



Towards the review of the European Union Water Framework Directive: Recommendations for more efficient assessment and management of chemical contamination in European surface water resources



Werner Brack^{a,b,*}, Valeria Dulio^c, Marlene Ågerstrand^d, Ian Allan^e, Rolf Altenburger^{a,b}, Markus Brinkmann^b, Dirk Bunke^f, Robert M. Burgess^g, Ian Cousins^d, Beate I. Escher^{a,h}, Félix J. Hernándezⁱ, L. Mark Hewitt^j, Klára Hilscherová^k, Juliane Hollender^l, Henner Hollert^b, Robert Kase^m, Bernd Klauer^a, Claudia Lindim^d, David López Herráez^a, Cécil Miègeⁿ, John Munthe^o, Simon O'Toole^p, Leo Posthuma^{q,r}, Heinz Rüdell^s, Ralf B. Schäfer^t, Manfred Sengl^u, Foppe Smedes^k, Dik van de Meent^v, Paul J. van den Brink^{w,x}, Jos van Gils^y, Annemarie P. van Wezel^{z,aa}, A. Dick Vethaak^{y,ab}, Etienne Vermeirssen^l, Peter C. von der Ohe^{ac}, Branislav Vrana^k

^a Helmholtz Centre for Environmental Research UFZ, Leipzig, Germany

^b RWTH Aachen University, Aachen, Germany

^c Institut National de l'Environnement Industriel et des Risques INERIS, Verneuil-en-Halatte, France

^d ACES - Department of Environmental Science and Analytical Chemistry, Stockholm University, Stockholm, Sweden

^e Norwegian Institute for Water Research (NIVA), Oslo, Norway

^f Oeko-Institut e.V. - Institute for Applied Ecology, Freiburg, Germany

^g U.S. Environmental Protection Agency, ORD, NHEERL, Atlantic Ecology Division, Narragansett, RI, USA

^h Eberhard Karls University of Tübingen, Tübingen, Germany

ⁱ Jaume I University, Castellón, Spain

^j Aquatic Ecosystem Protection Research Division, Environment Canada, Burlington, Ontario, Canada

^k Masaryk University, Research Centre for Toxic Compounds in the Environment (RECETOX), Brno, Czech Republic

^l EAWAG, Swiss Federal Institute of Aquatic Science and Technology, Dübendorf, Switzerland

^m Swiss Centre for Applied Ecotoxicology, Eawag-EPFL, Dübendorf, Switzerland

ⁿ IRSTEA – UR MALY, Villeurbanne Cedex, France

^o IVL Swedish Environmental Research Institute, Gothenburg, Sweden

^p Environmental Protection Agency, Dublin, Ireland

^q National Institute for Public Health and the Environment RIVM, Bilthoven, The Netherlands

^r Department of Environmental Science, Institute for Water and Wetland Research, Radboud University Nijmegen, The Netherlands

^s Fraunhofer Inst Mol Biol & Appl Ecol IME, Aberg 1, D-57392 Schmallenberg, Germany

^t University Koblenz-Landau, Landau, Germany

^u Bavarian Environmental Agency, D-86179 Augsburg, Germany

^v MERMAYDE, Groet, The Netherlands

^w Alterra, Wageningen University and Research Centre, P.O. Box 47, 6700 AA Wageningen, The Netherlands

^x Department of Aquatic Ecology and Water Quality Management, Wageningen University and Research Centre, P.O. Box 47, 6700 AA Wageningen, The Netherlands

^y Deltares, Delft, The Netherlands

^z KWR Watercycle Research Institute, Nieuwegein, The Netherlands

^{aa} Copernicus Institute, Utrecht University, Utrecht, The Netherlands

^{ab} VU University Amsterdam, Institute for Environmental Studies, Amsterdam, The Netherlands

^{ac} Amalex Environmental Solutions, Leipzig, Germany

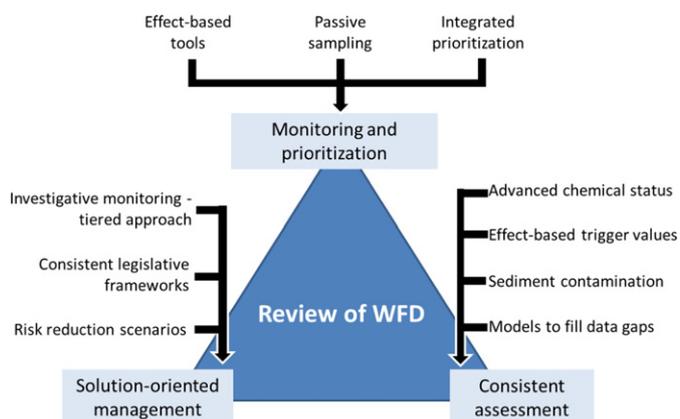
* Corresponding author at: Helmholtz Centre for Environmental Research UFZ, Leipzig, Germany.

E-mail address: werner.brack@ufz.de (W. Brack).

HIGHLIGHTS

- Improve monitoring and strengthen comprehensive prioritization of toxic pollutants
- Foster consistent assessment of water pollution
- Support solution-oriented management of chemicals in the water cycle

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:

Received 16 August 2016

Received in revised form 14 October 2016

Accepted 15 October 2016

Available online 28 October 2016

Editor: D. Barcelo

ABSTRACT

Water is a vital resource for natural ecosystems and human life, and assuring a high quality of water and protecting it from chemical contamination is a major societal goal in the European Union. The Water Framework Directive (WFD) and its daughter directives are the major body of legislation for the protection and sustainable use of European freshwater resources. The practical implementation of the WFD with regard to chemical pollution has faced some challenges. In support of the upcoming WFD review in 2019 the research project SOLUTIONS and the European monitoring network NORMAN has analyzed these challenges, evaluated the state-of-the-art of the science and suggested possible solutions. We give 10 recommendations to improve monitoring and to strengthen comprehensive prioritization, to foster consistent assessment and to support solution-oriented management of surface waters. The integration of effect-based tools, the application of passive sampling for bioaccumulative chemicals and an integrated strategy for prioritization of contaminants, accounting for knowledge gaps, are seen as important approaches to advance monitoring. Including all relevant chemical contaminants in more holistic “chemical status” assessment, using effect-based trigger values to address priority mixtures of chemicals, to better consider historical burdens accumulated in sediments and to use models to fill data gaps are recommended for a consistent assessment of contamination. Solution-oriented management should apply a tiered approach in investigative monitoring to identify toxicity drivers, strengthen consistent legislative frameworks and apply solutions-oriented approaches that explore risk reduction scenarios before and along with risk assessment.

© 2016 Published by Elsevier B.V.

1. Introduction

Water is a vital resource for natural ecosystems and human life, and therefore, as stated by the European Union (EU) Water Framework Directive, a “heritage which must be protected, defended and treated as such” (European Union, 2000). Especially freshwater is limited in quantity and in quality, and currently under a variety of increasing pressures; for example, climate change, overexploitation and contamination from point and diffuse sources, including agriculture, industry and households. Ensuring a high quality of water and a high level of protection from chemical contamination is fully in line with the major societal goals presented by the 7th Environmental Action Plan of the EU “Living well within the limits of our planet” (European Union, 2013a). Consistent with this, the earth’s capacity to assimilate chemical pollution has been proposed as one of the nine planetary or regional boundaries in relation to which anthropogenic impact needs to be reduced if unacceptable global or regional change is to be avoided (Rockström et al., 2009a; Rockström et al., 2009b; Steffen et al., 2015).

Threats to clean water (and other environmental compartments) have resulted in a number of regulations around the globe aiming to reduce the production and use of the most hazardous chemicals.

Nevertheless, despite significant achievements, toxic pollution still poses a substantial risk to almost half of the water bodies recently monitored in Europe (Malaj et al., 2014). Such risk assessment results are corroborated by diagnostic eco-epidemiological impact studies, in which changes in biodiversity associate with mixture exposures (Posthuma et al., 2016; Posthuma et al., 2016), but, due to lack of knowledge, current regulation of environmental quality is mostly based on a limited number of single chemicals. Consequently, and in agreement with the concepts of ecological, energy, carbon, and water footprints (Fang et al., 2014), the concept of a chemical footprint has been advanced to enable exploration of mixture threats for water systems. The chemical footprint has been defined as “a quantitative measure describing the environmental space needed to dilute net chemical pollution – commonly by a mixture – due to human activities to a level below a specified boundary condition” (Zijp et al., 2014). It is, however, very challenging to identify and quantify boundaries for chemical pollution either at local or global scales (Diamond et al., 2015) given the very large number of chemicals present in the environment, the wide-ranging sensitivity of natural species, and the vulnerability of ecosystems (Posthuma et al., 2014).

At present, man-made products containing >100,000 chemicals are registered in the EU, where 30,000 to 70,000 are in daily use (Loos et

al., 2009) (from a chemical universe of about 10^{60} unique compounds of molecular weight below 500 Da (Dobson, 2004)). A large (but unknown) fraction of those can be expected to find their way into the environment and water systems together with considerable numbers of environmental transformation products and manufacture by-products occurring in complex mixtures. It has recently been shown by the European Union's Joint Research Centre that Environmental Quality Standard (EQS) values are not sufficiently protective against mixture effects (Carvalho et al., 2014). The authors of this study identify “an urgent need to revise tools and paradigms used to assess the safety of chemicals” and stress the need for a mixture-oriented approach to setting water quality standards.

Safeguarding a non-toxic environment (European Union, 2013a) and protecting biodiversity and vital ecosystem functions and services (Reyjol et al., 2014) by minimizing exposure to mixtures of toxic substances and thus chemical footprints therefore remains a key challenge for European water policy including the Water Framework Directive (European Union, 2000) (WFD). This challenge translates into numerous requests to researchers from decision-makers and practitioners in the European Union, international river basin commissions, environmental and chemical agencies and water and wastewater utilities and their associations for information to support appropriate action. Specific challenges at the European scale include the identification, assessment and management of the most risky compounds and mixtures and the prediction of trends in compounds expected due to societal-change processes, such as increased population size and ageing. At the local scale, site-specific mixtures of unknown but complex composition, in some cases cause notable problems for the integrity of ecosystems, and for the production of drinking water, challenging water managers to identify and handle the risk drivers. The needs addressed by stakeholders thus range from methods for the proper diagnosis of current threats (e.g., the request for scientifically-sound and cost-efficient monitoring tools) to methods for the identification and prediction of future threats via modeling. Responses to meet these challenges should represent approaches supporting risk assessment at different scales, especially taking into account chemical mixture effects, scenarios for the prediction of upcoming risks, and the evaluation of abatement options, as well as encouraging enhanced consistency among different regulations.

The Water Framework Directive (European Union, 2000) and its daughter directives, the 2008/105/EC Environmental Quality Standards Directive (EQSD; European Union, 2008b), amended by the 2013/39/EU Directive, which contains the latest amendment of the list of priority substances (PS; European Union, 2013b), and the Groundwater Directive 2006/118/EC (GWD; European Union, 2006) amended by Directive 2014/80/EU (European Union, 2014a) are the main pieces of legislation for the protection and sustainable use of European freshwater resources. In addition, chemical-oriented regulations are in place to evaluate potential threats from man-made chemicals, so as to limit or stop emissions of the most hazardous ones. The water legislation has triggered extensive monitoring activities in all European Member States and, among other achievements, prescribes and supports the establishment of River Basin Management Plans for all EU river basins, which should lead to meeting the goals of good chemical- and ecological status. The WFD follows the receptor-oriented management principle and focuses on an assessment of biological, hydro-morphological, chemical and physico-chemical quality elements in all European river basins, acknowledging that ecological and human health impacts are multiple-stress responses. The WFD encompasses a holistic ‘response’ principle of “Good Ecological Status” assessment complemented by separate assessment of the Chemical Status. The latter is based on selected PS considered as EU-wide relevant contaminants for which compliance with Environmental Quality Standards (EQS) needs to be checked and ensured by all Member States. Discharges, emissions, and losses of priority substances should be progressively reduced and, in case of selected Priority Hazardous Substances phased out completely (European Union, 2013b) within 20 years. In addition to that, a watch list mechanism has

recently been established (Article 8b of the EQS Directive 2008/105/EC) (European Union, 2013b) for pollutants, including emerging pollutants, for which the available monitoring information today is considered insufficient. The 1st EU Watch List was published in 2015 (European Union, 2015a), in order to collect high quality monitoring data at European Union-wide level to support future chemical prioritization initiatives (European Union, 2013b). Currently, the operation of a voluntary Watch List for emerging pollutants in groundwater is under discussion between European Union Member States and the Commission, in accordance with revised Groundwater Directive.

