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MonitoringBase Surfactants – A Database Specifically for Storage of Environmental Data on Surfactants in Europe

A database has been developed in MS Access™ for storage and retrieval of environmental data of surfactants in Europe, as well as general information on major surfactant monitoring programs. The database contains measured concentrations (about 2100 data points) for 8 surfactant groups collected from scientific literature and unpublished reports. The quality of the monitoring data was evaluated and scored using an approach similar to the Klimisch method for judging ecotoxicology and toxicology data. The assignments involve four "Klimisch"-like categories (reliable without restriction, reliable with restriction, not reliable, not assignable), and are based on six key features of a monitoring study, of which three features were found the most important. The proposed evaluation and scoring approach is widely applicable and can easily be applied for other environmental contaminants.

Key words: Database, surfactants, monitoring, quality scoring system, european environment

MonitoringBase Surfactants – Eine Spezialdatenbank zur Speicherung von Umweltdaten der Tenside in Europa. Es wurde eine MS Access™-Datenbank zur Speicherung und Abfrage der Umweltdaten von Tensiden in Europa sowie zur grundsätzlichen Information über die wichtigsten Kontrollprogramme für Tenside entwickelt. Die Datenbank enthält die Messbedingungen (ungefähr 2100 Daten) für acht Tensidgruppen, die aus der veröffentlichten Fachliteratur und nicht veröffentlichen Berichten entnommen wurden. Die Zuverlässigkeit der Kontrolldaten wurde evaluiert und mit einem Ansatz, der der Klimisch-Methode zur Beurteilung von ecotoxikologischen und toxikologischen Daten ähnlich ist, bewertet. In die Bestimmung wurden vier Klimisch-ähnliche Kategorien einbezogen (zuverlässig ohne Einschränkung, zuverlässig mit Einschränkung, nicht zuverlässig, nicht bestimmbar). Sie basieren auf sechs Grundmerkmalen einer Kontrollstudie, von denen drei als besonders wichtig eingestuft wurden. Das vorgeschlagene Evaluierungs- und Bewertungsverfahren ist vielfältig einsetzbar und kann einfach auf andere Umweltverunreinigungen angewendet werden.

Stichwörter: Datenbank, Tenside, Kontrolle, Qualitätsbewertungssystem, europäische Umwelt

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1 Introduction

Over the last 20–30 years, considerable resources have been spent by the European detergent industries (Association Internationale de la Savonnerie, de la Détergence et des Produits d'Entretien (AISE)) and the surfactants producers (Comité Européen des Agents de Surface et leurs Intermédiaires Organiques (CESIO)), as well as governments and other parties, on the monitoring of surfactants in the environment. A number of surfactants, together with some of their degradation products, have been measured in different environments, from sewage treatment plants (STP) to the marine environment, and in a range of matrices, such as influent, effluent, water, sediment, soil to biota [e.g. 1–4]. Yet, the source of such data can vary from scientific publications in open literature to internal company and industry sector group reports, which may be more difficult to access. The objective of the current study was to develop a database (MonitoringBase Surfactants) suitable for the storage and retrieval of a wide range of measured environmental data for surfactants. The database is intended to include environmental data of anionic, non-ionic, cationic and amphoteric surfactants in various European environmental samples (i.e. water, sediment, agricultural soil, biota, waste water and sludge) for the period 1970 to 2005. The information in the database could have various applications. Field data can be used to explore spatial distribution, or as input for the validation of environmental models (e.g. exposure models, food chain models, GREAT-ER), or for the risk assessment of detergent-based surfactants in environmental compartments. The data can also be used to identify which surfactants reside in certain environmental compartments, confirm previous areas of interest for certain Universities and Research Institutes.

An additional feature of the MonitoringBase Surfactants project was the development of a system for appraising the quality of data from surfactant monitoring studies that would be included in the database. The evaluation and scoring system used is inspired by the approach developed by Klimisch [5], based on four categories, and which is now widely used in the assessment of (eco)toxicological studies for regulatory purposes. In our approach the assignment of these categories is determined by certain key features of a monitoring study, of which three were considered to be the most important (i.e. sample storage and transportation, analytical detection, and performance of the method).

This paper describes the database, the quality evaluation and scoring system, and presents a brief summary of the measured data stored in MonitoringBase Surfactants.

