries used** - number of measurements used to calculate I\_EXP; **entries >DL** - number of used measurements with concentrations higher than the corresponding determination limit; **Defaults I\_EFF** - shows the effect parameter(s) scored on the basis of defaults; **CONC/PNEC** - ratio between averaged EU-level exposure concentration and PNEC

CAS	Compound	Rank	I_PRIO	I_EXP	Sampl. Stat.	entries used	entries >DL	I_EFF	%_EFSd	%_EFSi	%_EFSH	Defaults I_EFF	CONC/PNEC
3424-82-6	DDE, o,p- isomer	1	76.68	9.76	25	183	133	7.86	36.4	38.2	25.5		2.53E+3
191-24-2	benzo-g,h,i-perylene	2	74.50	8.57	190	1709	1639	8.69	44.8	34.5	20.7		1.69E+4
56-55-3	benzo-a-anthracene	3	72.46	8.76	62	703	623	8.27	39.5	36.3	24.2		2.33E+3
205-99-2	benzo-b-fluoroanthene	4	72.45	8.77	215	1831	1755	8.26	39.5	36.3	24.2	EFSd	2.29E+3
207-08-9	benzo-k-fluoroanthene	5	71.70	8.31	209	1820	1678	8.63	42.0	34.8	23.2		4.23E+3
50-32-8	benzo-a-pyrene	6	71.42	8.55	215	1825	1718	8.35	40.1	35.9	23.9		2.26E+3
193-39-5	indeno(1,2,3-cd)pyrene	7	68.06	8.73	163	306	288	7.80	35.9	38.5	25.7	EFSd	3.86E+2
208-96-8	acenaphthylene	8	61.54	8.21	14	15	15	7.50	46.6	26.7	26.7	EFSd	2.22E+3
218-01-9	chrysene	9	61.04	9.44	29	93	92	6.47	25.8	46.4	27.8		1.90E+1
50-29-3	DDT, 4,4'- isomer	10	58.55	7.37	57	1065	759	7.94	52.2	25.2	22.7		6.22E+3
129-00-0	pyrene	11	58.15	9.28	47	120	110	6.27	39.4	31.9	28.7		2.79E+2
72-55-9	DDE, 4,4'- isomer	12	52.68	6.23	72	1284	1016	8.46	43.2	35.5	21.3		1.63E+2
118-74-1	hexachlorobenzene	13	52.02	6.77	124	1617	1465	7.68	34.9	39.0	26.0		1.08E+1
87-86-5	pentachlorophenol	14	51.77	6.84	20	66	61	7.57	36.6	39.6	23.8		1.67E+1
789-02-6	DDT, 2,4'- isomer	15	51.49	7.1	30	590	355	7.25	33.8	41.4	24.8		7.85E+0
86-73-7	fluorene	16	51.37	8.38	41	112	96	6.13	38.0	32.6	29.4		3.94E+1
72-54-8	DDD, 4,4'- isomer	17	51.30	7.45	55	924	794	6.89	56.4	43.6	0.0		2.74E+3
60-57-1	dieldrin	18	50.06	5.67	34	412	229	8.83	45.6	34.0	20.4		2.63E+2
85-01-8	phenanthrene	19	46.68	9.33	62	705	638	5.00	60.0	40.0	0.0		2.18E+3
72-20-8	endrin	20	45.35	5.71	16	177	69	7.94	62.2	37.8	0.0		8.09E+3
53-19-0	DDD, 2,4'- isomer	21	45.32	6.51	52	819	527	6.96	56.9	43.1	0.0		7.99E+2
206-44-0	fluoroanthene	22	45.28	9.15	226	1722	1701	4.95	39.4	60.6	0.0		3.36E+1
309-00-2	aldrin	23	42.73	5.3	13	371	172	8.06	40.5	37.2	22.3		8.64E+0

87-68-3	hexachlorobutadiene	24	41.53	6.09	17	344	218	6.82	29.6	44.0	26.4		0.31E+0
35693-99-3	PCB 52	25	41.27	6.31	56	152	134	6.54	54.1	45.9	0.0		1.22E+2
120-12-7	anthracene	26	41.21	8.1	55	580	520	5.09	60.7	39.3	0.0		4.08E+2

Table 15: (continued) Monitoring-based ranking of organic compounds sorbed to sediments

For explanation of abbreviations see top of table

CAS	Compound	Rank	I_PRIO	I_EXP	Sampl. Stat.	entries used	entries >DL	I_EFF	%_EFSd	%_EFSi	%_EFSh	Defaults I_EFF	CONC/PNEC
319-84-6	HCH, alpha- isomer	27	40.51	6.98	27	594	398	5.80	51.8	17.2	31.0		4.93E+1
959-98-8	endosulfan, alpha- isomer	28	40.22	7.01	20	75	45	5.74	82.6	17.4	0.0		3.10E+4
120-82-1	1,2,4-trichlorobenzene	29	39.59	6.97	55	790	658	5.68	33.1	35.2	31.7		7.81E-1
7012-37-5	PCB 28	30	39.59	5.84	49	135	101	6.78	55.7	44.3	0.0		1.38E+2
35065-28-2	PCB 138	31	39.30	6.6	86	204	191	5.95	49.6	50.4	0.0		2.24E+1
608-93-5	pentachlorobenzene	32	38.51	6.69	22	459	375	5.76	47.9	52.1	0.0		1.25E+1
35065-27-1	PCB 153	33	37.85	6.64	85	202	191	5.70	47.4	52.6	0.0		9.37E+0
91-20-3	naphthalene	34	37.50	8.98	38	291	256	4.18	52.2	47.8	0.0		5.88E+1
319-85-7	HCH, beta- isomer	35	36.62	6.85	27	822	528	5.35	47.6	18.7	33.7		7.45E+0
35065-29-3	PCB 180	36	35.29	6.49	80	190	179	5.44	44.8	55.2	0.0		2.79E+0
32534-81-9	diphenyl ether, pentabromo derivative	37	34.45	5.09	16	16	16	6.77	37.9	44.3	17.7		4.71E-1
37680-73-2	PCB 101	38	31.09	6.32	77	186	175	4.92	39.0	61.0	0.0		3.12E-1
1806-26-4	octylphenol	39	30.54	4.77	15	15	15	6.40	53.1	46.9	0.0	EFSd	6.12E+0
465-73-6	isodrin	40	29.03	4.81	4	131	45	6.04	50.3	49.7	0.0		1.67E+0
40088-47-9	2,2',4,4'-tetrabromodiphenyl ether	41	28.92	5.02	16	16	16	5.76	47.9	52.1	0.0	EFSd	8.55E-1
58-89-9	HCH, gamma- isomer (lindane)	42	28.04	5.77	53	953	689	4.86	58.9	41.1	0.0		4.13E+0
85-68-7	phthalic acid benzylbutyl-ester (BBP)	43	24.13	7.54	9	10	9	3.20	37.5	0.0	62.5		1.58E-1
83-32-9	acenaphthene	44	23.64	8.33	44	292	234	2.84	64.8	35.2	0.0		5.92E+0
108-70-3	1,3,5-trichlorobenzene	45	21.69	6.43	28	727	526	3.37	40.7	59.3	0.0		5.07E-2
106-46-7	1,4-dichlorobenzene	46	19.25	6.98	40	346	195	2.76	63.7	36.3	0.0		5.06E-1
13654-09-6	decabromobiphenyl	47	18.23	5.03	8	8	8	3.63	17.2	82.8	0.0	EFSd	1.49E-5

95-50-1	1,2-dichlorobenzene	48	17.22	6.68	22	292	129	2.58	61.2	38.8	0.0		1.60E-1
541-73-1	1,3-dichlorobenzene	49	16.77	6.57	33	364	211	2.55	60.8	39.2	0.0		1.22E-1
1163-19-5	bis(pentabromophenyl)-ether	50	16.54	7.52	20	20	20	2.20	100.0	0.0	0.0		6.10E+0
87-61-6	1,2,3-trichlorobenzene	51	14.73	6.23	32	761	527	2.36	57.7	42.3	0.0		3.54E-2
36355-01-8	hexabromobiphenyl	52	11.09	2.42	7	7	7	4.58	34.5	65.5	0.0	EFSd	1.69E-4

## 6.4 Monitoring-based ranking of metal compounds in the aquatic phase

The ranking of metal compounds was performed by using, in principle, the same procedure as for organic pollutants (multiplication of exposure index and effect index). However, since the effect scoring of metal compounds differs from that applied for the aquatic micropollutants (no consideration of the bioaccumulation potential for metal compounds, for reasons see chapter 5.3) metal compounds were ranked separately from the organic substances.

As already described in chapter 4.2, no modelling-based ranking was performed for metal compounds since the Mackay model cannot be applied to these compounds.

Several rankings were performed on the basis of variants of both the monitoring-based exposure scoring and the effect scoring (see chapters 4.1.3 and 5.3, respectively).

**Exposure indices** (I\_EXP) were calculated on the basis of the 90-percentiles of:

- the monitored concentrations of the dissolved fraction Variant I\_EXP\_1
- the monitored concentrations of the total amount (dissolved + particle bound fraction) Variant I\_EXP\_2
- calculated concentrations of the dissolved fraction (monitored concentrations of the total amount multiplied by the ratio factor "dissolved : total" for the respective metal [for further details see chapter 4.1.3]) Variant I\_EXP\_3

**Effect indices** (I\_EFF) were calculated as sum of the human toxicity score (EFS<sub>h</sub>, equal for all variants) and the direct effects score (EFS<sub>d</sub>). The latter score was derived from effect concentrations and metal background concentrations as follows:

- effect concentrations from toxicity tests - resulting PNECs and EFS<sub>d</sub>s refer to the dissolved fraction and are therefore compatible with the monitored dissolved concentration Variant I\_EFF\_1
- calculation of PNECs as described for variant I\_EFF\_1 and then replacement of PNECs lower than the highest reported background concentration for the dissolved fraction of the respective metal by that background concentration (the resulting EFS<sub>d</sub>s consider background levels and refer to the dissolved fraction) Variant I\_EFF\_2
- calculation of PNECs referring to total metal concentrations. PNECs derived according to variant 1 were divided by the ratio-factor "dissolved : total" for the respective metal [for details see chapter 4.1.3 (resulting EFS<sub>d</sub>s refer to the total amounts and are therefore compatible with the monitored total concentrations)] Variant I\_EFF\_3
- calculation of PNECs as described for Variant I\_EFF\_3 and then replacement of PNECs lower than the highest reported background concentration of the respective metal by that background concentration [total fraction] (resulting EFS<sub>d</sub>s account for background levels and are compatible with monitored total concentrations) Variant I\_EFF\_4

The following combinations of variants of exposure and effect scoring were used to calculate priority indices (I\_PRIO) and to establish ranking lists:

$$\begin{array}{lll} I\_EXP\_1 \times I\_EFF\_1 & I\_EXP\_2 \times I\_EFF\_3 & I\_EXP\_3 \times I\_EFF\_1 \\ I\_EXP\_1 \times I\_EFF\_2 & I\_EXP\_2 \times I\_EFF\_4 & I\_EXP\_3 \times I\_EFF\_2 \end{array}$$

The resulting ranks and priority indices for the metal compounds monitored in the aquatic phase are summarised in tables 16 and 17. The results demonstrate that changes in the ranking of metal compounds due to the combination of different variants of exposure and effect indices are only small. In this context it is worth noting that the consideration of background levels in the effects scoring (variants I\_EFF\_2 and I\_EFF\_4) has no substantial impact on the ranking of the assessed metal compounds.