The practical implementation of the WFD with regard to pollution by (toxic) chemicals has faced several challenges; however, at the same time it has also stimulated international collaborative initiatives and new research activities in the search for more effective and cost-efficient tools. The Common Implementation Strategy (CIS) (European Union, 2003a; European Union, 2015b) for the WFD was agreed upon by the Water Directors of the EU Member States in 2001 as a framework to address the challenges posed by the directive in a co-operative way at the EU level. In the scientific field, novel research activities led to funding of the large EU Collaborative Project SOLUTIONS (Brack et al., 2015) and to the various activities of the European monitoring network NORMAN (www.norman-network.net). The mission of those research efforts is to improve the evidence base for policy making and in particular, the identification, assessment and prioritization of emerging pollutants (Von der Ohe et al., 2011), with direct practical outcomes, such as the identification of River Basin Specific Pollutants (RBSPs), such as for Slovakia (Slobodnik et al., 2012) or the national watch list in France (Botta et al., 2012).

SOLUTIONS and NORMAN have identified several present-day challenges for monitoring, prioritizing, assessing, and managing risks posed by chemicals, which are presented herewith targeting the upcoming WFD review in 2019 (European Union, 2015b). These challenges are suggested to be addressed during the WFD review and updating processes. In this context, the aims of this paper are:

1. To analyze current challenges in water quality management in Europe, focusing on risks and impacts of chemicals and their mixtures;
2. To evaluate the state-of-the-art of the science and practices relevant to those challenges;
3. To suggest possible solutions to those challenges; and
4. To contribute to the regulatory review processes that are in place improving our water quality assessment and management approaches.

The present paper consists of ten chapters on problems and recommendations bundled in three overarching sections. This set is not meant to be exhaustive and various other subjects require attention. However, this approach represents the top-ten recommendations as discussed and agreed upon at two workshops at the General Assemblies of the NORMAN network and the FP7 Collaborative Project SOLUTIONS (Brack et al., 2015).

2. Approach

Based on the experience of the authors, we evaluated whether there exist fundamental, strategic and technical challenges regarding the practical implementation of the WFD. On the basis of this evaluation, we selected ten key problems that need special consideration in order to improve monitoring, strengthen comprehensive prioritization, foster consistent assessment, and support solution-oriented management. We assessed the identified problems, reflected upon our current status of knowledge and formulated recommendations accordingly. In the following section, a number of general and specific recommendations (Table 1) in support of the review process of the WFD are discussed. Note that the recommendations can be linked, by their cause, their background science, or their recommended actions. They are not arranged according to priority.

Table 1
Ten problems and recommendations for improving the success of WFD implementation.

No	Problem	Recommendation
Improve monitoring and strengthen comprehensive prioritization		
1	Absence of toxic stress cannot be monitored on a per-chemical basis due to large number of chemicals and mixtures.	Integrate effect-based tools into monitoring of water quality.
2	Concentrations and EQS for many hydrophobic chemicals in water are very low and evaluation of exceedance in water is hampered by insufficient analytical procedures and focus on whole water samples (although a move to monitoring such chemicals in biota has been made).	Apply passive sampling for improved compliance check of hydrophobic, bioaccumulative chemicals, with EQS and for temporally representative monitoring of polar substances.
3	Monitoring and assessment tends to emphasize well known and regulated chemicals and to overlook emerging compounds (although watch-list monitoring is helping to change the emphasis).	Use an integrated strategy for prioritization of chemical contaminants, taking knowledge gaps into account.
Foster consistent assessment		
4	Different groups of chemicals are addressed in two independent assessments (chemical status and status of River-Basin Specific Pollutants) hampering integrated evaluation. The use of only two quality classes (good and not good) neglects improvements and hampers prioritization of effective control measures.	Consider all relevant chemicals (priority substances and River Basin Specific Pollutants) and use a graded system to assess the chemical status of water bodies.
5	Effect-based monitoring and assessment is hampered by a lack of trigger values.	Define and use effect-based trigger values to address priority mixtures of contaminants.
6	Quality goals of WFD are frequently missed due to historical burdens of persistent organic pollutants (POPs) and metals in sediments.	Consider the toxicity and mobility of historical contaminants accumulated in sediments.
7	Incoherent and insufficient monitoring often leads to ignorance of relevant chemicals and peak concentrations resulting in unrecognized risks.	Consider exposure, effect and risk modeling as a tool to fill gaps in monitoring data and create incentives to extend the monitoring basis of chemical contamination across Europe.
Support solution-oriented management		
8	Strategies to identify causes of exceedance of effect-based trigger values and establish cause-effect relationships are missing.	Use a tiered approach of solution-oriented investigative monitoring including effect-directed analysis to identify toxicity drivers and abatement options.
9	Chemicals with the potential to affect water quality are covered by different regulatory instruments resulting in a lack of consistency.	Improve links across environmental-, chemical- and product-specific legislative frameworks and harmonize chemical legislation among Member States
10	There is often a mismatch between assessment outcomes and their usefulness for management.	Apply solutions-oriented approaches that explore risk reduction scenarios before and along with risk assessment.

3. Recommendations

3.1. Improve monitoring and strengthen comprehensive prioritization

The monitoring of ecological and chemical status is the basis for the management of water quality in European water bodies. Despite substantial efforts in many Member States to provide meaningful monitoring data for a comprehensive and harmonized assessment, the current methodologies still need significant improvement in order to be environmentally safe, efficient and scientifically sound. In their report on the “Ecological and chemical status and pressures in European waters” the European Environmental Agency (EEA) states: “The chemical

quality of water bodies has improved significantly in the last 30 years, but the situation as regards the priority substances introduced by the WFD is not clear. The assessment of chemical status presents a large proportion of water bodies with unknown status. Monitoring is clearly insufficient and inadequate in many Member States, where not all priority substances are monitored and the number of water bodies being monitored is very limited” (Solheim et al., 2012). Thus, significant improvement is required, which might include a paradigm shift towards a more effect-based and solution-oriented monitoring.

3.1.1. Recommendation 1: integrate effect-based tools (EBTs) into monitoring of water quality

3.1.1.1. Problem. The almost infinite number of stressor-receptor combinations (>100,000 compounds and their mixtures affecting numerous species in diverse water systems) may appear overwhelming with no solution in sight, whatever option for a chemical-by-chemical approach might be used or designed. The scale of the problem requires a novel, alternative perspective. A more holistic approach is required to address chemical pollution in the environment as a whole, using integrative parameters to capture and address possible effects.

3.1.1.2. Current status. Effect-based tools (EBTs) such as bioassays and biomarkers are integrative techniques for response assessment that allow a diagnosis of the degree of impact by toxic chemicals. EBTs detect cumulative effects, of general or specific kinds. In general, EBTs are particularly useful to contribute to bridging the gap between chemical contamination and ecological status, since they can cover a broad range of exposure histories and toxicity mechanisms in diverse organisms, and account for the additional risks posed by non-studied compounds and mixtures. In other words, the combined effects of mixtures of compounds (identified or not) are considered. Bioassays already provide the regulatory reference to derive environmental quality standards (EQS; European Union, 2011b) under the WFD and to evaluate Predicted No-Effect Concentrations (PNECs) under the REACH registration and other legislative chemical authorization processes (European Chemicals Agency, 2014). They are also applied to assess whole effluents from domestic wastewater treatment plants and different industrial sectors (Commission, 2007; Gartiser et al., 2009). Some tests are already recommended in the Best Available Techniques (BAT) reference documents (BREFs) under Industrial Emissions Directive (IED) (e.g. Manufacture of Organic Fine Chemicals, Common Waste Water and Waste Gas Treatment/Management Systems in the Chemical Sector). Indeed, bioassays integration in regulatory water quality monitoring is recommended (Hecker and Hollert, 2011; Wernersson et al., 2015) and supported by the fact that many of these methods are published as harmonized standard protocols, such as OECD guidelines and ISO standards (European Union, 2014b). In vitro and in vivo bioassays and biomarkers, supported by associated background documents and assessment criteria, have been successfully applied over the past few decades in monitoring programs by OSPAR (Oslo-Paris Commission) and other regional conventions for the marine and estuarine environment (Thain et al., 2008; Vethaak et al., in press). More recently, the International Council for Exploration of the Sea (ICES) and OSPAR have developed an integrated indicator framework and methodology for hazardous substances and their effects, which can provide a suitable approach for assessments of Good Environmental Status (GES) for Descriptor 8 of the Marine Strategy Framework Directive (MSFD) (European Union, 2008a) across European marine regions. The framework comprises a core set of biological tests that can be used in an integrated manner together with chemical contaminant measurements in biota, sediments and water across OSPAR maritime areas. It further comprises an assessment framework that integrates contaminant and biological effects monitoring data and that allows assessments to be made across matrices, sites, and regions (Vethaak et al., in press).

In the United States, the Clean Water Act authorizes the use of EBTs to quantify the occurrence of toxicity as a measure of the presence of chemicals. Recently, Ekman et al. published an example of the use of EBTs for monitoring the surface waters of the Great Lakes in North America as part of restoration initiative for that natural resource (Ekman et al., 2013).

However, there are still open questions that prevent application of effect-based tools for monitoring of water bodies. A major issue – for tests that are not in routine use – is whether sufficient inter-laboratory reproducibility can be achieved when evaluating the effects of representative aquatic pollutants and chemical mixtures. Particularly, the evaluation of the hazards of emerging contaminants, such as pharmaceuticals and personal care- and disinfection-by products, is a current priority in regulatory water quality monitoring (Brack et al., 2012; Loos et al., 2009).

A recent inter-laboratory study (ILS; Di Paolo et al., 2016) within the NORMAN network verified that a battery of bioassays, conducted in 11 different laboratories following their own protocols, produces comparable results when applied to the evaluation of blinded samples consisting of a water extract spiked with emerging pollutants as single chemicals or mixtures. Moreover, this ILS successfully demonstrated that a battery of bioassays is able to determine with high consistency and precision the aquatic toxicity of selected emerging pollutants in water extracts and identify mechanism-specific effects such as nuclear receptor-mediated responses. Such ILS activities represent an important step towards the implementation of bioanalytical monitoring tools in water quality assessment.

3.1.1.3. Recommendation. We recommend to adopt EBT as a key approach to addressing chemical (mixtures) interactions with aquatic organisms, thereby overcoming the poorly justified implicit assumption of ‘not known, not risky’ as happens in the current assessment regime. There is an urgent need to investigate and define a minimum and a higher tiered bioassay battery for the evaluation of water samples within the WFD. The applicability of such a battery of bioassays for diagnostic environmental risk assessment was discussed within a NORMAN Expert Group meeting in 2010 (Hamers et al., 2013). A toxicity profile was defined as a toxicological “fingerprint” of a sample, ranging from a pure compound to a complex mixture, obtained by testing the sample or its extract for its activity towards a battery of biological endpoints. The expert group concluded that toxicity profiling is an effective first tier tool for screening the integrated hazard of complex environmental mixtures with known and unknown toxicologically active constituents. In addition, toxicity profiles can be used for prioritization of sampling locations, for identification of hot spots, and – in combination with effect-directed analysis (EDA) or toxicity identification and evaluation (TIE) approaches – for establishing cause-effect relationships by identifying emerging pollutants responsible for the observed toxic potency. Both in the SOLUTIONS project and in the NORMAN network there are ongoing efforts to define such batteries. In the Netherlands, similar developments have recently resulted in the proposal for an operational bioassay test battery, including criteria to interpret the results of the set of bioassays (Van der Oost and Suarez Munoz, 2016). However, if this novel approach is to be implemented, several steps for consensus building need to be tackled, as explained in the following outlook.

3.1.1.4. Outlook. Technical progress on EBTs has been substantial so far, and based on the activities of the NORMAN network, the Joint Danube Survey 3, and the SOLUTIONS project, tailor-made batteries of bioassays with options for higher tiered investigations will be suggested within the coming months. A helpful conceptual basis for composing such batteries is the adverse outcome pathway concept (Ankley et al., 2010) linking molecular initiating events and key events at molecular/(sub)-cellular levels to adverse outcomes in organisms and populations. Many available fast-response EBTs focus on important molecular initiating events (MIEs), key events or can integrate several MIEs (Altenburger

et al., 2015). Measurable responses of these effect-based tools indicate potential for effects on higher levels of biological complexity.