2 MonitoringBase Surfactants development

MonitoringBase Surfactants was designed to help store and search for information on measured concentrations of surfactants in the European environment. The database contains general information on surfactant monitoring programmes in the European environment. It was, however, not made to be comprehensive and includes mainly the available data from major European monitoring programmes and industry reports.

MonitoringBase Surfactants contains data on a selected set of surfactants in effluents, influents, water, sediment and biota mainly determined in the European environment. The selection of compounds was made in collaboration with Environmental Risk Assessment and Management (ERASM) based on the production, use of surfactants and availability of data, and covers four key surfactant groups, i. e. anionics, non-ionics, cationics and amphoterics. For these groups, information on the programmes and measured concentrations of alcohol ethoxylates (AE), alcohol sulphates (AS), alkyl ether sulphates (AES), alkylphenol ethoxylates (APE), ditallowdimethylammonium chloride (DTDMAC), linear alkylbenzene sulphonates (LAS), nonylphenols (NP), octylphenols (OP) and soap (SOAP) were collected. No relevant information was found for betaines, and amine oxides.

Data on measured concentrations were retrieved from searches in Web of Science which contains references from peer-reviewed scientific journals dating back as far as 1899, but the search period for this study was restricted to 1970–2005. Several synonyms of the chemical names combined with the matrix of interest were used as search functions. Additionally, data from internal reports and external publications were received from ERASM and it's member companies. All publications and reports were reviewed and the quality of the data was scored for quality (see below), before uploading the data into the database. Information on the type of environment (i. e. fresh, marine, estuarine, terrestrial, STP), country and sea, sample location, matrix (i. e. water, sediment, sewage influent and effluent, sludge, soil, biota), date of sampling, sample type and number of samples (single, composite, pooled), measured concentration, general parameters (dry weight, lipid weight), quality scoring of the study, and references were stored. Each programme/study was accompanied with general information. Data on the programme title, organising country, type of study (monitoring, survey or laboratory study), status (planned, on-going or completed), start/end date of campaign, website, databank, contact details, if data were stored and a summary of the study were collected. Data from large monitoring programmes, which have their own databases, were not uploaded into MonitoringBase Surfactants as this would give only a single shot value of the database. Instead, links to the database were made by providing the url.

Technical aspects of the database: A user-friendly database was created in Microsoft Access 2000, which is compatible with the 2007 version as well. The database main menu offers two search options (Fig. 1). The first is a search for data on measured concentrations with search options on substance name, environment type, matrix, or country/sea. The second option is a search for information on European monitoring and survey programmes. In both search options the output is tabulated, and shows information on the project, environment type, location, substance, sample type, measured concentration, quality of the data, and reference (Fig 1). The tabulated data can be sorted on each parameter and copied to other programmes. More detailed information, such as start date, status, and contact details can also be retrieved. Finally, the retrieved data can also be exported to Word, Excel or printed showing all available information.

3 Evaluation of the quality of data

All studies were evaluated on the quality of sample collection, design of the study, sample storage and certain aspects of the analytical methodology. The quality scoring system used was based on the work of Klimisch [5] which describes an evaluation approach for the quality of experimental toxicological and ecotoxicological data. Four categories/codes of reliability are used: 1. Reliable without restriction, 2. Reliable with restriction, 3. Not reliable, and 4. Not assignable.

In appraising toxicological and ecotoxicological studies, any tests conducted and reported according to internationally accepted test guidelines (e. g. EU, EPA, FDA, OECD, ISO) and in compliance with the principle of Good Laboratory Practice (GLP) is normally given the highest grade of reliability (Klimisch – code 1, reliable without restriction). Studies in which the test parameters documented do not totally comply with the specific testing guidelines but are sufficient to accept the data or in which investigations are described which cannot be subsumed under a testing guideline, but are nevertheless well documented and scientifically acceptable are graded of lower reliability (Klimisch – code 2, reliable with restriction). Data from these two categories, which are submitted on behalf of industry (e. g. individual companies or consortia) are routinely accepted by regulators. Klimisch – code 3, not reliable – applies to studies, which for a number of reasons (e. g. unacceptable protocol, inappropriate test dosing, poor documentation, etc) are not sufficiently reliable enough to be accepted. The final code – 4, not assignable – is applied to studies or data from the literature, which do not give sufficient detail and cannot therefore be assigned to any of the previous categories.