## 6.5 Monitoring-based ranking of metal compounds in sediments

The calculation of priority indices for metal compounds sorbed to the sediment was not possible since effect indices could not be calculated. The reason is that toxicity tests for metal compounds with sediments and sediment dwelling organisms are hardly available and a transformation of  $PNEC_{water}$  to  $PNEC_{sediment}$  as conducted for the organic substances is not possible (for further details see chap. 5.2 and 5.4).

Thus, the direct effects assessment had to be replaced by a comparison of exposure concentrations with available information on internationally accepted quality objectives or maximum permissible levels for metals in soil. For this purpose the quality objectives for metal concentrations in sediment as set by the International Commission for the Protection of the Rhine (CIPR)<sup>[35]</sup> and the maximum permissible limits of metal concentrations in soil according to Annex A1 of Council Directive 86/278/EEC (sewage sludge disposal in agriculture)<sup>[36]</sup> were used. Effects on human health are accounted for by R-phrases and the respective score of the effect parameter "effects to humans" which is based on these R-phrases.

The comparison of exposure and desired levels as listed in table 18 indicates that, for the sediment, metals such as mercury, cadmium and zinc might be of higher relevance than for the water phase.

Table 16: Monitoring-based rankings of metal compounds in the aquatic phase (for explanation of variants refer to chap. 6.4)

**I\_PRIO** - priority index; **I\_EXP** - exposure index, **I\_EFF** - effects index; **%\_EFSd**, **%\_EFSh** - % contribution of the direct and human effect scores to **I\_EFF**;  
**Param. I\_EFF** - Parameter on which the calculation of the direct effect score of the effect index is based:  
**PNEC\_d** - PNEC based on effect concentrations referring to the dissolved metal compounds, **PNEC\_tc** - PNEC calculated from PNEC\_d by division with the ratio factor "dissolved : total" of the respective metal (see chapter 4.1.3); **BACKG\_d** - highest reported background concentration for the dissolved fraction (see table A24), **BACKG\_t** - highest reported background concentration for the total amount (dissolved and particle bound fraction (see table A24);  
**Sampl. Stat.** - number of sampling stations from which data were used to calculate **I\_EXP**; **entries used** - number of measurements used to calculate **I\_EXP**;  
**entries >DL** - number of measurements with concentrations higher than the corresponding determination limit

a) **I\_EXP\_1 X I\_EFF\_1**

CAS	Compound	Rank	I_PRIO	I_EXP_1	Sampl. Stat.	entries used	entries >DL	I_EFF_1	Param. I_EFF_1	%_EFS
7440-02-0	nickel (dissolved)	1	50.56	7.51	38	647	604	6.73	PNEC_d	73.3
7439-92-1	lead (dissolved)	2	47.69	7.38	61	773	315	6.46	PNEC_d	84.5
7440-43-9	cadmium (dissolved)	3	36.19	3.72	557	11556	6910	9.73	PNEC_d	79.4
7440-50-8	copper (dissolved)	4	33.38	5.93	21	625	580	5.63	PNEC_d	100.0
7440-38-2	arsenic (dissolved)	5	33.01	6.19	459	8829	7061	5.33	PNEC_d	100.0
7440-66-6	zinc (dissolved)	6	31.12	9.03	170	2528	2272	3.45	PNEC_d	100.0
7439-97-6	mercury (dissolved)	7	28.65	3.53	78	1680	880	8.12	PNEC_d	87.7
7440-47-3	chromium (dissolved)	8	26.53	6.14	144	2822	1807	4.32	PNEC_d	100.0

b) **I\_EXP\_1 X I\_EFF\_2**

CAS	Compound	Rank	I_PRIO	I_EXP_1	Sampl. Stat.	entries used	entries >DL	I_EFF_2	Param. I_EFF_2	%_EFS
7439-92-1	lead (dissolved)	1	43.78	7.38	61	773	315	5.93	BACKG_d	83.1
7440-02-0	nickel (dissolved)	2	38.37	7.51	38	647	604	5.11	BACKG_d	64.8
7440-66-6	zinc (dissolved)	3	30.74	9.03	170	2528	2272	3.40	BACKG_d	100.0
7440-43-9	cadmium (dissolved)	4	27.76	3.72	557	11556	6910	7.46	BACKG_d	73.2
7439-97-6	mercury (dissolved)	5	27.06	3.53	78	1680	880	7.67	BACKG_d	87.0
7440-47-3	chromium (dissolved)	6	26.53	6.14	144	2822	1807	4.32	PNEC_d	100.0
7440-50-8	copper (dissolved)	7	26.10	5.93	21	625	580	4.40	BACKG_d	100.0
7440-38-2	arsenic (dissolved)	8	25.56	6.19	459	8829	7061	4.13	BACKG_d	100.0



Table 16: (continued) Monitoring-based rankings of metal compounds in the aquatic phase (for explanation of variants refer to chap. 6.4)

**I\_PRIO** - priority index; **I\_EXP** - exposure index, **I\_EFF** - effects index; **%\_EFSd**, **%\_EFSh** - % contribution of the direct and human effect scores to **I\_EFF**;  
**Param. I\_EFF** - Parameter on which the calculation of the direct effect score of the effect index is based:  
**PNEC\_d** - PNEC based on effect concentrations referring to the dissolved metal compounds, **PNEC\_tc** - PNEC calculated from PNEC\_d by division with the ratio factor "dissolved : total" of the respective metal (see chapter 4.1.3); **BACKG\_d** - highest reported background concentration for the dissolved fraction (see table A24), **BACKG\_t** - highest reported background concentration for the total amount (dissolved and particle bound fraction (see table A24);  
**Sampl. Stat.** - number of sampling stations from which data were used to calculate **I\_EXP**; **entries used** - number of measurements used to calculate **I\_EXP**;  
**entries >DL** - number of measurements with concentrations higher than the corresponding determination limit

c) **I\_EXP\_2 X I\_EFF\_3**

CAS	Compound	Rank	I_PRIO	I_EXP_2	Sampl. Stat.	entries used	entries >DL	I_EFF_3	Param. I_EFF_3	%_EFSd	%
7440-02-0	nickel (total)	1	49.62	7.79	363	10895	7753	6.37	PNEC_tc	71.7	
7439-92-1	lead (total)	2	41.70	7.15	383	11569	8320	5.83	PNEC_tc	82.9	
7440-43-9	cadmium (total)	3	40.47	4.25	1193	35412	24275	9.52	PNEC_tc	79.0	
7440-50-8	copper (total)	4	36.58	6.96	414	12739	10699	5.26	PNEC_tc	100.0	
7440-38-2	arsenic (total)	5	36.48	6.96	454	13269	9986	5.24	PNEC_tc	100.0	
7440-47-3	chromium (total)	6	28.32	7.21	241	8893	6131	3.93	PNEC_tc	100.0	
7440-66-6	zinc (total)	7	26.74	8.67	306	10809	8879	3.08	PNEC_tc	100.0	
7439-97-6	mercury (total)	8	18.88	2.51	487	14257	8474	7.52	PNEC_tc	86.7	

d) **I\_EXP\_2 X I\_EFF\_4**

CAS	Compound	Rank	I_PRIO	I_EXP_2	Sampl. Stat.	entries used	entries >DL	I_EFF_4	Param. I_EFF_4	%_EFSd	%
7440-02-0	nickel (total)	1	38.82	7.79	363	10895	7753	4.98	BACKG_t	63.9	
7439-92-1	lead (total)	2	31.07	7.15	383	11569	8320	4.34	BACKG_t	77.0	
7440-38-2	arsenic (total)	3	27.84	6.96	454	13269	9986	4.00	BACKG_t	100.0	
7440-43-9	cadmium (total)	4	27.75	4.25	1193	35412	24275	6.53	BACKG_t	69.4	
7440-50-8	copper (total)	5	27.46	6.96	414	12739	10699	3.94	BACKG_t	100.0	
7440-47-3	chromium (total)	6	25.01	7.21	241	8893	6131	3.47	BACKG_t	100.0	
7440-66-6	zinc (total)	7	22.20	8.67	306	10809	8879	2.56	BACKG_t	100.0	
7439-97-6	mercury (total)	8	16.64	2.51	487	14257	8474	6.63	BACKG_t	84.9	
7440-39-3	barium (total)	9	14.18	9.50	22	225	224	1.49	BACKG_t	100.0	

Table 16: (continued) Monitoring-based rankings of metal compounds in the aquatic phase (for explanation of variants refer to chap. 6.4)

**I\_PRIO** - priority index; **I\_EXP** - exposure index, **I\_EFF** - effects index; **%\_EFSd**, **%\_EFSh** - % contribution of the direct and human effect scores to **I\_EFF**;  
**Param. I\_EFF** - Parameter on which the calculation of the direct effect score of the effect index is based:  
**PNEC\_d** - PNEC based on effect concentrations referring to the dissolved metal compounds, **PNEC\_tc** - PNEC calculated from **PNEC\_d** by division with the ratio factor "dissolved : total" of the respective metal (see chapter 4.1.3); **BACKG\_d** - highest reported background concentration for the dissolved fraction (see table A24), **BACKG\_t** - highest reported background concentration for the total amount (dissolved and particle bound fraction (see table A24);  
**Sampl. Stat.** - number of sampling stations from which data were used to calculate **I\_EXP**; **entries used** - number of measurements used to calculate **I\_EXP**;  
**entries >DL** - number of measurements with concentrations higher than the corresponding determination limit

e)  $I\_EXP\_3 \times I\_EFF\_1$ 

_1CAS	Compound	Rank	I_PRIO	I_EXP_3	Sampl. Stat.	entries used	entries >DL	I_EFF_1	Param. I_EFF_1	%_EFSd
7440-02-0	nickel (dis-calc)	1	47.94	7.12	363	10895	7753	6.73	PNEC_d	73.3
7439-92-1	lead (dis-calc)	2	38.62	5.98	383	11569	8320	6.46	PNEC_d	84.5
7440-43-9	cadmium (dis-calc)	3	37.66	3.87	1193	35412	24275	9.73	PNEC_d	79.4
7440-38-2	arsenic (dis-calc)	4	36.23	6.79	454	13269	9986	5.33	PNEC_d	100.0
7440-50-8	copper (dis-calc)	5	35.26	6.26	414	12739	10699	5.63	PNEC_d	100.0
7440-47-3	chromium (dis-calc)	6	27.99	6.48	241	8893	6131	4.32	PNEC_d	100.0
7440-66-6	zinc (dis-calc)	7	27.56	8.00	306	10809	8879	3.45	PNEC_d	100.0
7439-97-6	mercury (dis-calc)	8	11.39	1.40	487	14257	8474	8.12	PNEC_d	87.7