For a progressive operational application of EBTs in the WFD, we further suggest: 1) For endpoints for which the applicability of standardized bioassays and trigger values has already been demonstrated (Kase, 2016), *in vitro/in vivo* bioassays should be integrated in the WFD as screening tools to identify polluted water bodies (response above trigger values, see also Recommendation 5). These tools are (commercially) available and ready to use; 2) for less developed assays efforts are required for standardization of operating protocols, quality assurance/quality control procedures and data analysis methods. Researchers and users are working on a consensus on the criteria to judge the relevance and performance of each test for the different application fields; 3) An EU-wide discussion should be organized in order to reach consensus among experts and regulators about a purpose-tailored battery of bioassays and associated trigger values covering a range of toxic modes-of-action; 4) Since in the case of bioanalytical screening methods the result is expressed as Bioanalytical Equivalents (BEQ), guidance is needed on how to derive and use BEQ in addition to single substance concentrations resulting from chemical measurements. Experience with the application of this approach is already available in the food sector with the publication of Commission Regulation EU No 589/2014 of 2 June 2014 (European Union, 2014c). Here screening methods (which may comprise bioanalytical methods) are used to select those samples with levels of polychlorinated dibenzo-*p*-dioxins and furans and dioxin-like PCBs that exceed the maximum levels or the action levels (trigger values). These examples can serve as a model for implementation of these approaches in environmental monitoring. 5) Guidance for and harmonization of adequate enrichment techniques for the application of EBTs largely maintaining the original mixture composition in water such as large volume solid phase extraction (Brack et al., 2016) is required.

3.1.2. Recommendation 2: apply passive sampling together with monitoring of biota tissues for improved compliance check of hydrophobic, bioaccumulative substances with EQS and temporally-representative monitoring of polar substances

3.1.2.1. Problem. The evaluation of water EQS exceedance according to the WFD is typically based on the analysis of whole water samples and on the assessment of average concentrations in water bodies, using low frequency (e.g. monthly) spot sampling. However, it shall be mentioned that for 11 priority substances also EQS for biota are given (European Union, 2013b) and a move to monitoring these chemicals in biota has been made. Whole water sample concentrations of hydrophobic chemicals allow for only limited conclusions on exposure of, and risks to, aquatic organisms and thus hinder understanding of relationships between contamination and ecological status. Moreover, the large temporal variability in pollutant concentrations complicates the derivation of temporally-representative concentrations for assessment of the quality of water bodies, when using low frequency spot sampling.

3.1.2.2. Current status. Monitoring data reported by EU Member States and used in the prioritization process from 2008 to 2011 often lacked essential contextual information (i.e. metadata) and 72% of the data were below the limit of quantification (LOQ) (Heiss and Küster, 2015). Detection limits for several priority substances do not meet the minimum requirements on measurement uncertainty (<50% at concentration equal to EQS) and on the LOQ minimum performance criterion (i.e. $LOQ < 1/3 EQS$ (European Union, 2009a; Loos, 2012)). Water EQS values of many hydrophobic chemicals, including PBT (persistent, bioaccumulative and toxic) substances, are often beyond the capability of current analytical techniques. At the same time, the monitoring of hydrophobic substances in “whole water” samples for EQS compliance has

been questioned. Although this approach is in line with the precautionary principle for substances that strongly sorb to dissolved and particulate organic matter (DOM and POM), it severely hampers conclusions on effects and risks (Vignati et al., 2009). In agreement with the equilibrium partitioning theory (Di Toro et al., 1991), it has been demonstrated that bioaccumulation and toxicity of hydrophobic organic compounds are related to the freely dissolved concentration and chemical activity rather than total concentration (Reichenberg and Mayer, 2006). The natural variation in DOM and POM content makes whole water a highly temporally-variable mixture of matrices. Consequently, the PBT fraction partitioned to DOM and POM may lead to highly variable concentrations of hydrophobic substances in whole water, while the freely dissolved concentration and associated effects may remain constant (Traina et al., 1996). For PBT compounds, the EQS directive (European Union, 2013b) recently set EQS values as concentrations in biota. This approach allows for a better assessment of chemical exposure and associated toxicity to aquatic organisms than the analysis of whole water. This is not only because of higher (and thus better quantifiable) concentrations, but also because levels measured in organisms reflect the chemical activity in the environment in which they live. However, chemical monitoring in biota does not allow for a simple calculation of emission limits for pollutants (as was intended when using whole water analysis). Moreover, many new problems have appeared that are associated with the inherent variability of sampled biota and the fact that absence of a particular substance in biota does not automatically mean it is absent in the environment (i.e. metabolized substances). The latter has been considered in Directive 2013/39/EU for PAHs, which are recommended for monitoring in crustaceans and molluscs rather than in fish (European Union, 2013b). Partitioning passive sampling was developed three decades ago as an alternative approach to monitor hydrophobic organic pollutants in water in a time-integrated manner (Huckins et al., 1993), and is a well-established and cost-efficient method for the enrichment of hydrophobic organic pollutants from water samples that aids the detection and quantification of these chemicals at trace concentrations (Booij et al., 2016; Miège et al., 2015; Vrana et al., 2016).

Another aspect to be improved in the current EQS compliance checking regime is how representative water concentrations of polar substances are temporally. Environmental concentrations of polar substances often vary significantly in time. Rigidly-set low (e.g. monthly) sampling frequencies are unlikely to be suitable to provide representative information on pollutant concentrations. Various types and configurations of passive samplers exist today for hydrophilic compounds. In contrast to partitioning passive samplers for hydrophobic chemicals, passive samplers for polar substances are based on adsorbents. Although the conversion of chemical uptake by adsorption passive samplers to aqueous concentrations is still associated with larger uncertainty, estimates of time-weighted average substance concentrations via integrative passive sampling will improve temporal representativeness of monitoring in water bodies with highly variable concentrations (Miège et al., 2015).

3.1.2.3. Recommendation. We recommend combining biotic (organism tissues) and abiotic (passive sampling) measurements of hydrophobic substances for assessing their levels in aquatic environments thereby reducing the uncertainty in using biota or whole water samples for water quality assessment. Passive sampling is a powerful tool to complement and in many cases replace monitoring of PBT compounds in water and biota samples. It will also help to reduce/minimize the number of organisms to be sampled. Partitioning passive sampling is designed to provide estimates of freely dissolved concentrations (Vrana et al., 2005) which have been shown to be in many cases most appropriate to explain exposure and adverse effects in biota. Moreover, it allows direct comparison of measured water concentrations with concentrations in diverse compartments (water, sediment, biota), based on the assessment of chemical activity (Mayer et al., 2003) in those matrices.

The fact that passive sampling is a time-integrating technique in combination with the application of a sampling matrix (polymers) with well-defined and constant properties, makes it possible to achieve a lower inherent variability of exposure information compared to traditional grab sampling of whole water, sediment or biota, and thus is suitable for assessment of pollutant trends in water bodies. This approach will also help to identify compartments acting as a contaminant source or sink in the aquatic system (Lohmann et al., 2004) and thus inform management about the most effective control measures (e.g. do we need to remove contaminated sediments or do we have to address current wastewater effluents to reduce exposure of aquatic organisms to hydrophobic toxicants?). Finally, adsorptive passive sampling is recommended as it yields data that are more representative of the aqueous contamination in cases where the variability of a substance concentration in water is higher than the uncertainty associated with passive sampling (Poulier et al., 2014). While passive sampling together with chemical target analysis is readily available, directly linking passive sampling with EBTs is under debate since due to compound-specific uptake rates and partitioning coefficients the mixture in the sampler does not resemble the mixture in water (Brack et al., 2016).

3.1.2.4. Outlook. Considering the passive sampling of hydrophobic chemicals as a proxy for accumulation in a hypothetical organism without toxicokinetics, we believe that scientifically sound procedures can be derived for the conversion of passive sampling measurements to quality assessment criteria (EQS) on the basis of freely dissolved concentrations. If the emphasis is not on water quality but on the quantification of pollutant emissions or discharges, it should be recognized that transport of hydrophobic chemicals can be dominated by the particulate phases, not captured by passive sampling. Possible transport of hydrophobic chemicals can be assessed by additionally sampling the suspended matter or estimated by using the suspended matter concentration.

3.1.3. Recommendation 3: use an integrated strategy for the prioritization of chemical contaminants, taking knowledge gaps into account

3.1.3.1. Problem. Despite clear indications that the actual chemical stress in European water bodies is not adequately characterized by the assessment of the existing PS against EQS values (Moschet et al., 2014) alone, the prioritization, monitoring, and assessment under the WFD still tend to emphasize on regulated, well-known substances (Sobek et al., 2016), while emerging substances are not adequately addressed (Heiss and Küster, 2015). Given the number of chemicals produced, traded and used, we consider only a tiny percentage in our risk assessments. Often, a lack of information, such as sufficient data on the effects of a compound or on its environmental concentrations, may exclude compounds from current prioritization procedures (Dulio and Slobodnik, 2015). The current process means that the majority of compounds is excluded from the assessment, without any evidence of 'no harm'. As an example, during the last review of the list of priority pollutants, about 50% of the candidate substances were discarded because of a lack of data (Institut National de l'Environnement Industriel et des Risques, International Office for Water, 2009).

3.1.3.2. Current status. The present EQS Directive does not require the generation of any new data to feed into the prioritization process, apart from the data gathered through the watch list mechanism, but relies on the availability of data provided voluntarily by third parties (Heiss and Küster, 2015). Although the watch list mechanism now allows for a promising new procedure to identify and confirm relevant substances at the EU level, this procedure may be too slow and is not sufficiently integrated into a global prioritization scheme. Recently, the strengths and challenges of different prioritization strategies for emerging pollutants in Europe have been discussed in detail (Brack,

2015; Dulio and Slobodnik, 2015; Faust and Backhaus, 2015; Heiss and Küster, 2015). One of the most advanced prioritization schemes may be the categorization/prioritization approach suggested and demonstrated by the NORMAN network (Fig. 1, Dulio and von der Ohe, 2013).

It is based on data on the occurrence of chemicals and on predicted no-effect concentrations (PNECs derived from experimental data, QSAR or read-across predictions), and classifies chemicals into 6 categories depending on the information available, before starting the ranking exercise (Dulio and Slobodnik, 2015). These categories define the need for action, including: (1) priority regular monitoring; (2) watch list monitoring; (3) extension of the (eco)toxicological data set; (4) improvement of analytical methods; (5) extension of both monitoring and (eco)toxicological data and, finally; (6) classification of compounds as non-priority for regular monitoring due to estimated low risks. In many cases (eco)toxicological data are missing (Cat. 3 and 5). New databases such as the on-line ToxCAST dashboard (<https://actor.epa.gov/dashboard/#Chemicals>) may help to address this problem, allowing access to all the very recent results published for at least 9076 chemicals already tested under about 1192 biological assays (with all the QA/QC background and EC50 results). This strategy is currently used to screen, prioritize and review the US EPA Chemical Contaminant Lists before selecting the ones that have to be regulated. An example of a similar prioritization method has been implemented in Canada with its Chemicals Management Plan (CMP) (Government of Canada, 2014). The CMP was created to prioritize substances on the Canadian Domestic Substances List (DSL) published in 2006. In this prioritization study 4300 chemicals were designated subject to a risk assessment – these are referred to as ‘existing substances’. Approximately 500 of these have been assessed as persistent, bioaccumulative and toxic. Any substance not on the DSL is designated as a “new substance” and its import and manufacture are prohibited in Canada without prior notification; about 450 new substances notifications are received annually. Under the CMP, resources have been dedicated to research and monitoring, including biomonitoring, to provide essential information about the level of exposure to these

chemicals and their effects on human health and the environment. These data provide the basis for developing public health and environmental health policies and interventions, as well as for measuring the efficacy of control measures (Government of Canada, 2014).

3.1.3.3. Recommendation. A key objective for the prioritization of substances and for monitoring programs should be to minimize the risk of overlooking chemicals that might pose significant threats to ecosystems and environmental health. This may be achieved by prioritization of individual chemicals on a broader basis compared to currently used schemes. One of the main advantages of the NORMAN prioritization method is that it accounts for substances which otherwise would be excluded due to lack of data. The missing information on emerging substances that are prioritized in this way can then be tackled systematically as part of an integrated action-based prioritization process. It is well recognized that it is not possible to measure all chemical compounds present in the environment one-by-one. For this reason, extensive and Europe-wide coordinated efforts by national and regional authorities on non-target chemical screening is needed to extend the range of chemicals known to be present in the aquatic environment and thus build an information basis for prioritization based on environmental occurrence of compounds. New analytical tools are available today. For example, the complementary use of GC-QTOF MS and LC-QTOF MS allows a comprehensive screening of compounds of very different polarity and volatility (Hernández et al., 2015) and is a powerful approach for water analysis at present.