A similar system was used for appraising the quality of data arising from surfactant monitoring studies that were loaded into MonitoringBase Surfactants. However, monitoring studies do not have any accepted test guidelines, nor are generated to GLP standards, so it is necessary to develop a different set of selection criteria that will still allow them to be rated as Klimisch codes 1–4. In order to assign a monitoring study to one of the Klimisch codes, the main features of a successful monitoring study have been identified in Table 1. Six key features of a monitoring study have been identified which cover:

1. design and overall quality of the study
2. sample collection
3. sample storage, transportation and receipt
4. sample preparation
5. analytical detection
6. performance of the method

There are, however, three essential features in any monitoring study that need to be confirmed before any study can be considered to be "reliable", i. e. achieve Klimisch criteria 1 and 2. Those are key features 3, 5 and 6. In key feature 3 it is important to be able to confirm that the test substance has not degraded during the period between sampling and the start of sample preparation in the laboratory (e. g. by analysis of spiked field samples, by incorporation of suitable stabilising agent, from previous test data that confirms the stability of the material over a period of time, or based on a minimal time between sampling and analysis). An important aspect of key feature 5 is that the analytical method is sufficiently sensitive and specific enough to measure the test substance of interest to the required limit of determination required for the monitoring study objectives and that there is minimal interference from other constituents in the sample.

The last important key feature, number 6, is the recovery of the test substance through the analytical method which should be sufficiently high (> 70 %) and repeatable to give confidence that the monitoring data are valid (e. g. by analysis of spiked samples (i. e. recovery samples) through the analytical method).

A number of detailed criteria for evaluating each key feature are also included in Table 1 to assist in the evaluation of the quality of the monitoring study. These criteria may not necessarily applied in every case to the particular study under evaluation. For example, under "Sample storage, transportation and receipt", the use of an appropriate stabilizing agent may not be required for an analyte that is stable under the actual field conditions, or where there is analysis of samples directly in or close to the field operation. The evaluator must study the information and make a qualified judgment as to whether each key feature has been satisfactorily addressed in the monitoring study. Obviously, the more details that are