f)  $I\_EXP\_3 \times I\_EFF\_2$ 

CAS	Compound	Rank	I_PRIO	I_EXP_3	Sampl. Stat.	entries used	entries >DL	I_EFF_2	Param. I_EFF_2	%_EFSd
7440-02-0	nickel (dis-calc)	1	36.38	7.12	363	10895	7753	5.11	BACKG_d	64.8
7439-92-1	lead (dis-calc)	2	35.45	5.98	383	11569	8320	5.93	BACKG_d	83.1
7440-43-9	cadmium (dis-calc)	3	28.89	3.87	1193	35412	24275	7.46	BACKG_d	73.2
7440-38-2	arsenic (dis-calc)	4	28.05	6.79	454	13269	9986	4.13	BACKG_d	100.0
7440-47-3	chromium (dis-calc)	5	27.99	6.48	241	8893	6131	4.32	PNEC_d	100.0
7440-50-8	copper (dis-calc)	6	27.57	6.26	414	12739	10699	4.40	BACKG_d	100.0
7440-66-6	zinc (dis-calc)	7	27.22	8.00	306	10809	8879	3.40	BACKG_d	100.0
7439-97-6	mercury (dis-calc)	8	10.76	1.40	487	14257	8474	7.67	BACKG_d	87.0

Table 17: Comparison of metal compound ranks obtained by application of different combinations of variants for exposure and effect scoring (for explanation of variants refer to chap. 6.4)

Rank	Combinations of Variants for Exposure and Effect Scoring					
	I_EXP_1 X I_EFF_1	I_EXP_1 X I_EFF_2	I_EXP_2 X I_EFF_3	I_EXP_2 X I_EFF_4	I_EXP_3 X I_EFF_1	I_EXP_3 X I_EFF_2
1	nickel	lead	nickel	nickel	nickel	nickel
2	lead	nickel	lead	lead	lead	lead
3	cadmium	zinc	cadmium	arsenic	cadmium	cadmium
4	copper	cadmium	copper	cadmium	arsenic	arsenic
5	arsenic	mercury	arsenic	copper	copper	chromium
6	zinc	chromium	chromium	chromium	chromium	copper
7	mercury	copper	zinc	zinc	zinc	zinc
8	chromium	arsenic	mercury	mercury	mercury	mercury
9				barium		

Table 18: Exposure and effect related data of metal compounds in sediments

**I\_EXP** - exposure index; **Sampl. Stat.** - number of sampling stations from which data were used to calculate I\_EXP; **entries used** - number of measurements used to calculate I\_EXP; **entries used >DL** - number of measurements higher than the corresponding determination **CIPR** - International Commission for the Protection of the Rhine, quality objectives for concentrations of metal compounds in suspended sediment <sup>[35]</sup>  
**Dir. 86/278** - Council Directive 86/278/EEC (sewage sludge disposal in agriculture) <sup>[36]</sup>, maximum permissible concentration limit for the respective metal in soil dry matter according to Annex 1A of the Directive **CONC/CIPR, CONC/LIMIT** - ratios of EU-level 90-percentiles of monitored concentrations and the quality objectives set by CIPR or the maximum permissible level according to Directive 86/278 **EFSH** - score for "effects to humans" based on R-phrases

CAS	Compound	I_EXP	90-percentile conc. [mg/kg]	Sampl. Stat. (n)	entries used (n)	entries used >DL	Quality Objectives CIPR [mg/kg]	CONC/CIPR	Limit Conc. Dir. 86/278 [mg/kg]
7440-38-2	arsenic	4.76	28.68	441	2708	2680	40.0	0.7	-
7440-43-9	cadmium	3.46	10.00	328	2873	2849	1.0	10.0	1 - 3
7440-47-3	chromium	6.81	151.33	474	3409	3409	100.0	1.5	-
7440-50-8	copper	6.93	166.67	504	3153	3152	50.0	3.3	50 - 140
7439-92-1	lead	7.50	264.20	501	3091	3091	100.0	2.6	50 - 300
7439-97-6	mercury	2.83	6.00	196	2735	2701	0.5	12.0	1 - 1.5
7440-02-0	nickel	5.62	57.29	351	2909	2906	50.0	1.2	30 - 75
7440-66-6	zinc	9.53	1367.10	488	2833	2831	200.0	6.8	150 - 300

## 7 Processing and combination of ranked lists

As described in previous chapters, it is not possible to establish just one single risk-based list of candidate priority substances in an automated manner. Therefore it was decided to create within the COMMPS procedure several lists (herein after called candidate priority lists) and to select a finite number of priority substances on a case by case basis.

In COMMPS\_1, attempts were made to combine the monitoring-based and modelling-based lists via the correlation function of the exposure indices obtained by both ranking methods. The idea was to complete the upper section of the monitoring-based list with high ranking, but not monitored, substances on the modelling-based list by using the correlation function for the calculation of "virtual" exposure indices referring to the monitoring based exposure scoring. These virtual exposure indices had then been used together with the effect indices to derive priority indices and, thus, to identify the rank of the not monitored substances on the monitoring-based list. However, the exposure indices obtained by the two methods did not correlate and a combination of the two lists by the described procedure was not possible. A combined list was eventually established by application of a substance by substance expert judgement and the "ZIP-mechanism"<sup>[31]</sup>.

The correlation of the exposure indices obtained by the modelling-based and the monitoring-based approaches was also checked for the present version of COMMPS. Only 17 substances are candidates on both lists and again a correlation between the exposure indices obtained by the different methods is lacking (see figure 3 and table A31 in annex 1).

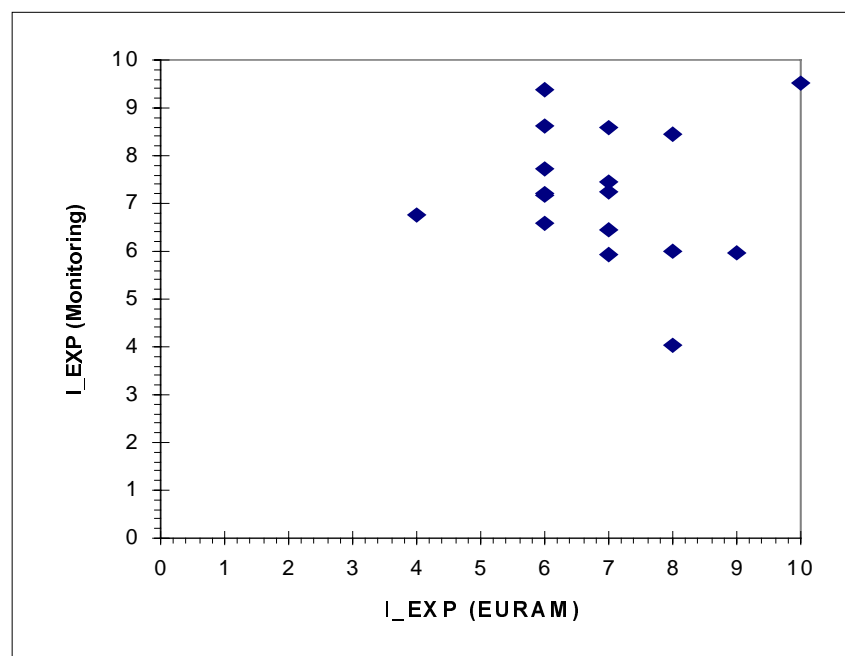


Figure 3: Correlation of modelling-based (EURAM) and monitoring-based exposure indices

In the present version of COMMPS the selection of priority substances was performed as follows:

As a first step, a number of top-ranked substances from the ranking lists are selected as candidate substances for the priority list. For this purpose, the high-ranked substances are screened and categorised on the basis of the following criteria:

1. Substances which occur normally as mixtures either because of their technical production conditions, such as trichlorobenzenes, or naturally, such as PAHs, are counted as one group, the rank of which is defined by the individual representative with the highest rank.
2. If a substance is already severely restricted or prohibited at European level (e.g. under Council Directive 79/117/EEC<sup>[14]</sup> and 76/769/EEC<sup>[15]</sup>) and no other significant use is known, the high rank of the substance on the monitoring or sediment list is most likely to be a "historic" pollution (particularly, if the substance is very persistent).
3. If an organic substance occurs mainly as breakdown product of a chemical, the source substance is included in the list with a rank given by that of the breakdown product. (This criterion was not applied in practice.)

The following tables present the candidate priority substances which were selected in this screening step following the above described criteria. In total, 20 substances (or groups of substances) have been respectively selected from the monitoring-based list and from the modelling-based list. Only 10 have been selected from the sediment-based list accounting for the lower weight which these findings have compared with the aquatic monitoring-based data<sup>3</sup>. 5 heavy metals have been selected (additionally mercury for discussion).

In a subsequent step, certain substances were selected as priority substances on the basis of a case by case judgement. It was not deemed appropriate to carry out this selection in an automated way by applying a rigid set of rules. However, a number of criteria have been used to decide whether the high rank of a substance on the risk-based lists can be justified. At the expert meeting on 2/3 July 1998 a majority of experts suggested that significantly more weight should be attributed to the evidence of the rank of a substance on the monitoring-based list compared to the modelling-based list due to the uncertainties of the latter. Taking this into account, the following two general principles were applied:

1. A substance which is listed on the monitoring-based candidate priority list is not excluded unless there is significant evidence that the high rank is not justified. Such evidence would be given if default values were used for the calculation of the effects score and that the defaults unjustifiably penalise the respective substance.
2. A substance which is listed on the modelling-based candidate priority list is only included in the final list if there is concrete additional evidence that the high rank of the substance is justified. This criterion requires to look at a number of aspects such as:
  - Use of default values for the effects scoring. In this case a substance is usually excluded from the final priority list, unless there is evidence that its high rank on the modelling based list might be justified.

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<sup>3</sup> The sediment-based list is considered to be of lower weight since it was not possible to base the effect scoring on tests with sediment or sediment dwelling organisms. Instead, the calculation of the direct effects scores (EFS<sub>d</sub>) was based on the aquatic phase PNECs. For this purpose a transformation was performed using the "equilibrium partitioning method" as outlined in the TGDs (for details see chap. 5.2).