3.1.3.4. Outlook. Enhanced efforts will be required to integrate suspect and non-target screening approaches into the prioritization process and to establish open access databases and multivariate analysis of environmentally detected chemical patterns and toxicity profiles. Prioritization results based on environmentally-observed concentrations may further be enhanced by modeling, and verification (and vice versa). The integrated prioritization process will support the identification of

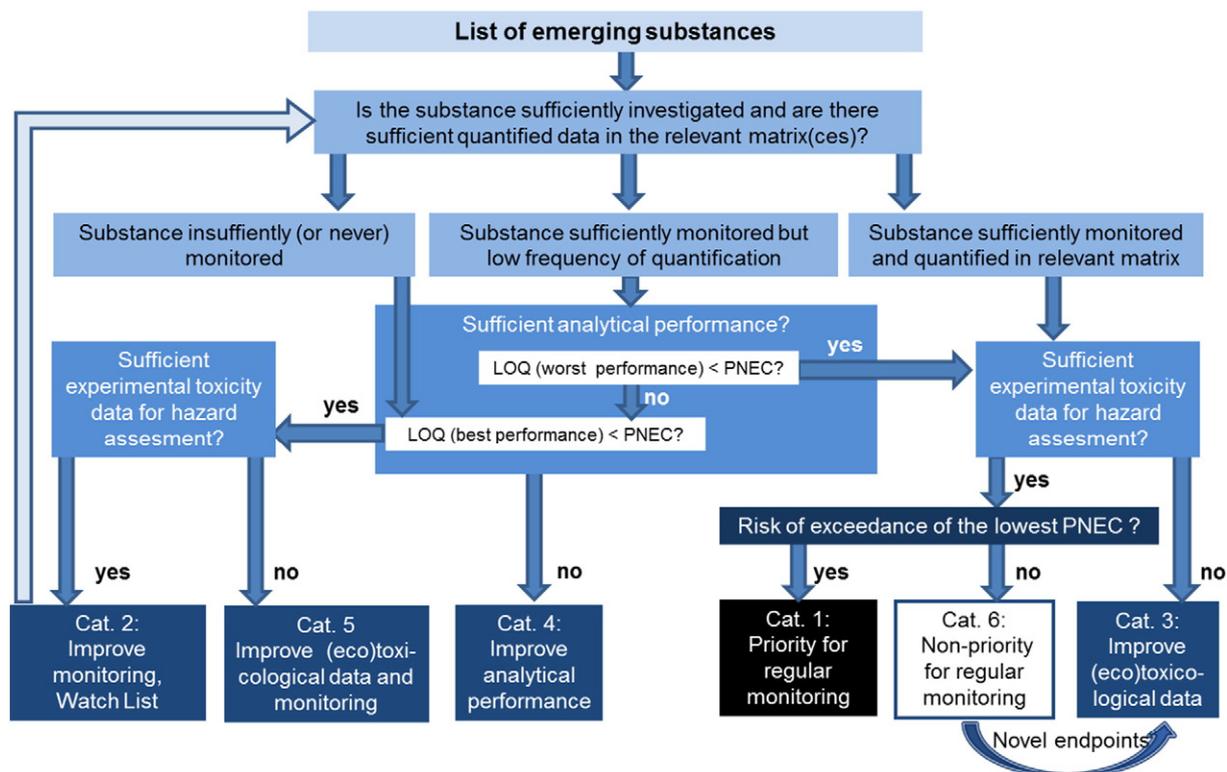


Fig. 1. Categorization/prioritization scheme suggested by NORMAN network (Dulio and von der Ohe, 2013).

frequently occurring chemicals and (e.g. source-related) mixtures that are to be considered. Altogether, a systematic link between the identification of emerging substances and a continuous prioritization process has to be organized. In this way the effort could focus on those compounds of current highest concern for human- and ecological impacts, and define measures to effectively reduce net chemical impacts.

3.2. Foster consistent assessment. The implementation of WFD triggered Europe-wide monitoring activity and yielded of an enormous amount of data of different quality. Recommendations on how to further improve data quality have been made above. Consistent, integrated and efficient assessment of these data is crucial to understand the degree to which chemical contaminants are responsible for the deterioration of aquatic ecosystems and to support solutions for efficient abatement. This may require the implementation of novel assessment approaches (e.g. for integrated assessment of chemical and effect-based monitoring data).

3.2.1. Recommendation 4: consider all relevant chemicals (PS and RBSP) and use a graded system to assess the chemical status of water bodies

3.2.1.1. Problem. So far, chemical pollution is addressed in two separate status assessments that do not have a clear relationship to each other: chemical status covers a few selected chemicals of Europe-wide concern (i.e. priority substances), while the so-called River Basin Specific Pollutants (RBSP) are considered as part of the ecological status. The current procedure makes an integrated assessment of chemical contamination difficult if not impossible.

3.2.1.2. Current status. Although it is recognized that the intention behind the WFD priority substances is to define a list of substances for which EU-wide measures should be applied by all Member States to reduce and/or phase-out their emissions in the aquatic environment, this limited list of substances seems arbitrary to describe the ‘chemical status’ – generally perceived as an integrative measure of chemical pollution – and inadequate for decision-making as the ‘chemical status’ and the ‘ecological status’ are dealt with by the WFD as two separate assessments (von der Ohe et al., 2009). A common assessment and sound interpretation of the data is further hampered by the fact that the sampling sites and periods used for the monitoring of chemical and biological quality elements are often not the same (Malaj et al., 2014). Moreover, the ecological status is described in five status classes (i.e. high, good, moderate, poor and bad), while the chemical status distinguishes only between two classes (i.e. water bodies achieving a “good” status and water bodies “failing to achieve good” status). Finally, the ecological status is mainly described in terms of general degradation with no information about the causes of the observed deterioration. Such metrics integrate effects from very different stressors, such as chemical pollution, hydromorphological degradation, eutrophication, and others. This makes it very difficult for water managers to specifically address relevant stress factors such as chemical contamination in their selection of risk mitigation measures. In other words, the diagnosis of the real impact of chemical mixtures is not organized in a single conceptual framework, in which clear associations could be identified between emission sources and net effects for all chemicals and their mixtures.

3.2.1.3. Recommendation. We recommend making both PS and RBSPs subject to a “chemical status” assessment. This will also account for cumulative effects and enable chemical pollution to be presented in one single sum parameter, and help to pinpoint those compounds that contribute most to the overall risk. In a first tier, the sum of the MEC/EQS ratios (Measured Environmental Concentrations/Environmental Quality Standards, a summation risk quotient, $RQ_{MEC/EQS}$) of all chemicals can be used to distinguish among sites potentially impacted by chemicals and those that most likely are not (Backhaus and Faust, 2012), providing

a full rank order when applied to a large set of studied sites. If this $RQ_{MEC/EQS}$ is above 1, then more sophisticated mixture toxicity models could be used to quantify overall ecotoxic pressure and expected local impacts in terms of predicted species loss, and to pinpoint the chemicals or the group of chemicals (considering their modes of action and targets) responsible for the identified risk (De Zwart and Posthuma, 2005; Posthuma and de Zwart, 2012; Posthuma et al., 2016). SOLUTIONS is providing a substantial basis to underpin, understand and apply these approaches, based on validated models (Altenburger et al., 2015; Brack et al., 2015). Moreover, we recommend a shift away from the current “good status/poor status” evaluation approach to a graded system for the evaluation of chemical status, considering the degree of exceedance of a given mixture risk threshold (e.g. $RQ > 10$; $RQ > 100$, etc.) or the quantitative value of the mixture toxic pressure proxy. In the former case, the risk of chemical pollution could thus be represented in five classes, by applying the same concept used for representation of the ecological status. The RQ equal to 1 could be defined as the border between good (i.e. below 1) and moderate (above 1) status. Anchoring the RQ or, in the case of single substances, the EQS value, at the border between good and moderate status allows the less than moderate status (i.e. poor and bad) and the better than good status (i.e. high) to be defined simply as exceedances or undercut ratios, using for example, order of magnitude steps to define expected magnitude-of-impact classes. This approach fits well with the observed temporal health status of aquatic communities (Schäfer et al., 2011; Von der Ohe et al., 2011), when considering that chemical concentrations in ambient media usually cover several orders of magnitude (Busch et al., 2016).

3.2.1.4. Outlook. Expanding on the idea of developing and using quantitative, comprehensive metrics for mixture risks, we propose that the ecological status analysis might also be improved by inclusion of stressor-specific metrics which are currently under development. Past applications of the SPEAR index (von der Ohe and Goedkoop, 2013) have shown to be promising, though other studies have questioned the stressor-specificity and its domain of application needs further scrutiny (i.e. independence from stream types and sizes). Overall, weight-of-evidence approaches that consider all site-specific information may be required to get to a realistic evaluation of the contribution of various stressors present, e.g. chemical and hydro-morphological degradation, after a less than good status has been determined using a general metrics. The introduction of a “Trophic and Hydro-morphological Status” in five classes, similar to the ecological status, might take account of the contribution of other major drivers of deterioration in a multiple stressed environment. The EU project MARS (Hering et al., 2015) is currently improving such indicators. These will enable integration of different stressors into a consistent classification system for assessing the status of aquatic systems in multiple-stressed environment that can be applied across different European water bodies. This approach is well in line with the findings of so-called Eco-epidemiological analyses of surface waters, in which monitoring data are used to diagnose magnitudes of ecological impacts as well as probable local causes. Application of such methods also provides quantitative insights into the relevance of causes of impacts (de Zwart et al., 2006; Kapo et al., 2014). Recently, the State of California in the U.S. adopted a framework for assessing sediment quality data combining benthic community metrics, sediment toxicity data, and empirical sediment quality guidelines to categorize coastal sediments into categories ranging from *unimpacted* to *clearly impacted* (Bay and Weisberg, 2012).

3.2.2. Recommendation 5: define and use effect-based trigger values to address priority mixtures of contaminants

3.2.2.1. Problem. The increasing awareness that chemicals cannot be tackled only as individual compounds but have to be assessed as components of mixtures of typically tens of thousands of known and

unknown substances, has triggered the development of EBTs, which we recommend to implement (see [Recommendation 2](#)). Thanks to the use of EBTs it is possible to address complex mixtures of only partially known and unknown composition, but in order to allow the implementation of biological-effect tests in the regulatory framework it is crucial to define common criteria for the interpretation of the results of these tests, i.e. effect-based trigger values for mode-of-action- (MoA)-specific and source-related priority mixtures as requested by the European Union ([European Union, 2012a](#)).

3.2.2.2. Current status. Effect-based trigger values can be used to aid the interpretation of effect-based monitoring data in combination with chemical measurement data and to differentiate between more or less polluted samples and tolerable and intolerable risks. They can be used as a tool to rank water bodies with regard to distance-to-target WFD 'good status'. Numerical values for non-specific cytotoxicity ([Tang et al., 2013](#)), oxidative stress response ([Escher et al., 2013](#)), photosynthesis inhibition ([Tang and Escher, 2014](#)), and a number of endocrine endpoints ([Escher et al., 2015](#)) were derived for Australian recycled water and the principles that guided the establishment of these values could also apply to the European situation. Advanced operational proposals are available for several MoAs, including endocrine disruption and photosynthesis inhibition ([Kienle et al., 2015](#)). Promising approaches have been outlined for drinking water contaminants, which might be adapted to surface water ([Brand et al., 2013](#); [Escher et al., 2015](#)).

3.2.2.3. Recommendation. The most straightforward way of defining effect-based trigger values for specifically-acting toxicants is the translation of available EQS for individual chemicals (with the same MoA) into bioanalytical equivalent concentrations (BEQs) measured with bioassays ([Escher et al., 2015](#)) in line with an approach regulating dioxin-like compounds in food commodities ([European Union, 2014c](#)). Further research efforts are required to develop effect-based trigger values also for apical endpoints.