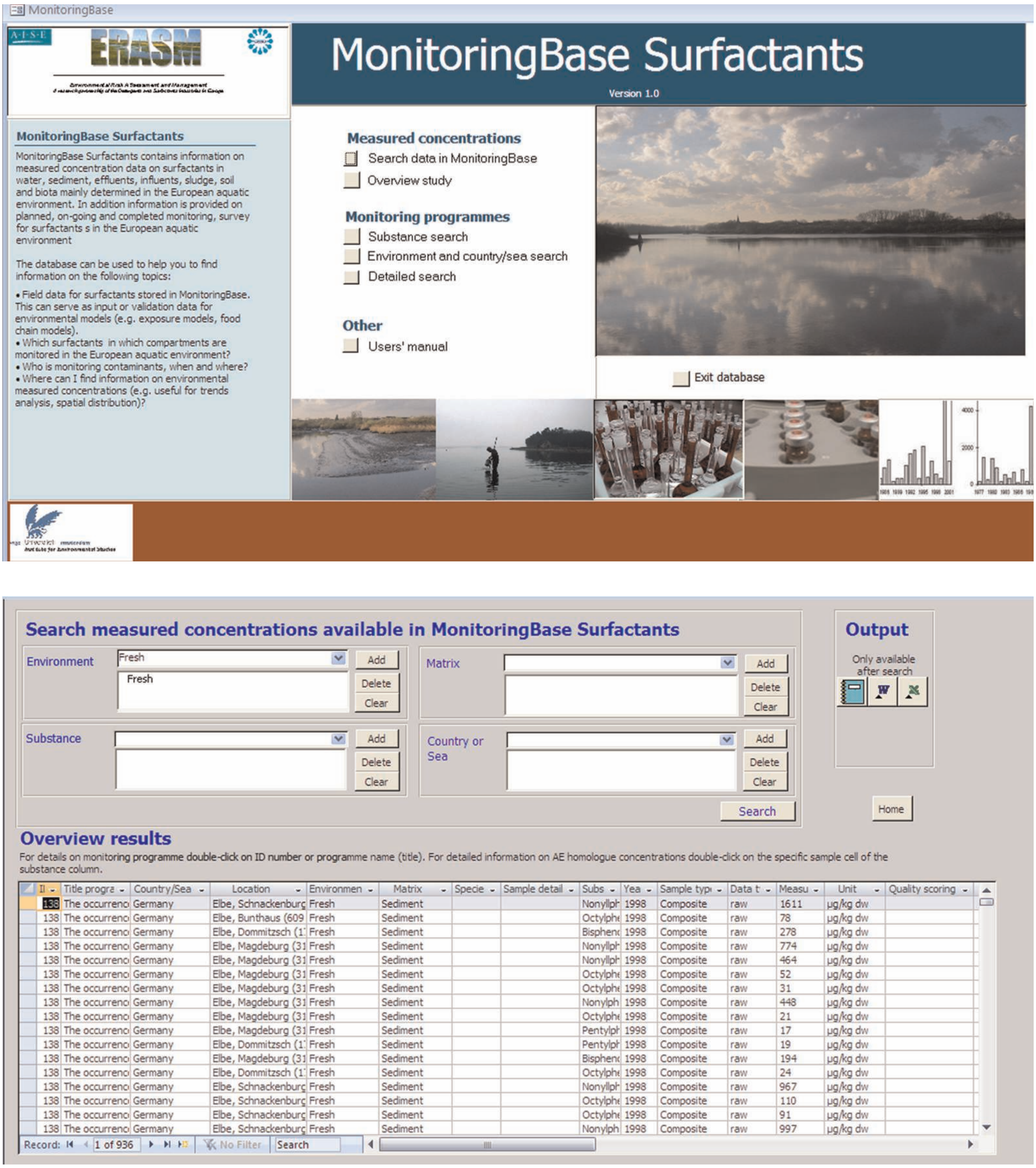

Figure 1 Opening screen of MonitoringBase Surfactants (above) and tabulated output (below) of a search

documented in the monitoring study, the easier it will be to evaluate whether the key features have been covered and thereby decide on the quality of the monitoring study.

After the key features have been satisfactorily evaluated in the monitoring study, it is then possible to assign the quality of the monitoring study and its data to the standard Klimisch codes (1–4) using the scoring system shown in Table 2. The details of the scoring and subsequent assignment of a monitoring study are summarized:

1. Any study must have the three essential key features (i.e. 3, 5 and 6) confirmed before it can be considered to be "reliable", i.e. Klimisch codes 1 and 2. If any of these key features is not sufficiently addressed then the study is assigned Klimisch code 3 (not reliable).

2. A monitoring study that has covered at least five and preferably six of these key features would be assigned to Klimisch code 1 – reliable without restriction. The essential features (key features 3, 5 and 6) would all be covered as well as 2 or 3 of the desirable features (1, 2 and 4).

3. A monitoring study that has only covered three or four of these key features would be assigned to Klimisch code 2 – reliable with restriction. The essential features (key features 3, 5 and 6) would all be covered as well as possibly one of the desirable features (1, 2 and 4), each weighing equal.

4 Measured surfactant concentrations

The database contains information from 36 studies, and includes more than 2100 measured concentrations for 8 surfactant groups. An overview of the stored data is shown in Table 3. The largest dataset was found for LAS (n = 647), followed by alkylphenol ethoxylates (n = 468), and nonylphenols (n = 373). Most data are reported for the fresh water environment (n = 936) and STP (n = 559), and less for the mar-