- A substance exhibits a high reactivity or hydrolyses in water (e.g. chlorine, hypochlorite). In this case, it can be expected that the high rank of the substance is mainly due to the high reported production volumes and insufficient consideration of its specific reactivity.
- There is additional information on actual monitoring data allowing for the calculation of an approximate rank on the monitoring-based list which can be directly compared with the rank of the selected monitoring-based substances. For this purpose, either literature data or the reported monitoring results of the substances which were excluded by the representativeness criterion may be used and aggregated to calculate an approximate monitoring-based exposure score.
- If additional monitoring data is not available and if a draft risk assessment report exists under Council Regulation (EEC) No. 793/93, the  $PEC_{\text{regional}}$  may be used to calculate an approximate risk-score (the  $PEC_{\text{regional}}$  is a model-based exposure value which is used in risk assessments for the exposure assessment for a standardised regional environment - normally, 200 x 200 km, 20 mio. inhabitants - assuming as a worst-case scenario that 10% of the overall production volume is produced/used in this area).
- Default values have been used for the exposure scoring (e.g. production volume, use pattern, degradation and distribution).

For the recommendations given in the second step, some other information was taken into account which relates to specific findings of possible pollution problems in compartments which are not included in COMMPS on a systematic basis. These include the following:

- Evidence of significant pressures on coastal and marine waters. OSPAR is currently developing a prioritisation method. There are preliminary findings of a Dutch study based on the SCREMOTOX model<sup>[37]</sup> (Screening Model for comparative risk assessment – North Sea) which have attempted to rank about 50 pollutants according to their relative risks in the total North Sea.
- Evidence of widespread groundwater pollution. In a draft report of the EEA on groundwater monitoring<sup>[38]</sup> an attempt has been made to prioritise substances detected in groundwater on the basis of the number of countries (including eastern European states) where groundwater concentrations above the drinking water limit of 0.1 µg/l were found.
- Specific concerns for the water treatment for drinking water supply. EAUREAU has proposed a number of substances for inclusion in the priority list which are likely to cause concern for the purification of raw waters.
- Suspected endocrine potential: Endocrine disrupters in the aquatic environment are an important but still controversial issue. There are local examples for xenobiotics (organochlorines) showing ecological effects due to endocrine disruption.

In the following chapters the candidate priority substances from the different ranking lists are discussed and a detailed reasoning for the inclusion/exclusion in the final priority list is provided.

## **7.1 Monitoring-based lists, aquatic phase, organic micropollutants**

Following the criteria given in the above introduction, several top-ranked substances from the monitoring-based ranking list of organic substances in the aquatic phase were not included in the respective candidate list (table 19):

- DDT-isomers and metabolites
- aldrin, dieldrin, endrin, and isodrin

The use of these substances as plant protection products is banned under Council Directive 91/117/EEC<sup>[14]</sup> and is prohibited for other areas in most Member States. For DDT only one production site is known in Europe which produces DDT as an intermediate product.



Table 19: Candidate priority substances from the monitoring-based ranking of organic substances in the aquatic phase. Comments and recommendations with regard to the inclusion/exclusion in the final priority list.

Rank	CAS	Compound	Comments	Recommendation for inclusion in the final priority list
1		PAH		Inclusion as a group because individual PAHs normally occur as mixtures (e.g. combustion products).
	193-39-5	indeno(1,2,3-cd) pyrene	The effect score of this compound is based on a default value but it can be reasonably assumed on the basis of the effect data of other PAHs that this default value describes the toxicity to the aquatic environment reasonably well. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances. Indeno(1,2,3-cd) pyrene has rank 1 on the monitoring-based list. Furthermore, there is some evidence for endocrine disrupting properties of this substance.	Inclusion in the final priority list as substance group PAH.
	56-55-3	benzo-a-anthracene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances. Benzo-a-anthracene has rank 2 on the monitoring-based list. Furthermore, there is some evidence for endocrine disrupting properties of this substance.	Inclusion in the final priority list as substance group PAH.
	191-24-2	benzo-g,h,i-perylene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances. Benzo-g,h,i-perylene has rank 3 on the monitoring-based list. Furthermore, there is some evidence for endocrine disrupting properties of this substance.	Inclusion in the final priority list as substance group PAH.
	205-99-2	benzo-b-fluoranthene	The effect score of this compound is based on a default value but it can be reasonably assumed on the basis of the effect data of other PAHs that the use of the default reflects the toxicity to the aquatic environment. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances. Benzo-b-fluoranthene has rank 5 on the monitoring-based list. Furthermore, there is some evidence for endocrine disrupting properties of this substance.	Inclusion in the final priority list as substance group PAH.
	207-08-9	benzo-k-fluoranthene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances. Benzo-k-fluoranthene has rank 7 on the monitoring-based list.	Inclusion in the final priority list as substance group PAH.

Table 19: (continued) Candidate priority substances from the monitoring-based ranking of organic substances in the aquatic phase.

Rank	CAS	Compound	Comments	Recommendation for inclusion in the final priority list
	50-32-8	benzo-a-pyrene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances. Benzo-a-pyrene has rank 8 on the monitoring-based list.	Inclusion in the final priority list as substance group PAH.
	91-20-3	naphthalene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances. Naphthalene has rank 23 on the monitoring-based list.	Inclusion in the final priority list as substance group PAH.
	120-12-7	anthracene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances. Anthracene has rank 24 on the monitoring-based list.	Inclusion in the final priority list as substance group PAH.
	206-44-0	fluoroanthene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances. Fluoroanthene has rank 37 on the monitoring-based list.	Inclusion in the final priority list as substance group PAH.
	83-32-9	acenaphthene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances. Acenaphthene has rank 55 on the monitoring-based list.	Inclusion in the final priority list as substance group PAH.
2	87-86-5	pentachlorophenol	The compound is already EU-wide restricted for many uses under Directive 76/769/EEC but is still in use e.g. as wood preservative. The emissions are controlled under 86/280/EEC. Pentachlorophenol has rank 6 on the monitoring-based list. Furthermore, there is some evidence for endocrine disrupting properties of this substance. EUREAU proposes the compound as a priority substance since it causes concern for water suppliers and waste water treatment operators in EU.	Inclusion in the final priority list.
3	76-44-8	heptachlor	No exclusion criterion applies. The EEA groundwater report <sup>[38]</sup> finds that the substance is found in at least two countries (including eastern European countries) in groundwater concentrations above 0.1 µg/l. Heptachlor has rank 10 on the monitoring-based list.	Inclusion in the final priority list.
4	2921-88-2	chlorpyrifos	No exclusion criterion applies. Chlorpyrifos has rank 12 on the monitoring-based list.	Inclusion in the final priority list.

Table 19: (continued) Candidate priority substances from the monitoring-based ranking of organic substances in the aquatic phase.

Rank	CAS	Compound	Comments	Recommendation for inclusion in the final priority list
5	118-74-1	hexachlorobenzene	No exclusion criterion applies. The compound is EU-wide restricted under Directives 79/117/EEC and 76/769/EEC but it still occurs as a by-product of certain chlorinating processes, e.g. production of perchloroethylene. The emissions are controlled under 86/280/EEC. Hexachlorobenzene has rank 13 on the monitoring-based list. Furthermore, there is some evidence for endocrine disrupting properties of this substance. EUREAU proposes the compound as a priority substance since it causes concern for water suppliers and waste water treatment operators in EU.	Inclusion in the final priority list.
6		monochloronitrobenzenes		Inclusion in the final priority list as substance group monochloronitrobenzenes because the individual compounds are normally produced as technical mixtures
	121-73-3	3-chloronitrobenzene	No exclusion criterion applies. 3-chloronitrobenzene has rank 14 on the monitoring-based list. EUREAU proposes the compound as a priority substance since it causes concern for water suppliers and waste water treatment operators in EU.	Inclusion in the final priority list as substance group monochloronitrobenzenes.
7		trichlorobenzenes		Inclusion in the final priority list as substance group monochloronitrobenzenes because the individual compounds are normally produced as technical mixtures.
	120-82-1	1,2,4-trichlorobenzene	No exclusion criterion applies. The adoption into the priority list is also supported by the draft risk assessment report under Council Regulation (EEC) 793/93 ( the use of 1,2,4-TCB may cause local problems for aquatic organisms). The emissions are controlled under 86/280/EEC. 1,2,4-trichlorobenzene has rank 17 on the monitoring-based list.	Inclusion in the final priority list as substance group trichlorobenzenes (TCB).
	108-70-3	1,3,5-trichlorobenzene	No exclusion criterion applies. The emissions are controlled under 86/280/EEC. 1,3,5-trichlorobenzene has rank 64 on the monitoring-based list.	Inclusion in the final priority list as substance group trichlorobenzenes (TCB).
	87-61-6	1,2,3-trichlorobenzene	No exclusion criterion applies. The emissions are controlled under 86/280/EEC. 1,2,3-trichlorobenzene has rank 78 on the monitoring-based list.	Inclusion in the final priority list as substance group trichlorobenzenes (TCB).

Table 19: (continued) Candidate priority substances from the monitoring-based ranking of organic substances in the aquatic phase.

Rank	CAS	Compound	Comments	Recommendation for inclusion in the final priority list
8	470-90-6	chlorfenvinphos	No exclusion criterion applies. Chlorfenvinphos has rank 18 on the monitoring-based list.	Inclusion in the final priority list.
9	330-54-1	diuron	No exclusion criterion applies. Diuron has rank 19 on the monitoring-based list.	Inclusion in the final priority list.
10	1582-09-8	trifluralin	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> , i.e. a Dutch model for a comparative risk assessment in the North Sea results in trifluralin being among the high priority substances (ranks 1-20 out of 52). Trifluralin has rank 21 on the monitoring-based list.	Inclusion in the final priority list.
11	67-66-3	trichloromethane	No exclusion criterion applies. The emissions are controlled under 86/280/EEC. Trichloromethane has rank 22 on the monitoring-based list.	Inclusion in the final priority list.
12	75-09-2	dichloromethane	No exclusion criterion applies. Dichloromethane has rank 25 on the monitoring-based list.	Inclusion in the final priority list.
13	107-06-2	1,2-dichloroethane	The compound is an intermediate in the production of PVC. The use of the compound as pesticide is EU-wide restricted under Directive 79/117/EEC. The emission is controlled by 86/280/EEC. 1,2-dichloroethane has rank 26 on the monitoring-based list.	Inclusion in the final priority list.
14	34123-59-6	isoproturon	No exclusion criterion applies. Isoproturon has rank 27 on the monitoring-based list.	Inclusion in the final priority list.
15	959-98-8	endosulfan, $\alpha$ - and $\beta$ -isomer	No exclusion criterion applies. The $\alpha$ -isomer has rank 30 and the $\beta$ -isomer has rank 51 on the monitoring-based list.	Inclusion in the final priority list as endosulfan without differentiation between the isomers.
16	15972-60-8	alachlor	No exclusion criterion applies. Alachlor has rank 31 on the monitoring-based list.	Inclusion in the final priority list.
17	87-68-3	hexachlorobutadiene	No exclusion criterion applies. There are probably only minor uses of the compound but it occurs as a by-product in the production of chlorinated compounds. The emissions are regulated under 86/280/EEC. Hexachlorobutadiene has rank 33 on the monitoring-based list. EUREAU proposes the compound as a priority substance since it causes concern for water suppliers and waste water treatment operators in EU.	Inclusion in the final priority list.