3.2.2.4. Outlook. Exploring future options of implementing EBTs with their trigger values, it is to be expected first that MoA-specific priority mixtures of chemicals can be addressed by specific in vitro assays (e.g. estrogenicity), which means that they provide a more comprehensive information basis for regulatory bodies to evaluate a chemical pressure. Current results of a recent European estrogen monitoring project initiated in 2014 as a result of activities of the WFD CIS sub-group on Chemical Monitoring and Emerging Pollutants (CMEP) and closely linked to the 'Chemicals' Working Group of DG Environment ([Kase, 2016](#)) indicate for receptor-mediated estrogenicity that the application of an effect-based trigger value of 0.4 ng/L (corresponding to the EQS value proposed by the Commission for 17 β -estradiol) allow sites polluted by wastewater to be distinguished from non-polluted sites. These findings are in agreement with recently published results on effect-based screening of endocrine active pharmaceuticals ([Kunz et al., 2015](#)) and other receptor-activating substances. For surface- and wastewater assessments the trigger value approach is a useful tool to differentiate between more and less polluted samples.

For source-related priority mixtures of predominantly non-specifically acting chemicals, integrative (non-specific) bioassays are the only currently available approach to monitor contamination in an (eco)toxicologically relevant way. They are valuable tools to obtain an integrated measure of the toxic burden of complex mixtures of chemicals associated with wastewater, particularly if only a minor fraction of the biological response can be explained by chemicals analyzed in the sample ([Neale et al., 2015](#)). This approach may involve benchmarks ([Escher et al., 2014](#)) and trigger values ([Escher et al., 2013](#)) for in vitro assays (e.g. for cytotoxicity or oxidative stress) as well as for in vivo assays for apical endpoints (e.g. algae, *daphnia* and fish embryos) related to WFD Biological Quality Elements (BQEs). Triggers that

effectively utilize critical effect sizes for adult fish health and benthic community structure are part of Canadian monitoring programs below mining and pulp mill discharges ([Munkittrick et al., 2009](#)) and have been designed to address the effects of point source discharges of complex mixtures.

3.2.3. Recommendation 6: consider the toxicity and mobility of chemicals accumulated in sediments

3.2.3.1. Problem. Although, currently, contaminated sediments prevent achievement of the quality goals of the WFD (exceeding biota-EQS) to reach a "good chemical status" because of a number of legacy substances such as mercury, PCDD/Fs and dioxin-like PCBs ([Förstner et al., 2016](#)), there are still no scientifically sound and legally binding quality standards for sediments available that consider bioavailability as a key to risk assessment.

3.2.3.2. Current status. So far, legally binding Europe-wide EQS values exist only for the «surface water» and «biota» matrices. While the Member States are obliged to perform trend monitoring for those priority substances that tend to accumulate in sediment and/or biota, they may decide at their own discretion whether to include river basin-specific sediment EQS values in their River Basin Management Plans. Although all Member States must take measures to ensure that concentrations of priority substances in sediment and/or biota do not significantly increase ([European Union, 2013b](#)), there are no harmonized European-wide quality goals for the «sediment» matrix. Due to the great complexity of the interrelationship between concentrations in water, sediment and biota, defining meaningful common sediment EQS values is challenging. Quantitative Europe-wide correlations between EQS values for biota and EQS values for sediments are currently thought by many stakeholders to be impossible as a result of the great differences in, e.g., biogeochemistry, particle size distribution, and transport frequency of sediments in different catchment areas ([WFD Navigation Task Group, 2011](#)). A recent cooperation project between the German Federal Institute of Hydrology and RWTH Aachen University (DioRAMA; [Eichbaum et al., 2013](#)) has identified the rapidly desorbing or bioavailable fraction of sediment-borne dioxin-like contaminants as the central determinant of biological effects in exposed fish. These assessments have been performed thanks to the generation of novel experimental datasets ([Brinkmann et al., 2015](#); [Eichbaum et al., 2016](#)), using advanced computational models ([Brinkmann et al., 2014](#)).

In addition to the risks of contaminated sediments under average flow conditions, re-suspension of highly contaminated sediments may be a key driver for apparent toxicity in aquatic systems and sediment stability has been identified as an important and emerging factor that needs to be considered in the implementation of the WFD. For several European river basins, including Neckar, Rhine and Elbe, highly contaminated old sediments can be described as "potential chemical time bombs" ([Stachel et al., 2005](#); [Stigliani, 1988](#); [Stigliani, 1991](#)). The frequency of re-suspension of sediments and the intensity of flood events such as the flood on the River Elbe in 2002 are expected to increase in the future because of climate change.

3.2.3.3. Recommendation. In light of these findings and with regard to the increasingly promising experiences with passive sampling procedures in determining the freely dissolved fraction of hydrophobic contaminants in sediments ([Ghosh et al., 2014](#); [Mayer et al., 2014](#)), we recommend to consider establishing EQS for sediments based on the freely dissolved fraction, that can be determined using passive sampling, rather than total concentrations (see [Recommendation 2](#)). Because the freely dissolved fraction integrates all mentioned confounding factors that have impeded derivation of Europe-wide EQS values for sediment so far, this approach would greatly facilitate common quality goals for all Member States. In addition, unlike for passive sampling of water, where the sampling rates are chemical-specific, with passive sampling

of sediments the ratios of chemicals in the passive sampling extract remain unchanged relative to the whole sediment (Jahnke et al., 2016). This allows the application of passive sampling for sediments not only for chemical analysis but also for EBTs. For determining the risk of sediment contamination (1) standardized protocols to assess the impact of re-suspended sediments on biota are required (Förstner et al., 2016) and (2) sediments' stability to erosion should be acknowledged as an important parameter. We recommend that this aspect should receive particular attention when balancing the partially conflicting quality goals of the WFD, the European Floods Directive, and the Marine Strategy Framework Directive (since marine systems can be considered the ultimate recipients of historically contaminated sediments).

3.2.3.4. Outlook. Recently, it became evident that in addition to classical POPs and metals, more polar chemicals may play an important role in risks from contaminated sediments. These chemicals include polar polyaromatic compounds (Lübcke-von Varel et al., 2012; Lübcke-von Varel et al., 2011) as well as surfactants, pharmaceuticals and personal care products (Smital et al., 2013). Monitoring approaches and trigger values are therefore also required for these chemicals in sediments as a direct source of exposure for benthic organisms. The development of reliable approaches for the determination of freely dissolved concentrations of these compounds in sediment pore water is a future challenge in sediment risk assessment. In the U.S., the Superfund Program (which regulates and remediates contaminated sites) is developing a set of interstitial water remedial goals (IWRGs) based on passive sampling-generated freely dissolved concentrations and water-only toxicity values to allow for the management of contaminated sediment sites based on interstitial water concentrations (i.e., freely dissolved) and not total concentrations of contaminants (Burkhard et al., 2015).

3.2.4. Recommendation 7: consider exposure, effect and risk modeling as a tool to fill gaps in monitoring data and create incentives to extend the monitoring basis of chemical contamination across Europe

3.2.4.1. Problem. Although the WFD intended to align monitoring and assessment of freshwater resources on a European scale, one can observe a lack of consistency with respect to number and quality of monitoring data provided by current sampling efforts. Fewer compounds monitored and less frequent monitoring efforts often result in underestimation of risks (Malaj et al., 2014) and diagnosed ecological impact (Posthuma et al., 2016). Moreover, the low frequency of monitoring may miss exposure variability altogether, especially when e.g. the peak concentrations after the use of plant protection products are overlooked due to wrong sampling times. These kinds of problems still are a bottleneck for prioritization and assessment (Heiss and Küster, 2015). Prioritization, assessment and management require a clear basis for diagnosing impact magnitudes and causes, as well as for predicting the efficacy of management plans.

3.2.4.2. Current status. Malaj et al. (2014) evaluated the Waterbase dataset of the European Environmental Agency and reported great differences among various Member States with respect to the intensity and density of monitoring. The authors identified a set of chemicals that pose acute risks at different European monitoring sites and found a clear correlation: the higher the number of these chemicals monitored in a river basin the higher the resulting estimated risk (based on exceedance of the respective threshold values). This might disincentivize comprehensive monitoring efforts and give a false impression of compliance with water quality standards. Protective water quality monitoring urgently needs a reversal of these counter-productive incentives.

As an option to support and supplement high quality monitoring, advanced spatial explicit emission, fate and transport modeling are becoming increasingly important tools (Lindim et al., 2016b). They become especially powerful when coupled to hydrological modeling

(Hrachowitz et al., 2016). As shown for PFOS and PFOA in the Danube River catchment and Europe wide, it is possible to predict pollutants concentrations with high spatial and temporal resolution (Lindim et al., 2015; Lindim et al., 2016a) but they require careful parameterization to achieve high accuracy. New approaches for estimating environmental partitioning (Endo and Goss, 2014) are facilitating the prediction of the fate and transport of a wider range of organic chemicals including polar and ionic organic substances. Remaining challenges in fate and transport modeling, which are both being addressed within the SOLUTIONS project, are the estimation of spatially and temporally-resolved environmental emission rates of chemicals (Breivik et al., 2012) and the estimation of realistic environmental transformation rates (Boethling et al., 2009). Once proven reliable through model evaluation, these models can be used to predict seasonal variability and peak concentrations and they allow the analysis of hypothetical emissions scenarios for studying the effect of mitigation measures. Fate and transport models may also be used to study pollutants with intermittent or cyclic releases, for example, pesticides, which are not covered by typical sampling designs (Mottes et al., 2014). Within the SOLUTIONS project, scientists are attempting to model larger numbers of REACH- and other chemicals in all European river basins in order to predict which chemicals may create problems, where, when and why (Brack et al., 2015). The modeling of predicted environmental concentrations in European water systems – including their spatio-temporal variability – can be followed by evaluating the local mixture exposure levels with the toxic pressure proxy. The whole approach may thus include effect modeling, which thereby integrates (as appropriate) emission quantification, chemical fate and population and ecosystem-level models (De Laender et al., 2015; Focks et al., 2014a; Focks et al., 2014b; Schuwirth and Reichert, 2013) and empirical modeling of sensitivity (Rico and Van den Brink, 2015). It offers scope for a priority ranking of sites of interest (with expectedly large impacts), and of the most relevant compounds at given sites, while these predicted results can be validated by diagnostic approaches towards studying ecological impacts of mixtures at the same scales (Posthuma et al., 2016).

3.2.4.3. Recommendation. In cases where Member States are not able to fulfill their legal obligations for monitoring or in cases where more than the pollutants generally agreed upon are expected to be of relevance monitoring should be supported and enforced with modeling. If monitoring data are lacking it should be made an obligation to preliminary use modeled data for chemical occurrence. Water quality assessment could thus proceed based on reasonable worst case concentrations for chemicals giving the incentive to fill data gaps with enhanced monitoring efforts. Risk modeling should include the prediction of joint effects of similarly and dissimilarly acting chemicals, based on the concepts of concentration addition (Altenburger et al., 2000) and independent action (Faust et al., 2003), applied to measured or predicted per-chemical concentrations.

3.2.4.4. Outlook. Using effect modeling approaches, predicted local exposures to single compounds or mixtures of chemicals can be translated into quantitative estimates of toxic effects on individuals, populations and communities, and so build quantitative relationships between the chemicals and the ecological status. Producing these and other modeling data provides the insights needed for full spatial and temporal coverage, which even the best monitoring data fail to achieve. In fact, measured and modeled data could best be used to obtain a comprehensive overview of both the spatio-temporal variability of exposures and impacts, while their comparison would imply a cross-validation option (models verified by data vice versa). This would help to provide incentives to expand modeled data by monitoring data wherever predicted impact problems emerge. Further, exposure and impact modeling, increasingly cross-validated with measured concentrations or impacts, will also facilitate the prediction of future exposures and impacts. A key challenge for spatially and temporally resolved modeling of

chemicals is the availability of accurate environmental emission rates. To estimate these, up-to-date and accurate information on quantities in commerce (production and imports) as well as a detailed breakdown on chemical function are critically needed in Europe for developing accurate emission estimates. This requires a maximum in transparency and could follow the approach by the Nordic countries providing exposure-related information for substances in preparations in the SPIN database including quantity and risk indices (KEMI Swedish Chemical Agency, 2014). Scenarios on climate change, demographic change, urbanization, health care development, food production, technological developments etc. can be translated to expectations on chemical emissions and included into modeling as an early warning for upcoming risks. Trend analysis of pharmaceutical concentrations in surface waters (Ter Laak et al., 2009), demographic projections of future pharmaceutical consumption (van der Aa et al., 2011), and changes in disease patterns and pharmaceutical use in response to climate change (Redshaw et al., 2013) together with river basin transport and fate models (Lindim et al., 2016b) may be used, for example, to estimate future pharmaceutical loads in river water. Modeling can help exploring which types of chemicals pose the highest threats, and which molecular structures and characteristics should be avoided. Modeling can also support 'benign by design' chemicals, thereby putting safe design upfront in the process of developing and using chemicals (Eissen et al., 2002).