No	Feature	Further criteria for evaluating whether a key feature has been properly covered in the monitoring study
1.	Design and overall quality of study	**Desirable** to show that sufficient forethought has gone into the design of the monitoring study as well as data collection and retention. Includes: • Protocol with clearly defined objectives of the study, accurate locations for sampling (e.g. GIS coordinates), sampling/storage details and a validated analytical methodology to be applied to samples. • Raw data are archived and could be accessed by authorized person to check on the accuracy of data and calculations, if required. • Study has been carried out by an experienced group of workers with monitoring expertise. • Study has been audited internally (within company or group) and/or externally (Journal review).
2.	Sample collection	**Desirable** to collect samples of suitable volume and to minimise the possibility of contamination. Additional samples (blank/spiked) will enable further checks to be made in the laboratory, if needed. Includes: • Use of appropriate containers for the study/analyte of interest. • Method of sampling and type of sample to be taken (composite or grab sample) is detailed. • Inclusion of "blank" and "spiked field" samples. • Care is taken to minimise the possibility of contamination. during sampling (e.g. prewashing of sample containers) • Sufficient sample is taken for analysis requirements and to avoid any sub-sampling.
3.	Sample storage, transportation and receipt	**Essential** to prove that the test substance has not degraded during the period between sampling and the start of sample preparation in the laboratory. Includes: • Previous information on the stability of the analyte(s) of interest. • Use of appropriate stabilising agent to minimise sample deterioration. • Storage conditions in field/lab at suitable temperature to minimise sample deterioration. • Check on efficiency of preservation made (e.g. by analysis of "spiked field" samples at laboratory). • Details of shipment and receipt ("chain of custody") are provided where appropriate.
4.	Sample preparation	**Desirable** to minimise interference from other compounds in the analysis and thereby achieve a sufficiently low limit of determination for the analyte of interest. Includes: • Validated method for isolation of analyte of interest. • Isolation removes compounds likely to interfer in method. • Isolation achieves low limit of determination required.
5.	Analytical detection	**Essential** that the analytical method is sufficiently sensitive and specific enough to measure the test substance of interest, without interference and to the required limit of determination. Includes: • Published/industry accepted and validated analytical method has been employed. • Preferably specific method (e.g. GC/MS, LC/MS). Non-specific methods can give rise to an overestimation of the level of the surfactant of interest due to the presence of structurally similar substances. • Allows quantification of all analytes of interest. • Little or no interference observed in the region of interest, confirmed by analysis of reagent blanks and field blanks. • Sufficiently low limit of determination with details of such parameters (e.g. LoD, LoQ, MDL).
6.	Performance of the method	**Essential** that there is satisfactory recovery of the test substance to give confidence that the monitoring data are valid. Includes: • A set of recoveries for the analytes of interest have been carried out at different spiking levels to cover the likely monitoring concentrations. • Recovery data are $>$70% and with acceptable standard deviation. • Appropriate external standard has been used for recovery. • Internal standard, if appropriate, has been used in method.

Table 1 Six key features of a satisfactory monitoring study of surfactants

ine (n = 251), estuarine (n = 298) and terrestrial (n = 126) environments. For the fresh water environment measured concentrations are mainly reported for water (n = 650) and sediment (n = 301) and some data for pore water (n = 36). For biota, data (n = 26) on nonylphenols (NP), octylphenols (OP) and alkylphenol ethoxylates (APEs) in fresh water and estuary fish are available; data on other surfactants were not found. The dataset on the APE degradation products (NP and OP) is not comprehensive as this was outside the scope of the surfactant database, but was taken from a previous effort (MonitoringBase, www.cefic-lri.org).

The database can be used to provide information on the surfactant profile in the fresh water European environment. The profile of surfactants in fresh waters is dominated by LAS (median 15 µg/L), followed by AS (median 1.7 µg/L), and AES (median 1.0 µg/L), as shown in Fig. 2. Both the nonylphenol ethoxylate (NPE) and octylphenol ethoxylate (OPE) median concentrations are much lower, 0.035 and 0.001 µg/L, respectively. Interestingly, the concentration range (95 % confidence intervals) for most surfactants are limited to one order of magnitude. This indicates that the variation in surfactant concentrations between European countries (Germany, United Kingdom, The Netherlands, Italy, Spain) is relatively small. For NP and OP, the degradation products of NPE and OPE, the median concentrations are 0.25 and 0.001 µg/L, respectively, which indicate that the NP concentrations are approximately one order of magnitude higher than the parent compound (NPE).

In European fresh water sediment (Germany, United Kingdom, The Netherlands, Italy) the surfactant profile is

Klimisch criteria	Score against the 6 key features of a satisfactory monitoring study	Examples of such studies
1 – reliable without restriction	5–6	LAS, AE and AS/AES monitoring studies carried out by ERASM and SDA (now ACI) as part of risk assessment exercises. Other monitoring studies carried out by national authorities (e.g. UK DoE or water authorities). Such studies include most, if not all, of the key aspects of a monitoring study (see Table 1). **Such studies address, as a minimum, the 3 essential key features of a monitoring study (see Table 1)**
2 – reliable with restriction	3–4	Includes studies or data from the literature or reports in which certain features of the study have been overlooked or not completely covered (e.g. lack of detailed protocol, recovery studies carried out at only one concentration). However, despite this, the study has sufficient features covered well for an assessor to consider the data to be scientifically acceptable. **Such studies address, as a minimum, the 3 essential key features of a monitoring study (see Table 1)**
3 – not reliable	0–2	Obvious and unacceptable problems associated with the study. **For example, one or more of the 3 essential aspects of a monitoring study have not been sufficiently covered such that there are serious doubts about the accuracy of the actual results.**
4 – not assignable	Insufficient details provided to rate the quality of the study.	This includes studies or data from the literature, which do not give sufficient experimental details and which are only listed in short abstracts or secondary literature (books, reviews).