Table 19: (continued) Candidate priority substances from the monitoring-based ranking of organic substances in the aquatic phase.

Rank	CAS	Compound	Comments	Recommendation for inclusion in the final priority list
18		hexachlorocyclohexanes (HCHs)		Inclusion as a group since the substances are normally produced as technical mixtures.
	319-84-6	HCH, $\alpha$ -isomer	<p>Products of HCH containing less than 99% of Lindane (<math>\gamma</math>-HCH) are prohibited under Council Directive 79/117/EEC.</p> <p>The emission of HCHs is regulated under 84/491/EEC. <math>\alpha</math>-HCH is synthesized as by-product of Lindane production in one known plant in Europe (Rumania) but cracked down on site in the course of Lindane purification.</p> <p>Exclusion criteria are not clearly fulfilled.</p> <p>HCH, <math>\alpha</math>-isomer, has rank 34 on the monitoring-based list.</p>	Inclusion in the final priority list as substance group HCHs.
	319-86-8	HCH, $\delta$ -isomer	<p>Products of HCH containing less than 99% of Lindane (<math>\gamma</math>-HCH) are prohibited under Council Directive 79/117/EEC.</p> <p>The emission of HCHs is regulated under 84/491/EEC. <math>\delta</math>-HCH is synthesized as by-product of Lindane production in one known plant in Europe (Rumania) but cracked down on site in the course of Lindane purification.</p> <p>Exclusion criteria are not clearly fulfilled.</p> <p>HCH, <math>\delta</math>-isomer, has rank 35 on the monitoring-based list.</p>	Inclusion in the final priority list as substance group HCHs.
	319-85-7	HCH, $\beta$ -isomer	<p>Products of HCH containing less than 99% of Lindane (<math>\gamma</math>-HCH) are prohibited under Council Directive 79/117/EEC.</p> <p>The emission of HCHs is regulated under 84/491/EEC. <math>\beta</math>-HCH is synthesized as by-product of Lindane production in one known plant in Europe (Rumania) but cracked down on site in the course of Lindane purification.</p> <p>Exclusion criteria are not clearly fulfilled.</p> <p>HCH, <math>\beta</math>-isomer, has rank 38 on the monitoring-based list.</p>	Inclusion in the final priority list as substance group HCHs.
	58-89-9	HCH, $\gamma$ -isomer (lindane)	<p>The emission of HCHs is regulated under 84/491/EEC. <math>\gamma</math>-HCH is produced in one known plant in Europe (Rumania). Lindane is still in use for several purposes. The substance has been proposed for adoption in the priority list because of specific concern for drinking water suppliers (EUREAU).</p> <p>Lindane has rank 45 on the monitoring-based list.</p>	Inclusion in the final priority list as substance group HCHs.

Table 19: (continued) Candidate priority substances from the monitoring-based ranking of organic substances in the aquatic phase.

Rank	CAS	Compound	Comments	Recommendation for inclusion in the final priority list
19	1912-24-9	atrazine	No exclusion criterion applies. The EEA groundwater report <sup>[38]</sup> states that the substance is found in at least six countries (including eastern European countries) in groundwater concentrations above 0.1 µg/l. The Screamotox-study <sup>[37]</sup> finds for the total North Sea that atrazine is within the priority ranks 1-20 out of 52 ranked substances. Atrazine has rank 36 on the monitoring-based list. Furthermore, there is some evidence for endocrine disrupting properties of this substance.	Inclusion in the final priority list.
20		simazine	No exclusion criterion applies. The EEA groundwater report <sup>[38]</sup> states that the substance is found in at least six countries (including eastern European countries) in groundwater concentrations above 0.1 µg/l. Simazine has rank 39 on the monitoring-based list.	Inclusion in the final priority list.

Following the recommendations presented in table 19, twenty final priority substances have been selected (table 20).

**Table 20: Priority organic micropollutants in the aquatic phase, monitoring-based list**

<b>Number</b>	<b>Compound</b>
1	PAHs
2	pentachlorophenol
3	heptachlor
4	chlorpyrifos
5	hexachlorobenzene
6	monochloronitrobenzenes
7	trichlorobenzenes
8	chlorfenvinphos
9	diuron
10	trifluralin
11	trichloromethane
12	dichloromethane
13	1,2-dichloroethane
14	isoproturon
15	endosulfan
16	alachlor
17	hexachlorobutadiene
18	HCHs
19	atrazine
20	simazine

## **7.2 Modelling-based list, aquatic phase, organic micropollutants**

The modelling-based list has been screened and evaluated on a case by case basis using the above mentioned criteria. The candidate substances are discussed in table 21. Comments and recommendations for inclusion in or exclusion from the final priority list are included as well.

Table 21: Candidate priority substances from the modelling-based ranking of organic substances in the aquatic phase. Comments and recommendations with regard to the inclusion/exclusion in the final priority list.

Rank	CAS	Compound	Comments	Recommendations for inclusion in the final priority list
1	7681-52-9	hypochlorite, sodium salt	The compound is used as bleaching agent, e.g., in household, laundry, paper, pulp and textile industry, as disinfectant for glass, ceramics and water as well as algacide and molluscicide in cooling water for power stations. Beside other uses it is also applied as a sanitiser in swimming pools, in treatment of thiol spills, as dye oxidiser and as an antiseptic. In natural water decomposition of sodium hypochlorite takes place within a few seconds <sup>[40, 41, 42]</sup> . EURAM calculations use defaults for: production volume, use pattern, distribution and biodegradability	Exclusion due to high instability in water. The modelled high exposure rank is probably due to an insufficient consideration of the specific reactivity.
2	7782-50-5	chlorine	The compound is used in manufacture of chlorinated lime, in bleaching of all kinds of fabric, for purifying water and as disinfectant. Many other minor uses are published. The stability of free chlorine in natural water is very low because it is a strong oxidising agent and rapidly oxidises inorganic compounds. It also oxidises organic compounds, but more slowly than the inorganic substances <sup>[40, 43, 44]</sup> . EURAM calculations use defaults for: production volume, use pattern, distribution and biodegradability	Exclusion due to high instability in water. The modelled high exposure rank is probably due to an insufficient consideration of the specific reactivity.
3	87-68-3	hexachlorobutadiene	The compound is a by-product in the production of chlorinated compounds. The emissions are regulated under 86/280/EEC. EURAM calculations use defaults for: production volume and use pattern, but the high rank of the substance is confirmed also on the basis of monitoring-results (the compound is recommended for inclusion in the final priority list via the aquatic monitoring-based list). EUREAU proposes the compound as a priority substance since it causes concern for water suppliers and waste water treatment operators in EU.	Inclusion in the final priority list.
4	71-43-2	benzene	The compound is known to cause adverse effects mainly because of its cancerogenic properties. Also, accumulation (e.g. in the food chain) may occur. Under Council Directive 76/769/EEC certain uses of the substance have been restricted (exceptions: e.g. content in motor fuels). The exposure score is uncertain because the EURAM calculation is based on uses of defaults for distribution, production volume and use pattern. However, if the monitoring data are used without considering the European-wide representativeness the compound would obtain the rank 2 on the monitoring-based list. This finding supports the high rank of the substance.	Inclusion in the final priority list since there is additional evidence for the high rank.



Table 21: (continued) Candidate priority substances from the modelling-based ranking of organic substances in the aquatic phase.

Rank	CAS	Compound	Comments	Recommendations for inclusion in the final priority list
5	11138-47-9	perboric acid, sodium salt	The compound is used as a constituent in detergents. Boron compounds are known to have a phytotoxic potential in concentrations exceeding optimum levels. No detailed information about emissions and impacts was available in literature. The exposure score is uncertain because the EURAM calculation is based on defaults for distribution, production volume and use pattern.	Exclusion from the final priority list because of low certainty of exposure rank.
6		trichlorobenzenes		Inclusion in the final priority list as substance group trichlorobenzenes because the individual compounds are normally produced as technical mixtures.
	120-82-1	1,2,4-trichlorobenzene	EURAM calculations use defaults for production volume and use pattern but the high rank of the substance is confirmed on the basis of monitoring-results (the compound is recommended for inclusion in the final priority list via the aquatic monitoring-based list) The adoption into the priority list is supported by the draft risk assessment report under Regulation 793/93 which concludes that the use of 1,2,4-TCB may cause local problems for aquatic organisms. The emissions are controlled under 86/280/EEC.	Inclusion in the final priority list as substance group trichlorobenzenes (TCB) since there is additional evidence for the high rank..
7	85535-84-8	chloroalkanes, C10-13	The risk assessment under Regulation 793/93/identified a significant risk to the aquatic ecosystem for certain uses.	Inclusion in the final priority list since there is additional evidence for the high rank..
8	98-95-3	nitrobenzene	Nitrobenzene is mainly used for the production of aniline. It is furthermore used for preparing dinitrobenzenes, m-chloronitrobenzene and nitrobenzene-sulfonic acid, and also as solvent. Emissions from industrial production are likely to be the main source for exposure. The EURAM calculation uses defaults for production volume and use pattern. However, monitoring data have been reported by one Member State. Approximately 15% of the measurements were above the corresponding determination limit. If these monitoring data are used without considering the European-wide representativeness the compound would obtain the rank 26 on the monitoring-based list. This finding supports the high rank of the substance.	Inclusion in the final priority list since there is additional evidence for the high rank.

Table 21: (continued) Candidate priority substances from the modelling-based ranking of organic substances in the aquatic phase.