3.3. Support solution-oriented assessment

Improved monitoring and data evaluations will help to significantly advance available data sets and to understand contamination and corresponding risks. However, solution-focused assessment will be the key to translate these findings into efficient management. This may require improved investigative monitoring to identify toxicity drivers, better consistency across environmental-, chemical- and product-specific legislative frameworks, and an exploration of risk reduction scenarios before and along with risk assessment.

3.3.1. Recommendation 8: use a tiered approach of solution-oriented investigative monitoring including effect-directed analysis to identify toxicity drivers and abatement options

3.3.1.1. Problem. Including effect-based tools and trigger values in monitoring schemes will help to bridge the gap between chemical contamination and ecological status, and will provide indications on toxic chemicals as a probable cause of deterioration. This may help reduce efforts for chemical monitoring, but where effect-based trigger values are exceeded, solution-focused procedures are required to identify the drivers of the measured effects in order to initiate effective management activities. This is part of the investigative monitoring required by WFD in cases, for example, "where the reason for any exceedance of environmental objectives is unknown" (European Union, 2003a). However, a consistent strategy on how to establish cause-effect relationships is missing.

3.3.1.2. Current status. Effect-directed analysis (EDA) as a combination of biotesting, sequential fractionation and subsequent analytical identification of toxicants in active fractions has been successfully applied as a tool for the identification of drivers of toxicity in complex environmental mixtures including water, sediment and even biota. Several review papers (Brack, 2003; Hewitt and Marvin, 2005) and a recently published in-depth overview (Brack et al., 2016) provide valuable guidance for use in practice and a compilation of interesting case studies. EDA has been shown to be very helpful in establishing cause-effect relationships at specific sites of concern where significant adverse effects have been observed. Thus, the approach has already been suggested as a relevant tool for toxicant identification after effect-based monitoring in the context of WFD implementation (Wernersson et al., 2015).

However, although automation and integration of biotesting, fractionation and analysis in EDA may significantly enhance the throughput of this methodology (Zwart et al., 2015), the approach is still time-consuming. Thus, recently, virtual EDA has been discussed as an alternative approach applying multivariate statistics rather than fractionation for reduction of complexity of complex mixtures and identifying chemical signals correlating with observed effects (Eide et al., 2004; Hug et al., 2015). Both approaches may complement each other as tools for the identification and confirmation of candidate toxicants. However, a conceptual integration into existing monitoring and assessment schemes is still lacking.

3.3.1.3. Recommendation. We recommend a tiered approach for the most efficient assessment and selection of abatement options involving toxicant identification where necessary (Fig. 1). In Tier 1 we suggest performing a simple assessment of whether exceedance of effect-based trigger values can be explained by the fraction of treated and untreated municipal wastewater in a water body. If that is the case, at least in smaller water bodies, direct abatement by upgrading wastewater treatment might be an option without further in-depth analysis of drivers of toxicity. In cases where observed BEQ_{bio} exceed the expectations based on wastewater fractions a specific source of toxicity may be assumed and drivers should be identified. The fraction of wastewater in a water body can be identified by marker compounds such as carbamazepine (untreated and treated wastewater) and caffeine (untreated wastewater). In vitro bioassay-based benchmarks for micropollutants in wastewater have been documented for Australia (Escher et al., 2014). Such benchmarks for wastewater and wastewater-impacted surface waters are still missing for Europe but can be derived from correlations between fractions of wastewater in a water body and measurable BEQ_{bio} . Tier 2 investigations are required if (1) justification of abatement demands more information, (2) exceedance of benchmarks based on the fraction of wastewater suggest specific sources of toxicity or (3) many pollution sources contribute to the overall load typically of larger waterbodies. In cases where the fraction of wastewater does not correlate with the BEQ_{bio} agricultural land-use and the use of pesticides for plant protection but also industrial production may be drivers of toxicity (Malaj et al., 2014; Hug et al., 2015). In Tier 2, effect-based screening will be combined with more in depth chemical target and non-target screening that allows for mass balances between biologically and chemically derived BEQs (Neale et al., 2015) supplemented by multivariate approaches to identify chemical signals co-varying with effects (Hug et al., 2015). These approaches help identify individual or groups of drivers of effects and their contribution to mixture effects and thus identify sources and suggest abatement measures. Such an approach has been applied in Canada to determine the causes of endocrine disruption in fish downstream of pulp and paper facilities, the sources of these substances in the papermaking process (Hewitt et al., 2008) and mill operating conditions to reduce these effects (Martel et al., 2011). Tier 3 is required for those sites where major effects cannot be explained by identified and quantified chemicals and thus no targeted measures are possible. It may also help as a confirmation step for Tier 2 to further substantiate abatement options. As a tier 3 approach we recommend EDA (Brack, 2003) as a powerful tool to identify such drivers of toxicity in different matrices. This site-specific approach may address water, sediment or biota extracts and is based on a combination of biotesting, sequential reduction of complexity by fractionation and extensive target and non-target analysis of toxic fractions (Brack, 2003). EDA is the ultimate tool to establish cause-effect relationships between (groups of) individual chemicals and measurable effects in biotests. A similar tiered approach is proposed in the U.S. to assess contaminated sediments (Burgess et al., 2012). This approach combines monitoring (e.g., whole sediment concentrations, bioaccumulation, passive sampling), equilibrium partitioning modeling, and effects measures (toxicity, benthic community status) to assess the magnitude of contaminant impacts

and evaluate abatement options. Like the approach presented in Fig. 2, the U.S. EPA contaminated sediments approach may culminate with a toxicant identification step (i.e., toxicity identification evaluation – TIE).

3.3.1.4. Outlook. Rapid development of automated EDA systems based on multi-endpoint, high throughput and low volume biotesting (Dix, 2009) together with efficient micro- to nanofractionation (Booij et al., 2014; Kool et al., 2011) and automated workflows for non-target analysis of active fractions involving innovative software tools for in silico MS fragmentation, chromatographic retention prediction and estimates on toxicity (Brack et al., 2016) will make this tool increasingly applicable in monitoring of specific toxicity such as neurotoxicity, nuclear receptor-mediated effects, photosynthesis inhibition etc. Non-specific effects on whole organisms or cell lines are often caused by the complex mixture rather than by individual chemicals (or simple mixtures thereof that can be isolated). In these cases the overall contamination, loads, rather than individual toxicants, will need to be reduced.

3.3.2. Recommendation 9: improve links across environment-, chemical- and product-specific regulations and harmonize chemical legislation among Member States to improve abatement efficacy

3.3.2.1. Problem. Chemicals with the potential to affect water quality are covered by a large number of regulations in the EU, but there are significant inconsistencies between the various regulatory frameworks, particularly in procedures for updating their lists of chemicals, collection and availability of information on e.g. sources, occurrence and effects, implementation and compliancy checks, and their individual focus on a small subset of all (>100,000) chemicals currently used. As a result, there are significant gaps in coverage of the full range of chemicals, and the goals of the WFD are difficult to achieve.

3.3.2.2. Current status. The WFD is receptor-oriented and represents a regulatory framework for the protection and restoration of the aquatic

environment including groundwater bodies. It is based on a retrospective risk assessment by monitoring of toxic chemicals in European water resources and has a strong focus on aquatic ecosystems but states also that drinking water should be able to be produced with a reduced level of purification treatment required. Thus, a strong interconnection between WFD and Drinking Water Directive (DWD, European Union, 1998) is required. Article 7 WFD states that drinking water should be able to be produced with a reduced level of purification treatment required. However, drinking water concerns are inadequately reflected by current prioritization of chemicals within the WFD. The DWD defines chemical parameters for some compounds, such as pesticides and their transformation products (0,1 µg/L), which are not included in the WFD.

There are several sector- or product-specific directives and regulations focusing on the control of specific substances (Plant Protection Products Regulation (European Union, 2009b; European Union, 2011a), and Biocidal Products Regulation (European Union, 2012c), EMEA Guidelines for risk assessment of veterinary and human pharmaceuticals (European Union, 2010c; European Medicines Agency, 2006; European Medicines Agency, 2008) which are based on a prospective risk assessment. REACH is the main policy framework for prospective chemical risk assessment and thus for regulation of industrial chemicals. In addition to these regulatory instruments the presence of selected chemicals in products (Directive on waste electrical and electronic equipment, WEEE (European Union, 1998; European Union, 2012b) and Directive on the restriction of the use of hazardous substances in electrical and electronic equipment, RoHS (European Union, 2003b) is regulated. Lastly, emission-oriented regulations focus on emissions to the environment, such as the Industrial Emissions Directive (IED; European Union, 2010b), Sewage Sludge Directive (SSD; European Union, 1986), but with very limited coverage of chemical contaminants. In addition to the variety in purpose and form of regulatory control of chemicals in Europe, chemicals that are an integral part of imported articles cannot be subject to authorization under REACH and therefore cannot be addressed by source-related management if prioritized under WFD. Here other restrictions need to be applied.

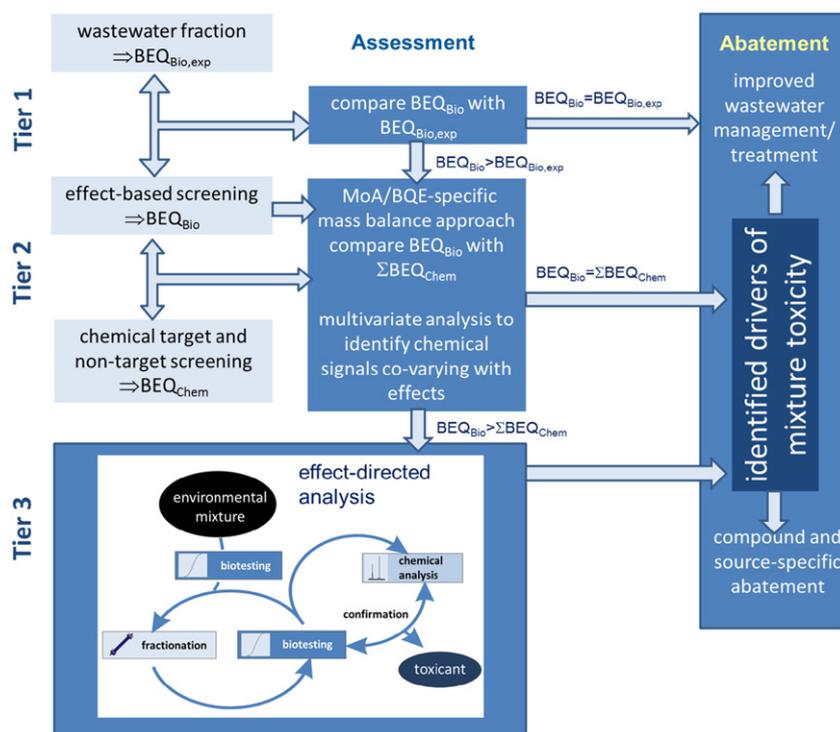


Fig. 2. Recommended tiered approach for enhanced investigative monitoring. Terms are defined as: BEQ_{Bio} : biologically derived BEQs, $BEQ_{Bio,exp}$: BEQ_{Bio} expected from benchmarking for a specific fraction of wastewater, BEQ_{Chem} : BEQ derived from chemical analysis.

Lists of Priority (PS) and Priority Hazardous Substances (PHS) are established under the WFD. For the latter, the WFD requires the cessation or phasing-out of discharges, emissions, and losses. However, essential sources of emissions of PHS fall outside the domain governed by water legislation. Major sources of e.g. PFOS and 4-nonylphenol are production processes, the use of these substances, release from products and, for nonylphenol, formation as a degradation product. With regard to commercially used chemicals the substances regulated as PHS by the WFD are also restricted or identified as substances of very high concern (SVHC) under REACH. However, identification as SVHC does not in itself mean any use restrictions. The restrictions in REACH are in many cases limited to a particular use, which means that all other uses are allowed (Molander et al., 2012). Overall, it can be concluded that structural links between water legislation and complementary source-related regulations are missing.