Table 2 Assignment of monitoring studies to the standard Klimisch categories (1–4)

Surfactant	Nr of studies	Measured data	Environment	Matrix	Reference
Alcohol ethoxylates (AE)	11	148	STP, marine	Effluent, influent, sludge sediment	[4, 6–13, 27, 28]
Alcohol sulphates (AS)	6	84	STP, fresh	Effluent, influent, water, sediment	[2, 4, 7, 13–15]
Alkyl ether sulphates (AES)	4	100	STP, fresh	Effluent, influent, water, sediment	[2, 4, 7, 13, 14, 15, 16, 29]
Alkylphenol ethoxylates (APE)	4	588	Estuarine, marine, fresh	Water, sediment, biota	[3, 29–31]
Ditallowdimethylammonium cation (DTDMAC)	1	10	Marine	Sediment	[28]
Linear alkyl benzene sulphonates (LAS)	21	647	STP, fresh, estuarine, marine, terrestrial	Effluent, influent, sludge, water, sediment, soil	[1, 2, 3, 4, 7, 13, 15, 16, 18–26, 28, 32–34]
Linear alkyl benzenes (LAB)	1	27	STP, terrestrial	Influent, sludge, soil	[19]
Nonylphenols (NP)	5	373	Estuarine, marine, fresh	Water, sediment, biota	[3, 29–31, 35]
Octylphenols (OP)	3	78	Estuarine, Marine, fresh	Water, sediment, biota	[29–31]
SOAP	3	58	STP	Influent, effluent	[4, 7, 13]

Table 3 Overview of studies and measured concentrations

limited to LAS, NPE, OPE NP and OP (Fig 3). The concentration difference between LAS and NPE is within one order of magnitude (median concentrations 3 250 and 969 µg/kg dry weight, respectively). On the contrary, the concentration of LAS in the water phase was about 400 times higher than NPE.

One of the most studied environmental compartments for surfactants are STPs. A high percentage of studies (23/36 = 64 %) examined the occurrence and fate of surfactants in sewage treatment plants [1, 2, 4, 6–26]. The concentrations of European STP influents and effluents for AE, AES, APE, AS, LAS, NP and OP are shown in Fig. 4. The highest levels are found in influents for SOAP (median 28 mg/L) and the lowest for AS (median 0.5 mg/L). Obviously, levels in effluent are much lower; three orders of magnitude for AE and AES, and two orders of magnitude for AS, LAS and SOAP. This suggests that AE and AES are somewhat more efficiently removed than AS, LAS and SOAP. The general picture is in agreement with detailed studies that determined the removal of surfactants in STPs, showing generally high removal of surfactants in the sewage treatment process.

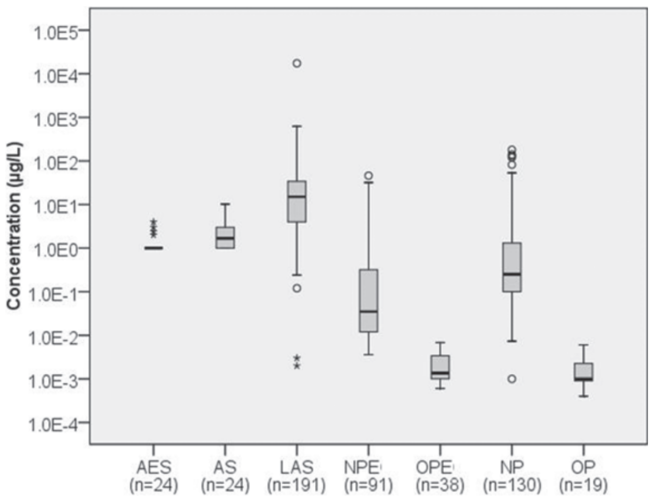

Figure 2 Box-Whisker plot of water concentrations (µg/L) of alkyl ether sulphates (AES), alcohol sulphates (AS), linear alkyl benzene sulphonates (LAS), nonylphenol ethoxylates (NPE), octylphenol ethoxylates (OPE), nonylphenols (NP), and octylphenols (OP) determined in European fresh water systems. Indicated are the median, quartiles, outlier (o) and extreme (*) values based on a designated number (n) of data points for each surfactant