Rank	CAS	Compound	Comments	Recommendations for inclusion in the final priority list
9	77-78-1	dimethylsulfate	The compound is used in manufacturing of dyes, colours, perfumes, and solvents for separation of mineral oils. It is a methylating agent for amines and phenols. DMS enters the environment during its production and use as an industrial methylating agent. If released into water, it will hydrolyse with a half-life time of appr. 1.2 hours. It would not be expected to bioconcentrate in fish due to its low logPow-value (0.03). (Ref. <sup>[45, 46, 47]</sup> ) The EURAM calculation used defaults for degradability, production volume and use pattern. It ranks fairly high in the modelling-based list due to these defaults.	Exclusion due to high reactivity and the low certainty of the exposure rank. The modelled high exposure rank is probably due to an insufficient consideration of the hydrolysis.
10	61790-33-8	amines, tallow-alkyl-	There is little information on exposure and use pattern in literature. EURAM uses defaults for use pattern and the distribution in the environment.	Exclusion from the final priority list because of lack of information and the uncertainty of the exposure rank.
11	101-77-9	4,4'-methylenedianiline	The compound is used e.g. for polyurethane manufacturing and as epoxy hardener. EURAM calculations use defaults for the use pattern. No monitoring data is available but the draft report under Council Regulation (EEC) No. 793/93 provides for a PEC <sub>regional</sub> , which allows to calculate an approximate rank of 57 which can be compared with the rank of other selected substances of the monitoring-based list. This demonstrates that the high rank is not supported by monitoring data and the substances should be excluded from the list.	Exclusion from final priority list since no significant releases are expected. The PEC <sub>regional</sub> used for the risk assessment suggests that the substance would have a lower rank on the monitoring-based list compared with those which were selected from this list.
12	8012-95-1	mineral oil	This group comprises a large number of individual substances with different physico-chemical properties and degradation. Therefore, no straightforward assessment can be given for the whole group. Furthermore, the EURAM exposure rank is highly uncertain due to the use of defaults for the use pattern, distribution in the environment and biodegradation.	Exclusion from the final priority list because of low certainty of exposure rank.
13	78-00-2	tetraethyl lead	TEL is manufactured through a radical reaction of chloroethane with lead-sodium alloy. TEL is/was added as antiknock agent to Otto motor fuels. It also is used as intermediate in the production of organomercury fungicides. Due to the physical properties it is mainly discharged into the atmosphere. Through rain-out, wash-out and dry deposition TEL can migrate from the air to soil and surface waters. Due to reduction measures in motor fuels, the overall emissions have significantly decreased in the last years. The compound has been evaluated comprehensively by the German Beratergremium für umweltrelevante Altstoffe (Advisory Committee for environmentally Relevant Existing Substances) <sup>[48]</sup> . Reported results for an occurrence in the hydrosphere are scarce, highly varying and mostly below the determination limit. EURAM calculations used defaults for biodegradability and use pattern.	Exclusion from final priority list since there is no other evidence which justifies the high rank of the substance and since no significant releases into water are expected due to the physical properties.

Table 21: (continued) Candidate priority substances from the modelling-based ranking of organic substances in the aquatic phase.

Rank	CAS	Compound	Comments	Recommendations for inclusion in the final priority list
14	117-81-7	phthalic acid, 2-ethylhexylester (DEHP)	<p>The PEC<sub>regional</sub>, which is given in the draft risk assessment report under Council Regulation (EEC) No. 793/93 (not finalised at technical level) can be used to calculate an approximate priority rank of 8 on the monitoring-based list. Comparison with the selected substances from the monitoring-based ranking supports the high rank of the substance.</p> <p>A recent Danish study<sup>[49]</sup> has shown that DEHP is one of the major phthalate compounds in surface waters (accounting for about 70% of the total mass flow of phthalates and nonylphenols in rivers and 50% in sewage treatment plants)</p> <p>Furthermore, there is some evidence for endocrine disrupting properties of this substance.</p>	Inclusion in the final priority list since there is additional evidence for the high rank of the substance.
15	683-18-1	dibutyltin dichloride	<p>The compound ranks relatively high due to the high model exposure index. In the EURAM exposure scoring defaults are only used for the production volume.</p> <p>However, if the available monitoring data for the aquatic phase and the sediment are used without considering the European-wide representativeness the compound would obtain rank 53 on the monitoring-based list for the aquatic phase and rank 42 on the sediment list. This finding does not support the high rank of the substance on the modelling based list.</p>	Exclusion of dibutyltin dichloride from the final priority list since there is no additional evidence which justifies the high rank of the substance.
16	106-89-8	epichlorohydrin	<p>The compound has been evaluated comprehensively by the German Beratergremium für umweltrelevante Altstoffe (Advisory Committee for Environmentally Relevant Existing Substances)<sup>[50]</sup>. Results are cited directly from the summary of the report:</p> <p>The compound is used for further processing to synthetic glycerine, to epoxide resins and to wet binder for paper and to other special chemicals. Through manufacture, processing and use of the resulting products emissions of epichlorohydrin into the atmosphere and hydrosphere can occur. Some information is available on the occurrence in the environment: For the USA no data is available on the occurrence of epichlorohydrin in the hydrosphere, but 2-5 µg/l have been detected in drinking water. The compound is hydrolysed fairly rapidly (half-life time = 6,5 d at 20° C and pH = 5-9). In the modified MITI test, after 14 d about 60% degradation were found for freshwater. Effect concentrations are above the reported concentrations in drinking water.</p> <p>EUREAU proposes the compound as a priority substance since it causes concern for water suppliers and waste water treatment operators in EU</p> <p>Information on concentrations in the hydrosphere were not available for European countries up to 1992<sup>[50]</sup>, while in USA three positive findings without detailed specifications were reported in 1976.</p> <p>EURAM calculation used defaults for production volume and use pattern.</p>	Exclusion from the final priority list since there is no clear additional evidence supporting the high rank of the substance. Due to rapid hydrolysis, concentration levels in the aquatic environment are expected to be low.

Table 21: (continued) Candidate priority substances from the modelling-based ranking of organic substances in the aquatic phase.

Rank	CAS	Compound	Comments	Recommendations for inclusion in the final priority list
17	62-53-3	aniline	From reference <sup>[51]</sup> it can be concluded that the compound is present in the hydrosphere at concentrations below 100 ng/l. Assuming a aniline concentration of 100 ng/l and performing the ranking procedure as for monitored compounds would result in approximately rank 50 on the monitoring-based list. Thus, the substance would obtain a lower rank on the monitoring-based list as those compounds selected from this list. EURAM calculation used defaults for the production volume and use pattern.	Exclusion from the final priority list since there is no additional evidence which justifies the high rank of the substance.
18	10039-54-0	bis(hydroxylammonium)-sulphate	EURAM calculations use defaults for: production volume, use pattern, distribution and biodegradability. No additional information on exposure and use pattern can be found in literature.	Exclusion from the final priority list since there is no additional evidence which justifies the high rank of the substance.
19		octylphenols - nonylphenols	Nonylphenols are placed on ranks 38 and 39 of the modelling-based list. Monitoring data have been provided but the substance was excluded on the basis of the European representativeness criterion. If this criterion was neglected the substance had obtained a rank of 21 on the monitoring-based list which is even higher than the rank of 4-tert.-octylphenol.	Inclusion in the final priority list as substance group octylphenols - nonylphenols. The occurrence of the individual compounds in the aquatic environment is mainly a result of the breakdown of alkylphenol-ethoxylates.
	140-66-9	1,1,3,3-tetramethyl-4-butylphenol (4-tert-octylphenol)	The production of the compound as well as its use as a chemical intermediate may result in the release into the aquatic environment. The compound may also be formed as a degradation product of alkylphenol surfactants in wastewater. If released into the atmosphere it is degraded by reaction with photochemically produced hydroxyl radicals with an estimated half-life of about 9 hours. An estimated Koc-value of 18.000 suggests that the substance will be immobile in soil and sediment. Rapid infiltration studies indicate, however, that 4-(1,1,3,3,-tetramethylbutyl) phenol has some mobility in sandy or gravelly soils and is able to reach groundwater although in lower concentrations as the original effluent. Biodegradation may be an important fate process in the water column. The compound is expected to accumulate in aquatic organisms based on estimated BCF-value of 6000. (Ref. <sup>[52, 53, 54, 55, 56]</sup> ). If the rank of the substance is calculated using the provided monitoring data without applying the criterion of European-wide representativeness the substance would have a rank of 34 on the monitoring-based list. This confirms the high rank of this substance.	The compound should be included in the final priority list as group "octylphenols - nonylphenols" because there is additional evidence which supports the high rank.
20	84-66-2	Phthalic acid diethylester (DEP)	EURAM calculations use defaults for production volume and use pattern Several phthalates were monitored and reported, e.g. in a recent Danish study <sup>[49]</sup> indicating some evidence for their exposure. However, no specific concentrations were available for DEP which allow to verify the high rank. The substance should therefore be excluded from the priority list, though endocrine disrupting properties cannot be ruled out.	Exclusion from the final priority list because there is no additional evidence which supports the high rank.

In summary, it is recommended to exclude the following candidate substances from the modelling-based priority list:

- Hypochlorite (sodium salt), chlorine, dimethyl sulfate, epichlorhydrin because of high reactivity or hydrolysis in water.
- Perboric acid (sodium salt), mineral oils, tetraethyl lead, tallow-alkylamines, bis(hydroxylammonium)sulphate and DEP because of high uncertainty of the ranking (defaults were used for production volume, use pattern and distribution) or because there is no information available which allows to verify the likeliness of their high rank.
- Aniline and dibutyltin dichloride, because there are monitoring data available which suggest that the substance would have a lower rank on the monitoring-based list compared with those which were selected from this list.
- 4,4'-methylenedianiline because the  $PEC_{\text{regional}}$  used for the risk assessment under Council Regulation (EEC) No. 793/93 suggests that the substance would have a lower rank on the monitoring-based list compared with those which were selected from this list.
- Hexachlorobutadiene and trichlorobenzene have been already selected on the basis of the monitoring-based list.

It is recommended that the remaining candidate substances from the modelling-based candidate list (table 21) should be included in the final priority list since there is additional evidence for their high rank.

Nonylphenol is a substance which has been proposed for inclusion in the priority list by a number of experts because of its generally acknowledged endocrine disrupting effects and wide-spread occurrence (mainly as a breakdown product of nonylphenol-ethoxylates). The substance is placed on ranks 38 (unbranched C-chain) and 39 (branched isomer) on the modelling-based list. Monitoring data have been provided but the substance was excluded on the basis of the European representativeness criterion. If this criterion was neglected the substance had obtained rank 21 on the monitoring-based ranking list which is even higher than the rank of 4-tert.-octylphenol. Therefore, it is suggested to include also this substance - as group "octylphenols - nonylphenols", covering all isomers of the C<sub>8</sub> and C<sub>9</sub> alkyl chains – in the priority list.

It should be mentioned that tributyltin was recommended by several parties as a priority substance. The EURAM exposure score for tributyltin oxide is confidential since there is, apparently, only one enterprise producing/importing this high production volume chemical (HPVC) in volumes exceeding 1000 tons per year (table A21). Consequently, while monitoring data was provided, the substance has been excluded on the basis of the European representativeness criterion. It is remarkable that the substance would have obtained rank 1 on the monitoring-based ranking list.

To conclude, the substances listed in table 22 are recommended for inclusion in the final priority list.

**Table 22: Priority organic micropollutants in the aquatic phase, modelling-based list**

Number	Compound
1	chloroalkanes, C10-13
2	benzene
3	nitrobenzene
4	ci(2-ethylhexyl)phthalate (DEHP)
5	octylphenols - nonylphenols

### 7.3 Monitoring-based lists, sediment, organic micropollutants

The same procedure as for the aquatic phase was followed for the monitoring-based sediment ranking list. The candidate list is presented in table 23 <sup>4</sup>.