In addition to PS and PHS the WFD requires monitoring of RBSPs. EQS values for RBSPs are not established at the European level but set by the individual Member States. This may lead to serious disagreements about the quality status of a water body when a river crosses the border even if the concentrations do not change. A recent study found differences in applied EQS values for RBSPs of several orders of magnitude, suggesting different protection levels across Europe (Carvalho et al., 2016). The same discrepancy exists for groundwater threshold values derived in different countries (Scheidleder, 2012).

3.3.2.3. Recommendations. For an increased efficiency of WFD implementation, drinking water relevance of chemicals should be considered in prioritization and monitoring. It could be helpful in this respect that provisional drinking water quality standards - as described in TGD 27 (European Union, 2011b) - are in fact derived within the process of prioritization, striving for a reduced level of drinking water treatment according to art. 7 WFD. Also, a coupling of legal requirements in the DWD to the WFD could contribute to a more coherent implementation of EU policy. Compounds identified as PS and PHS in the WFD, RBSPs or groundwater contaminants should also be evaluated in relation to coverage by other regulations and, if necessary, included in the corresponding priority lists for implementation of restriction measures via specific cross-compliance mechanisms (in those regulations). As a first step in the direction of harmonization and better alignment regulatory instruments and in the interest of closing gaps and loop holes, risk assessment and prioritization procedures employed in different instruments should be evaluated and compared. We recommend that a common safety threshold for European waters (e.g. PNEC_{freshwater}) for all RBSPs should be derived according to common principles that can be applied in all chemical legislation and by all Member States to assess the risks in a consistent way. To derive these values, all reliable and relevant ecotoxicity data should be reviewed and assessed, including both studies run under “Good Laboratory Practice” conditions submitted by industry as well as appropriate and well-documented literature studies. In order to ensure the quality of ecotoxicity studies applied for risk assessment, the CRED (Criteria for Reporting and Evaluating Ecotoxicity Data) method has been published. This applies explicit criteria to evaluate the quality (reliability and relevance) of a study in a more harmonized and transparent way (Moermond et al., 2016). In this context, post-authorization monitoring could offer assurance that the use of authorized active ingredients is indeed not posing unacceptable risks to the environment. Similarly, better harmonization and transparency of the establishment of groundwater threshold values is recommended to achieve better comparability of the results.

To increase emission control from point sources, better coherence between WFD and the IED should be explored. Currently, the IED sets limitations only to large installations and defines technologies to be implemented for air and water emission treatment in the Best Available Techniques (BAT) reference documents (BREFs). In the recently approved BREF for chemical industry (European Union Joint Research Centre, 2014) the conclusions include BAT recommendations on

pretreatment of waste water to remove toxic and non-biodegradable compounds which can inhibit the regular water treatment or are insufficiently abated. A first step of policy harmonization would be further evaluation of whether the technologies described in the BREFs are efficient for reducing emissions of PS, PHS, RBSPs and groundwater contaminants.

Substitution for safer alternatives and development of “Green chemistry” are a key activity that needs to be continuously encouraged to prevent accumulation of toxic chemicals in society and the environment. Today, regulatory or monitoring authorities have limited possibilities to collect information on uses and emission sources of all chemicals which have been prioritized according to procedures set up to protect the aquatic environment, and even less possibility to develop and enforce regulations outside their own area. To a large extent, though, the necessary information is currently available in other regulatory frameworks such as REACH, and should be utilized.

3.3.2.4. Outlook. In line with these recommendations the EU Commission is currently performing a fitness check on chemical legislation (excluding REACH) in the EU under the REFIT process (European Union, 2015c; European Union, 2016). This process provides opportunities to harmonize chemical legislation and make procedures for prioritization and risk assessment as well as abatement more efficient. To minimize risks of negative impacts on humans and the environment, the most stringent restriction in all legislations should be adopted. Specifically for the WFD, this would entail that chemicals prioritized under the procedures relevant for the aquatic environment should be considered for identification as SVHC substances or for restrictions under REACH. Furthermore, a joint database system on uses and sources of chemicals should be developed. With such a joint system, authorities responsible for different regulatory frameworks on chemicals would be able to cooperate and develop joint abatement strategies when necessary.

3.3.3. Recommendation 10: apply solutions-oriented approaches that explore risk reduction scenarios before and along with, rather than after, risk assessment

3.3.3.1. Problem. Although the strict trigger values defined for ecological and chemical status are effective as generally agreed upon objectives, it is clear that incentives for and appraisal of improvement should be acknowledged even if the final goals (good ecological and chemical status) cannot be achieved within the given time frame. Often large gaps exist between assessment and management, while at the same time tools for prioritization of abatement options are lacking. The problem of a serious mismatch between assessment outcomes (science-based evaluations) and their usefulness in the context of effective management has been widely noted (Abt et al., 2010; Finkel, 2011).

3.3.3.2. Current status. The WFD assessments are based on the so-called one-out-all-out principle that requires managing a less-than-good quality status if one parameter fails the respective EQS. This has been confirmed by the Water Directors, who agreed that progress indicators are not an alternative to the overall status assessment on the basis of the on-out all-out principle, but additional useful information (Water and Marine Directors of the European Union, Candidate and EFTA Countries, 2013). The one-out-all-out principle logically works out as a signal that identifies water bodies where the situation is not completely ideal, but also as a signal that creates a full-warning impression when one criterion fails, even when the exceedance is small, while the same conclusion would be drawn in the case of non-compliance with multiple criteria. Further, it may result in non-compliance due to factors that are beyond the jurisdiction of water managers. Such examples include the diffuse long-range trans-boundary atmospheric deposition of mercury and polycyclic aromatic hydrocarbons (PAHs), persistent and bio-accumulating legacy pollutants or persistent and mobile chemicals infiltrating groundwater. For those chemicals, local emission

reductions would help to limit further deterioration but will not help to reduce environmental levels, as has been shown for mercury monitored in biota. Goals impossible to achieve have in practice resulted in a lack of efforts to improve water quality with respect to chemicals, as long-term abatement efforts appeared not to result in compliance (Posthuma et al., 2016). Consequently, a system that requires and rewards gradual improvements towards a given environmental quality target might help to define a best possible status, or a best possible trajectory to improve the status, in cases of “less stringent environmental objectives” according to Art. 4.5. WFD (European Union, 2000). Further, this approach would focus efforts on available efficient abatement options rather than Member States applying for exemption from compliance, thereby ignoring the worsening problem completely.

3.3.3.3. Recommendations. Research in chemical water quality is currently focused mainly on problem and risk analysis. Relatively little attention is paid to mitigation opportunities, whereas this is a common strategy for other environmental problems, such as climate change. We recommend implementation of a solution-focused paradigm in water quality assessment and management. In the environment chemicals are not the only stressors and prioritization of possible mitigation options might trigger effective and innovative approaches. Moreover, we propose to apply not only a risk-oriented view – with an output providing a ‘warning’ – but also a more holistic approach in the format of a sustainability assessment. That is: an evaluation of a current situation based on multiple parameters and metrics, together with considerations of options for sets of solutions, whereby sustainable, integrated scenarios for solutions are identified and implemented. This reduces risks while maximizing progress towards sustainable development. A focus on sustainable abatement options at an early stage, rather than assessment of the current status, may support the development of a consensus among the various relevant social actors, and stimulate coherent implementation and cross-sectoral learning. This has been illustrated by Reichert et al. (2015) and Zijp et al. (2016), who took the management of river rehabilitation and the sustainable management of slightly contaminated sediments, respectively, as examples. Both of these studies followed structured but slightly different decision-making processes which are integrated in Fig. 3. The use of a solution-focused paradigm has supported the definition and implementation of solution strategies for complex environmental management problems, which failed when the focus was on risks only (Zijp et al., 2016).

We also suggest the implementation of integrated abatement options that address several stressors in one measure, or increase the incentive to reduce chemical releases. Examples include the installation of buffer strips along river banks that offer protection from both pesticide pollution and the input of excess nutrients from arable lands. In this sense, embedding the key threats of chemical mixtures in a wider context is of utmost importance. Landscapes intensively influence riverscapes, so that the exploration of abatement options should encompass a broad view which includes land use and land management as major driving forces of stress, and of optional solutions. Sustainable, multi-effective abatement options would also increase habitat diversity and hence the biological diversity of both terrestrial and aquatic communities alike. Other options could be found beyond the field of the natural sciences, e.g. by the introduction of fees on chemical use in order to enforce the “polluter pays” principle and to finance broad-scale measures such as the introduction of additional sewage treatments to remove organic pollutants in intensively inhabited areas (see also Recommendation 8).

3.3.3.4. Outlook. The approach of solution-focused assessments can be optimized when supported by a so-called ‘mitigation database’. Such a database, for which the conceptual foundations were laid recently (Van Wezel et al., submitted) consists of a data model which enables the storage of all kinds of abatement options and strategies (by kind,

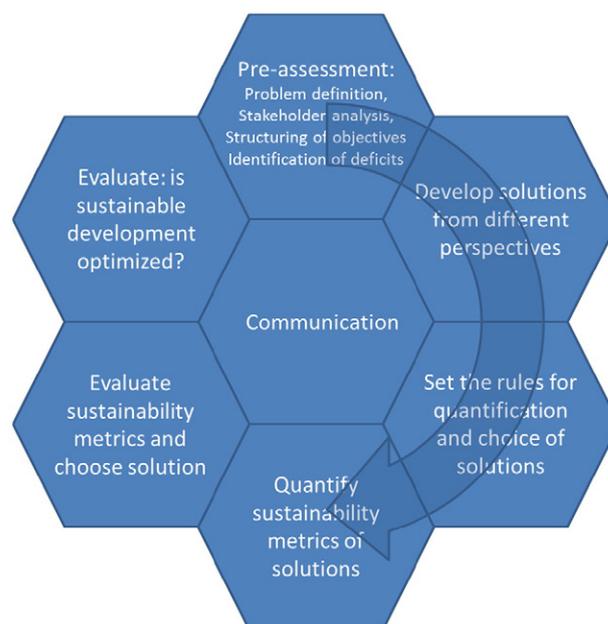


Fig. 3. Main process steps (clockwise) for solution-focused sustainability assessment according to Zijp et al. (2016) involving ideas by Reichert et al. (2015). A key principle is continuous improvement via an adaptive management strategy (continuous abatement efforts identified and implemented, decided upon evaluation of the success of ongoing abatement). Sustainability metrics are quantitative values to characterize sustainability (e.g. human health risks, ecosystem risks, costs etc.).

and name), and thereupon the predicted or observed efficacy in reducing emissions, concentrations or impacts (quantitatively, by compound group, by abatement technique). It stores and makes available for use the suite of technical and non-technical options for reducing chemical threats via the water system. Mitigation options can be defined along the whole pathway of a chemical's life cycle, whilst accounting for the characteristics of the water cycle. Early in the chemical's life cycle, non-technological mitigation options relevant on large spatial scales dominate, while later in the life cycle technological options relevant at regional scale dominate (Van Wezel et al., submitted). An efficient mitigation strategy combines both preventive and curative options, thereby accounting for abatement costs and trade-offs, i.e., optimizing sustainable development of abatement approaches. Such a mitigation database can be coupled to hydrological models on a river basin or global scale (see previous recommendation). Improvement of environmental quality by implementation of sets of mitigation options can be expressed in different, typically non-linearly related, terms of (1) decreased concentrations, (2) diminished adverse effects on environmental and human health (e.g., a chemical footprint), or (3) better possibilities to obtain water system services. In the case of water treatment, measures could be given a paramount importance if water bodies support or have the potential to support protected species, high biodiversity or important ecosystems services such as drinking water production or recreational fishery, or if pollution loads have a strong impact on downstream ecosystems (Coppens et al., 2015). One example may be the spatially smart abatement of pharmaceuticals in surface waters by prioritizing the impact of sewage treatment plants on susceptible functions such as drinking water abstraction and valuable ecosystems (Coppens et al., 2015).