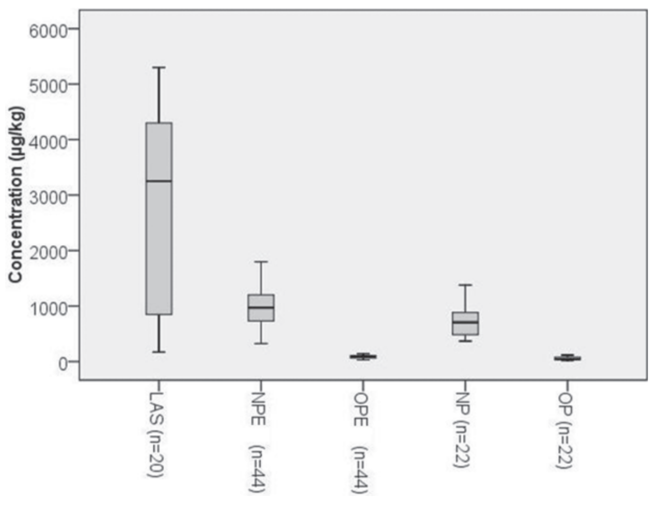

Figure 3 Box-Whisker plot of sediment concentrations (µg/kg) of linear alkylbenzene sulphonates (LAS), nonylphenol ethoxylates (NPE), octylphenol ethoxylates (OPE), nonylphenols (NP), and octylphenols (OP) in European fresh water systems. Indicated are the median and quartiles

5 Conclusions

The main conclusions are:

- A database was developed to store and retrieve measured environmental data for 8 groups of surfactants in Europe found in scientific publications and grey literature (reports).
- An evaluation and scoring approach was developed based on six key features to judge the quality of the monitoring data. This approach is widely applicable and can easily be applied to other environmental contaminants.
- The broad picture that emerges of surfactant removal in STPs, and the resulting concentrations in different matrices such as water and sediments, is in line with the current understanding of their environmental fate, and the values used in risk assessment models.

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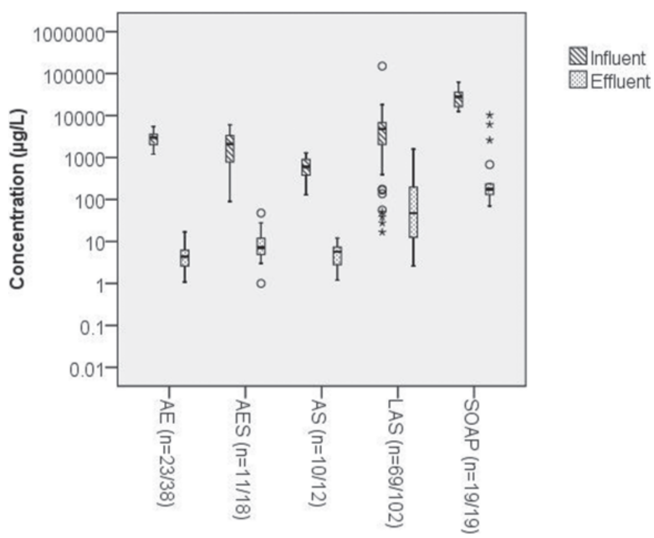

Figure 4 Box-Whisker plot of concentrations (µg/L) of alcohol ethoxylates (AE), alkyl ether sulphates (AES), alcohol sulphates (AS), linear alkyl benzene sulphonates (LAS), and soap (SOAP) determined in influents and effluents of European sewage treatment plants (Germany, United Kingdom, The Netherlands, Italy, Spain). Indicated are the median, quartiles, outlier (o) and extreme (*) values based on a designated number of data points for each surfactant (n = influent/effluent)

Ordering a copy of the database: *MonitoringBase Surfactants is available upon written request from the ERASM secretariat (www.erasm.org).*

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