Following the criteria described in the introduction of chapter 7 several top-ranked substances from the monitoring-based sediment ranking list were not included in the sediment candidate list (table 23):

- aldrin, dieldrin, endrin, and isodrin
- DDT and metabolites

The use of these substances as plant protection products is banned under Council Directive 91/117/EEC and is prohibited for other areas in most Member States. For DDT only one production site is known in Europe which produces DDT as an intermediate product.

- PCBs

This group of substances (except mono- and dichlorinated products) has been restricted in marketing and use by Council Directive 76/769/EEC.

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<sup>4</sup> The candidate list based on sediment monitoring data as presented in table 22 is the corrected version of the respective list in the final draft report dated March 1999 and presented at the COMMPS meeting of 19 April 1999. In the previous version hexachlorobutadiene was erroneously excluded from the ranking. The rank of hexachlorobutadiene on the sediment final priority list is 4. Thus, the inclusion of hexachlorobutadiene in the ranking of substances monitored in sediment and its rank among the top 10 on the sediment priority list results also in the withdrawal of phthalic acid benzylbutyl-ester (BBP) from the final list because this substance now obtains only rank 11.

Table 23: Candidate priority substances from the monitoring-based ranking of organic substances in sediments. Comments and recommendations with regard to the inclusion/exclusion in the final priority list.

Rank	CAS	Compound	Comments	Recommendations for inclusion in the final priority list
1		PAHs		Inclusion as a group because individual PAHs normally occur as mixtures (e.g. combustion products).
	191-24-2	benzo-g,h,i-perylene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Benzo-g,h,i-perylene is on rank 2 on the monitoring-based sediment list. Furthermore, there is some evidence for endocrine disrupting properties of this substance.	Inclusion in the final priority list as substance group PAH.
	56-55-3	benzo-a-anthracene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Benzo-a-anthracene is on rank 3 on the monitoring-based sediment list. Furthermore, there is some evidence for endocrine disrupting properties of this substance.	Inclusion in the final priority list as substance group PAH.
	205-99-2	benzo-b-fluoroanthene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Benzo-b-fluoroanthene is on rank 4 on the monitoring-based sediment list. Furthermore, there is some evidence for endocrine disrupting properties of this substance.	Inclusion in the final priority list as substance group PAH.
	207-08-9	benzo-k-fluoroanthene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Benzo-k-fluoroanthene is on rank 5 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.
	50-32-8	benzo-a-pyrene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Benzo-a-pyrene is on rank 6 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.

Table 23: (continued) Candidate priority substances from the monitoring-based ranking of organic substances in sediments.

Rank	CAS	Compound	Comments	Recommendations for inclusion in the final priority list
	193-39-5	indeno(1,2,3-cd)pyrene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Indeno(1,2,3-cd)pyrene is on rank 7 on the monitoring-based sediment list. Furthermore, there is some evidence for endocrine disrupting properties of this substance.	Inclusion in the final priority list as substance group PAH.
	208-96-8	acenaphthylene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances) Acenaphthylene is on rank 8 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.
	218-01-9	crysene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Crysene is on rank 9 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.
	129-00-0	pyrene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Pyrene is on rank 11 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.
	86-73-7	fluorene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Fluorene is on rank 16 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.
	85-01-8	phenanthrene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Phenanthrene is on rank 19 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.
	206-44-0	fluoroanthene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Fluoroanthene is on rank 22 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.



Table 23: (continued) Candidate priority substances from the monitoring-based ranking of organic substances in sediments.

Rank	CAS	Compound	Comments	Recommendations for inclusion in the final priority list
	120-12-7	anthracene	No exclusion criterion applies The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Anthracene is on rank 26 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.
	91-20-3	naphthalene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Naphthalene is on rank 34 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.
	83-32-9	acenaphthene	No exclusion criterion applies. The Scremotox-study <sup>[37]</sup> finds for the total North Sea that PAHs are within the priority ranks 1-20 out of 52 ranked substances Acenaphthene is on rank 44 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group PAH.
2	118-74-1	hexachlorobenzene	No exclusion criterion applies. The compound occurs as a by-product upon production of chlorinated compounds such as tetrachloroethylene. The compound is EU-wide restricted under Directives 79/177/EEC and 76/769/EEC. The emission is controlled under 86/280/EEC. Hexachlorobenzene is on rank 13 on the monitoring-based sediment list. Furthermore, there is some evidence for endocrine disrupting properties of this substance. EUREAU proposes the compound as a priority substance since it causes concern for water suppliers and waste water treatment operators in EU.	Inclusion in the final priority list.
3	87-86-5	pentachlorophenol	The compound is already EU-wide restricted for many uses under Directive 76/769/EEC but is still in use e.g. as wood preservative. The emission is controlled under 86/280/EEC Pentachlorophenol is on rank 14 on the monitoring-based sediment list. Furthermore, there is some evidence for endocrine disrupting properties of this substance. EUREAU proposes the compound as a priority substance since it causes concern for water suppliers and waste water treatment operators in EU.	Inclusion in the final priority list.

Table 23: (continued) Candidate priority substances from the monitoring-based ranking of organic substances in sediments.

Rank	CAS	Compound	Comments	Recommendations for inclusion in the final priority list
4	87-68-3	hexachlorobutadiene	No exclusion criterion applies. There are probably only minor uses of the compound but it occurs as a by-product in the production of chlorinated compounds. The emissions are regulated under 86/280/EEC. Hexachlorobutadiene has rank 24 on the monitoring-based sediment list. EUREAU proposes the compound as a priority substance since it causes concern for water suppliers and waste water treatment operators in EU.	Inclusion in the final priority list
5		hexachlorocyclohexanes (HCHs)		Inclusion as a group since the substances are normally produced as technical mixtures.
	319-84-6	HCH, $\alpha$ - isomer	Products of HCH containing less than 99% of Lindane ( $\gamma$ -HCH) are prohibited under Council Directive 79/117/EEC. The emission of HCHs is regulated under 84/491/EEC. The compounds are not produced in Europe. HCHs are still in use for several purposes (especially Lindane). Exclusion criteria are not clearly fulfilled. $\alpha$ -HCH is on rank 27 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group HCHs.
	319-85-7	HCH, $\beta$ - isomer	Products of HCH containing less than 99% of Lindane ( $\gamma$ -HCH) are prohibited under Council Directive 79/117/EEC. The emission of HCHs is regulated under 84/491/EEC. The compounds are not produced in Europe. HCHs are still in use for several purposes (especially Lindane). Exclusion criteria are not clearly fulfilled. $\beta$ -HCH is on rank 35 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group HCHs.
	58-89-9	HCH, $\gamma$ - isomer (lindane)	The emission of HCHs is regulated under 84/491/EEC. The compound is not produced in Europe. Lindane is still in use for several purposes. The substance has been proposed for adoption in the priority list because of specific concern for drinking water suppliers (EUREAU). Exclusion criteria are not clearly fulfilled. Lindane is on rank 42 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group HCHs.
6	959-98-8	endosulfan ( $\alpha$ - and $\beta$ - isomer)	No exclusion criterion applies. $\alpha$ -endosulfan is on rank 28 on the monitoring-based sediment list.	Inclusion in the final priority list as group ( $\alpha$ - and $\beta$ - isomer).

Table 23: (continued) Candidate priority substances from the monitoring-based ranking of organic substances in sediments.

Rank	CAS	Compound	Comments	Recommendations for inclusion in the final priority list
7		trichlorobenzenes		Inclusion in the final priority list as substance group monochloronitrobenzenes because the individual compounds are normally produced as technical mixtures.
	120-82-1	1,2,4-trichlorobenzene	No exclusion criterion applies. The adoption into the priority list is also supported by the draft risk assessment report under Regulation 793/93 ( the use of 1,2,4-TCB may cause local problems for aquatic organisms). The emission is controlled under 86/280/EEC. 1,2,4-trichlorobenzene has the rank 29 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group trichlorobenzenes (TCB).
	87-61-6	1,3,5-trichlorobenzene	No exclusion criterion applies. The emissions are controlled under 86/280/EEC. 1,3,5-trichlorobenzene has the rank 45 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group trichlorobenzenes (TCB).
	87-61-6	1,2,3-trichlorobenzene	No exclusion criterion applies. The emissions are controlled under 86/280/EEC. 1,2,3-trichlorobenzene has the rank 51 on the monitoring-based sediment list.	Inclusion in the final priority list as substance group trichlorobenzenes (TCB).
8	608-93-5	pentachlorobenzene	No exclusion criterion applies. Pentachlorobenzene has the rank 32 on the monitoring-based sediment list.	Inclusion in the final priority list.
9		brominated diphenylethers		Inclusion in the final priority list as substance group brominated diphenylethers because the individual compounds are normally produced as technical mixtures.
	32534-81-9	diphenyl ether, penta-bromo derivative	No exclusion criterion applies. The compound has the rank 37 on the monitoring-based sediment list	Inclusion in the final priority list as substance group brominated biphenylethers.
	40088-47-9	2,2',4,4'-tetrabromodiphenyl ether	No exclusion criterion applies. The compound has the rank 41 on the monitoring-based sediment list	Inclusion in the final priority list as substance group brominated biphenylethers.
	1163-19-5	bis(pentabromophenyl)-ether	No exclusion criterion applies. The compound has the rank 50 on the monitoring-based sediment list	Inclusion in the final priority list as substance group brominated biphenylethers.

Table 23: (continued) Candidate priority substances from the monitoring-based ranking of organic substances in sediments.

<b>Rank</b>	<b>CAS</b>	<b>Compound</b>	<b>Comments</b>	<b>Recommendations for inclusion in the final priority list</b>
10	1806-26-4	octylphenol	No exclusion criterion applies. Furthermore, there is some evidence for endocrine disrupting properties of this substance. Octylphenol has the rank 39 on the monitoring-based sediment list.	Inclusion in the final priority list.

Based on the recommendations presented in table 23, two further final priority substances/substance groups have been selected (table 24). Substances/groups which are already recommended for inclusion in the final priority list via the aquatic monitoring-based or modelling based candidate lists are not presented (i.e. PAHs, hexachlorobenzene, pentachlorophenol, hexachlorobutadiene, HCHs, endosulfan, trichlorobenzenes, octylphenols).

**Table 24: Priority organic micropollutants in the sediment, monitoring-based list**

Number	Compound
1	pentachlorobenzene
2	brominated diphenylethers

#### 7.4 Monitoring-based lists, metals and metal compounds

Based on the ranking of the metals in the aquatic phase, it is recommended to include the top five heavy metals as listed in table 25.

**Table 25: Priority metals**

Number	Compound
1	nickel
2	lead
3	cadmium
4	copper
5	arsenic

This recommendation is partially supported by the Scremotox study<sup>[37]</sup>, a comparative risk assessment for the North Sea. This study results in copper, zinc, nickel, chromium, mercury and cadmium being among the high priority substances with ranks between 1 and 20 out of 52 chemicals.

Mercury has a very low rank on the aquatic risk-based ranking list. This certainly reflects the fact that past measures against mercury pollution have been particularly successful. There is, however, some evidence that mercury concentrations in sediments are still significant and of relatively higher concern in relation to other heavy metals. While no clear recommendation can be given, many experts clearly suggested to include mercury in the priority list. For this reason, the substance should be discussed at the experts meeting in the light of the provided data.

## 8 References

- [1] Council Regulation (EEC) No 793/93 of 23 March 1993 on the evaluation and control of risks of existing chemical substances, OJ No. L84, 5.4. 1993
- [2] List I and II of Council Directive 76/464/EEC, OJ No. C 176 of 14.7.1982
- [3] Third North Sea Conference: Annex 1A (List of priority substances agreed by the Third North Sea Conference) and 1D (Reference list of substances agreed by the Third North Sea Conference [e.g. Annex 1D to the Hague Declaration], for further selection of priority substances), in: Oslo and Paris Conventions for the Prevention of Marine Pollution, Working Group on Diffuse Sources (DIFF), Oslo: 20-24 October 1997, Summary Record DIFF 97/19/E-1, Annex 8
- [4] Priority lists 1-3 identified under Council Regulation No 793/93: OJ, No. L 131/4 of 26.5.1994, Annex (first list); OJ No. L 231/19 of 28.9.1995, Annex (second list); OJ No. L 25/13 of 28.1.1997, Annex (third list)
- [5] List of substances identified as of concern by OSPAR in the period 1991-1996, which are part of the OSPAR Work-Programme, Annex 3, in: Ministerial Meeting of the OSPAR Commission, Sintra: 22 - 23 July 1998, Draft Summary Record OSPAR 98/14/1, Annex 34 (Ref. N° 1998-16).
- [6] HELCOM lists of priority substances, HELCOM 12/18, Annex 6, HELCOM 14/18, paragraph 6.40 and HELCOM recommendations 19/5, Appendix 3)
- [7] Council Directive 91/414/EEC, OJ No. L230 of 19.8.1991, pg. 1
- [8] Council Regulation 3600/92, OJ No. L366 of 15.12.1992, pg. 10
- [9] Technical Guidance Documents in Support of the Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and the Commission Regulation 1488/94 on Risk Assessment for Existing Substances
- [10] Liste der gefährlichen Stoffe und Zubereitungen nach § 4a GefStoffV [list of hazardous substances and preparations acc. §4a of the German ordinance on protection from hazardous substances] in: Verordnung zum Schutz vor gefährlichen Stoffen (Gefahrstoffverordnung - GefStoffV) of October 26, 1993, last update April 15, 1997
- [11] TRGS 905: Verzeichnis krebserzeugender, erbgutverändernder oder fortpflanzungsgefährdender Stoffe [inventory of carcinogenic, mutagenic or reproduction endangering substances], edition June 1997, last update October 1, 1997
- [12] MAK- und BAT-Werte [maximum workplace concentrations and biological tolerance values for occupationally handled substances and materials], Liste 1997 edited by the Deutsche Forschungsgemeinschaft, Mitteilung 33 der Senatskommission zur Prüfung gesundheitsschädlicher Arbeitsstoffe vom 1. Juli 1997
- [13] Registry of Toxic Effects of Chemical Substances (RTECS), edition January 1998, retrieved from the CHEM-BANK database, edition February 1998
- [14] Council Directive 79/117/EEC, Prohibition for the Placing on the Market of Plant Protection Products Containing Certain Active Substances, OJ No L33, 8.2. 1979, pg. 36
- [15] Council Directive 76/769/EEC, Restrictions on the Marketing and Use of Certain Dangerous Substances and Preparations, OJ No L262, 27.9. 1976
- [16] HSDB (CD-ROM) Hazardous Substances Data Bank, Program of the U.S. National Library of Medicine (1995)
- [17] ECDIN (CD-ROM) - Environmental Chemicals Data and Information Network (1992): Commission of the European Communities Environment Institute ISPRA, Italien
- [18] Aquire (Online-Datenbank): Chemical Information System, Oxford Molecular Group
- [19] Handbook of acute toxicity of chemicals to fish and aquatic invertebrates (1980): Johnson, WWE, Finley MT

- [20] Report R&D-Project No. 102 04 109 of the German Environmental Agency: "Anwendung eines Auswahlschemas zur Identifizierung gewässerrelevanter, gefährlicher Stoffe"
- [21] Ch. R. Worthing et al. (eds.) (1991): The Pesticide Manual, A World -Compendium, 9. Edition, published by BCPC, Unwin Brothers Ltd., Old Working Surrey
- [22] VCI-Existing Chemicals: Daten zur Beurteilung der Wirkung auf Mensch und Umwelt
- [23] UBA-Texte 44/94 (1994: Zielvorgaben für gefährliche Stoffe in Oberflächengewässern, i. A. des Bund/Länder-Arbeitskreises „Qualitätsziele,, (BLAK QZ), Umweltbundesamt, Berlin
- [24] UBA-Texte 52/94 (1994: Ableitung von Zielvorgaben zum Schutz oberirdischer Binnengewässer für die Schwermetalle Pb, Cd, Cr, Cu, Ni, Hg und Zn , i. A. des Bund/Länder-Arbeitskreises „Qualitätsziele,, (BLAK QZ), Umweltbundesamt, Berlin
- [25] Perkow, W. und H. Ploss (1996): Wirksubstanzen der Pflanzenschutz- und Schädlingsbekämpfungsmittel, Paul Parey Verlag, April 1996
- [26] Report R&D-Project No. 101 05 016 of the German Environmental Agency (UBA): Weiterentwicklung von Indikatorensystemen für die Umweltberichterstattung (1996)
- [27] BUA-Report: Beratergremium für umweltrelevante Altstoffe der Gesellschaft Deutscher Chemiker, Hirzel Verlag, Stuttgart
- [28] Schudoma, D. et al., 1994: Ableitung von Zielvorgaben zum Schutz oberirdischer Binnengewässer für die Schwermetalle Blei, Cadmium, Chrom, Kupfer, Nickel, Quecksilber und Zink. UBA-Texte 52/94, Umweltbundesamt, Berlin
- [29] G. Niebeck, Rijksinstituut voor Integraal Zoetwaterbeheer en Afvalwaterbehandeling RIZA, pers. communication: In December 1997, a working group proposed environmental quality criteria for air, water and soil in The Netherlands. They also prepared a table with background concentrations for metals in surface waters.
- [30] J. Mannio, Finnish Environment Institute, pers. communication: 10-percentile of Lapland lakes survey (J. Mannio et al., Sci. Total Environ. 160/161 (1995): 433-439) considered as present ambient background for Finland.
- [31] Proposal for a List of Priority Substances in the Context of the Draft Water Framework Directive. Fraunhofer Institut für Umweltchemie und Ökotoxikologie, Schmallenberg, Germany, 13<sup>th</sup> August 1998. The project was funded by the European Commission and by the German Umweltbundesamt. The report was finalized following the expert meeting on 2/3 July 1998.
- [32] Dr. habil. Steffen Uhlig, quo data Gesellschaft für Qualitätsmanagement und Statistik mbH, personal communication.
- [33] S. Uhlig, 1999: Assessment of options of the statistical treatment and evaluation of monitoring data within the COMMPS procedure. Final Report – Draft, 9 March 1999. Study contract: B4-3040/98/000784/MAR/E1
- [34] B.G. Hansen, A.G. van Haelst, K. van Leeuwen, P. van der Zandt, 1999: Priority Setting for Existing Chemicals: The European Union Risk Ranking Method. Environ. Toxicol. Chem. Vol 18, No 4 (scheduled for March 1999)
- [35] International Commission for the Protection of the Rhine, 1994: Rhine Action Programme. Data sheets for the quality objectives. German edition. Printed by RIZA, Lelystad, NL
- [36] Council Directive 86/278/EEC of 12 June 1986 on the protection of the environment, and in particular of the soil, when sewage sludge is used in agriculture. OJ No L 181 04.07.86 p.6
- [37] A.C. Baart, J.G. Boon, 1998: Scremotox - A screening model for comparative ecotoxicological risk assessment - North Sea. Prepared by WL-delft hydraulics for the Dutch Ministry of Housing, Spatial Planning and Environment, The Hague
- [38] A. Scheidleder et. al., 1999: Groundwater Quantity and Quality in Europe. Final Version 1999, in preparation. EEA, Copenhagen
- [39] Council Directive 76/464/EEC on pollution caused by certain dangerous substances discharged into the aquatic environment of the Community
- [40] The Merck Index. 10th edition. Rathway, New Jersey: Merck & Co., Inc., 1983

- [41] Kirk-Othmer, 1978: Encyclopedia of Chemical Technology. 3rd edition, Volumes 1-12. New York, John Wiley and Sons
- [42] A.G. Gilman et al. (eds.), 1985: Goodman and Gilman's, The pharmacological Basis of Therapeutics. 7th edition, New York: Macmillan Publishing Co.
- [43] US-EPA; Ambient Water Quality Criteria Doc.: Chlorine p. 12 (1981) EPA 440/3-78-005
- [44] J.D. Johnson, Water Chlorination: Envir. Impact and Health Effects 1: 37-63 (1978)
- [45] GEMS; Graphical Exposure Modelling System
- [46] CLOGP Data Base. Office of Toxic Substances, US-EPA
- [47] W.J. Lyman et al., 1982: Handbook of Chemical Property Estimation Methods. Environmental Behaviour of Organic Compounds. McGraw-Hill NY p. 4.1-4.33
- [48] Beratergremium für umweltrelevante Altstoffe (BUA) der Gesellschaft Deutscher Chemiker, 1993: BUA Report No. 130, Hirzel Verlag, Stuttgart
- [49] J. Vikesoe et al., 1998: Sources of phthalates and nonylphenols in municipal waste water, NERI report No. 225
- [50] Beratergremium für umweltrelevante Altstoffe (BUA) der Gesellschaft Deutscher Chemiker, 1992: BUA Report No. 90, Hirzel Verlag, Stuttgart
- [51] G. Rippen: Handbuch Umweltchemikalien, ecomed-Verlag, Landsberg, Loseblattsammlung
- [52] S.R. Hutchins et al., 1984. Water Res. 18, 1025-36
- [53] W.M. Meylan and P.H. Howard, 1995. J. Pharm. Sci. 84, 83-92
- [54] S.R. Hutchins et al., Appl. Environ. Microbiol. 48, 1039-45 (1984)
- [55] W.M. Meylan and P.H. Howard, 1991. Environ. Toxicol. Chem. 10, 1283-93
- [56] R.L. Swann et al., 1983. Res. Rev. 85, 23
- [57] Council Directive 98/8, Biocides Directive, OJ L 123, 24.April 1998, pg. 1