4. Summary and conclusions

The WFD, as a directive for all European Union Member States, has successfully safeguarded the protection, restoration, and sustainable use of EU water resources. The planned revision of the WFD in 2019 offers the opportunity of advancing its conceptual basis (which is now

almost 20 years old), and bringing the practices for water quality assessment and management up to date. In the present paper, we have evaluated the WFD in practice, and identified various options for improvement regarding monitoring, setting of priorities, assessments, and management. Based upon a summary of identified problems, we have assessed the state-of-the-art in the relation to common practice and with regard to scientific developments relevant to important improvement for the implementation of the WFD. Based on these considerations we have made ten recommendations. We are convinced that the consideration of these findings will advance WFD implementation, which is crucial for protecting ecosystems and human health by reducing the chemical footprints of man-made practices in industry, agriculture and domestically. Globally, the WFD is currently seen as a model for the implementation of water quality protection, receiving a great deal of interest from regulators and scientists worldwide. In brief, the current status of the options for further supporting the improvement of the WFD can be summarized as a versatile toolbox, whose tools can be applied to promote safer and more cost-efficient monitoring, assessment and management of European water resources, supported by the integration of effect-based tools and benchmarks, mixture risk assessment, passive sampling, non-target chemical screening effect-directed analysis. These efforts provide the scientific underpinnings which allow for the ultimate achievement of the important goals of the WFD including more comprehensive prioritization schemes, better European-scale fate and risk modeling, improved solutions-focused assessments, and the consistent regulation of water quality and chemical production. These developments provide a contemporary scientific and practical basis to support achievement of the aims of the WFD.

Acknowledgments

This article has been supported by, and prepared as a common outcome of the NORMAN network (www.norman-network.net) on emerging pollutants and the SOLUTIONS project (European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement no. 603437). Andreas Kortenkamp, University of Brunel, is acknowledged for proof reading. The views expressed herein do not necessarily reflect the views or policies of the authors' agencies. Bo N. Jacobsen and Giordano Giorgi are acknowledged for their comments.

References

Abt, E., Rodricks, J.V., Levy, J.I., Zeise, L., Burke, T.A., 2010. Science and decisions: advancing risk assessment. *Risk Anal.* 30, 1028–1036.

Altenburger, R., Ait-Aissa, S., Antczak, P., Backhaus, T., Barceló, D., Seiler, T.-B., et al., 2015. Future water quality monitoring – adapting tools to deal with mixtures of pollutants in water resource management. *Sci. Total Environ.* 512–513, 540–551.

Altenburger, R., Backhaus, T., Boedeker, W., Faust, M., Scholze, M., Grimme, L.H., 2000. Predictability of the toxicity of multiple chemical mixtures to *Vibrio fischeri*: mixtures composed of similarly acting chemicals. *Environ. Toxicol. Chem.* 19, 2341–2347.

Ankley, G.T., Bennett, R.S., Erickson, R.J., Hoff, D.J., Hornung, M.W., Johnson, R.D., et al., 2010. Adverse outcome pathways: a conceptual framework to support ecotoxicology research and risk assessment. *Environ. Toxicol. Chem.* 29, 730–741.

Backhaus, T., Faust, M., 2012. Predictive environmental risk assessment of chemical mixtures: a conceptual framework. *Environ. Sci. Technol.* 46, 2564–2573.

Bay, S.M., Weisberg, S.B., 2012. Framework for interpreting sediment quality triad data. *Integr. Environ. Assess. Manag.* 8, 589–596.

Boethling, R., Fenner, K., Howard, P., Klečka, G., Madsen, T., Snape, J.R., et al., 2009. Environmental persistence of organic pollutants: guidance for development and review of POP risk profiles. *Integr. Environ. Assess. Manag.* 5, 539–556.

Booij, K., Robinson, C.D., Burgess, R.M., Mayer, P., Roberts, C.A., Ahrens, L., et al., 2016. Passive sampling in regulatory chemical monitoring of nonpolar organic compounds in the aquatic environment. *Environ. Sci. Technol.* 50, 3–17.

Booij, P., Vethaak, A.D., Leonards, P.E.G., Sjöllema, S.B., Kool, J., de Voogt, P., et al., 2014. Identification of photosynthesis inhibitors of pelagic marine algae using 96-well plate microfractionation for enhanced throughput in effect-directed analysis. *Environ. Sci. Technol.* 48, 8003–8011.

Botta, F., Dulio, V., Andres, S., Feray, C., Morin, A., 2012. A watch list of emerging pollutants for surface water monitoring in France. http://www.norman-network.net/sites/default/files/files/bulletins/newsletter_norman_3a-r.pdf. NORMAN Bull.: 7–8.

Brack, W., 2003. Effect-directed analysis: a promising tool for the identification of organic toxicants in complex mixtures. *Anal. Bioanal. Chem.* 377, 397–407.

Brack, W., 2015. The challenge: prioritization of emerging pollutants. *Environ. Toxicol. Chem.* 34, 2181.

Brack, W., Ait-Aissa, S., Burgess, R.M., Busch, W., Creusot, N., Di Paolo, C., et al., 2016. Effect-directed analysis supporting monitoring of aquatic environments – an in-depth overview. *Sci. Total Environ.* 544, 1073–1118.

Brack, W., Altenburger, R., Schüürmann, G., Krauss, M., López Herráez, D., van Gils, J., et al., 2015. The SOLUTIONS project: challenges and responses for present and future emerging pollutants in land and water resources management. *Sci. Total Environ.* 503–504, 22–31.

Brack, W., Dulio, V., Slobodnik, J., 2012. The NORMAN network and its activities on emerging environmental substances with a focus on effect-directed analysis of complex environmental contamination. *Environ. Sci. Eur.* 24, 29.

Brand, W., de Jongh, C.M., van der Linden, S.C., Mennes, W., Puijker, L.M., van Leeuwen, C.J., et al., 2013. Trigger values for investigation of hormonal activity in drinking water and its sources using CALUX bioassays. *Environ. Int.* 55, 109–118.

Brevik, K., Arnot, J.A., Brown, T.N., McLachlan, M.S., Wania, F., 2012. Screening organic chemicals in commerce for emissions in the context of environmental and human exposure. *J. Environ. Monit.* 14, 2028–2037.

Brinkmann, M., Eichbaum, K., Kammann, U., Hudjetz, S., Cofalla, C., Buchinger, S., et al., 2014. Physiologically-based toxicokinetic models help identifying the key factors affecting contaminant uptake during flood events. *Aquat. Toxicol.* 152, 38–46.

Brinkmann, M., Eichbaum, K., Reininghaus, M., Koglin, S., Kammann, U., Baumann, L., et al., 2015. Towards science-based sediment quality standards-effects of field-collected sediments in rainbow trout (*Oncorhynchus mykiss*). *Aquat. Toxicol.* 166, 50–62.

Burgess, R.M., Driscoll, S.B.K., Ozretich, R.J., Mount, D.R., Reiley, M.C., 2012. Equilibrium partitioning sediment benchmarks (ESBs) for the protection of benthic organisms: procedures for the determination of the freely dissolved interstitial water concentrations of nonionic organics. In: United States Environmental Protection Agency (Ed.), EPA/600/R-02/012.

Burkhard, L., Mount, D.I., Burgess, R.M., 2015. Deriving Sediment Interstitial Water Remediation Goals (IWRGs) for the Protection of Benthic Organisms from Direct Toxicity. U.S. EPA, Office of Research and Development, Washington, DC 20460 (draft).

Busch, W., Schmidt, S., Kühne, R., Schulze, T., Krauss, M., Altenburger, R., 2016. Micropollutants in European rivers: a mode of action survey to support the development of effect-based tools for water monitoring. *Environ. Toxicol. Chem.* <http://dx.doi.org/10.1002/etc.3460>.

Carvalho, N.R., Marinov, D., Loos, R., Chirico, N., Napierska, D., Lettieri, T., 2016. Monitoring-based Exercise: Second Review of the Priority Substances List Under the Water Framework Directive. Draft. In: Joint Research Centre I, editor.

Carvalho, R.N., Arukwe, A., Ait-Aissa, S., Bado-Nilles, A., Balzamo, S., Baun, A., et al., 2014. Mixtures of chemical pollutants at European legislation safety concentrations: how safe are they? *Toxicol. Sci.* 141, 218–233.

Commission O. OSPAR Hazardous Substances Committee, 2007. OSPAR Practical Study 2005 on Whole Effluent Assessment.

Coppens, L.J.C., van Gils, J.A.G., ter Laak, T.L., Raterman, B.W., van Wezel, A.P., 2015. Towards spatially smart abatement of human pharmaceuticals in surface waters: defining impact of sewage treatment plants on susceptible functions. *Water Res.* 81, 356–365.

De Laender, F., Morselli, M., Baveco, H., Van den Brink, P.J., Di Guardo, A., 2015. Theoretically exploring direct and indirect chemical effects across ecological and exposure scenarios using mechanistic fate and effects modelling. *Environ. Int.* 74, 181–190.

de Zwart, D., Dyer, S.D., Posthuma, L., Hawkins, C.P., 2006. Predictive models attribute effects on fish assemblages to toxicity and habitat alteration. *Ecol. Appl.* 16, 1295–1310.

De Zwart, D., Posthuma, L., 2005. Complex mixture toxicity for single and multiple species: proposed methodologies. *Environ. Toxicol. Chem.* 24, 2665–2676.

Di Paolo, C., Ottermann, R., Keiter, S., Ait-Aissa, S., Bluhm, K., Brack, W., et al., 2016. Bio-assay battery interlaboratory investigation of emerging contaminants in spiked water extracts – towards the implementation of bioanalytical monitoring tools in water quality assessment and monitoring. *Water Res.* (submitted).

Di Toro, D.M., Zarba, C.S., Hansen, D.J., Berry, W.J., Swartz, R.C., Cowan, C.E., et al., 1991. Technical basis for establishing sediment quality criteria for nonionic organic chemicals using equilibrium partitioning. *Environ. Toxicol. Chem.* 10, 1541–1583.

Diamond, M.L., de Wit, C.A., Molander, S., Scheringer, M., Backhaus, T., Lohmann, R., et al., 2015. Exploring the planetary boundary for chemical pollution. *Environ. Int.* 78, 8–15.

Dix, D.J., 2009. Identifying toxicity pathways with ToxCast high-throughput screening and applications to predicting developmental toxicity. *Birth Defects Res. A Clin. Mol. Teratol.* 85, 394.

Dobson, C.M., 2004. Chemical space and biology. *Nature* 432, 824–828.

Dulio, V., Slobodnik, J., 2015. In response: the NORMAN perspectives on prioritization of emerging pollutants. *Environ. Toxicol. Chem.* 34, 2183–2185.

Dulio, V., von der Ohe, P.C., 2013. NORMAN prioritisation framework for emerging substances. http://www.norman-network.net/sites/default/files/files/Publications/NORMAN_prioritisation_Manual_15%20April2013_final%20for%20website-f.pdf. NORMAN Association. Network of reference laboratories and related organisations for monitoring and bio-monitoring of emerging environmental substances (ISBN: 978-2-9545254-0-2).

Eichbaum, K., Brinkmann, M., Buchinger, S., Hecker, M., Engwall, M., van Bavel, B., et al., 2013. The diORAMA project: assessment of dioxin-like activity in sediments and fish (*Rutilus rutilus*) in support of the ecotoxicological characterization of sediments. *J. Soils Sediments* 13, 770–774.

Eichbaum, K., Brinkmann, M., Nuesser, L., Buchinger, S., Reifferscheid, G., Codling, G., et al., 2016. Bioanalytical and instrumental screening of the uptake of sediment-borne, dioxin-like compounds in roach (*Rutilus rutilus*). *Environ. Sci. Pollut. Res.* 1–15.

Eide, I., Neverdal, G., Thorvaldsen, B., Arneberg, R., Grung, B., Kvalheim, O.M., 2004. Toxicological evaluation of complex mixtures: fingerprinting and multivariate analysis. *Environ. Toxicol. Pharmacol.* 18, 127–133.

- Eissen, M., Metzger, J.O., Schmidt, E., Schneidewind, U., 2002. 10 years after Rio - concepts on the contribution of chemistry to a sustainable development. *Angew. Chem., Int. Ed.* 41, 414–436.
- Ekman, D.R., Ankley, G.T., Blazer, V.S., Collette, T.W., Garcia-Reyero, N., Iwanowicz, L.R., et al., 2013. Environmental reviews and case studies: biological effects-based tools for monitoring impacted surface waters in the Great Lakes: a multiagency program in support of the Great Lakes restoration initiative. *Environ. Pract.* 15, 409–426.
- Endo, S., Goss, K.-U., 2014. Applications of polyparameter linear free energy relationships in environmental chemistry. *Environ. Sci. Technol.* 48, 12477–12491.
- Escher, B.I., Allinson, M., Altenburger, R., Bain, P.A., Balaguer, P., Busch, W., et al., 2014. Benchmarking organic micropollutants in wastewater, recycled water and drinking water with in vitro bioassays. *Environ. Sci. Technol.* 48, 1940–1956.
- Escher, B.I., Neale, P.A., Leusch, F.D.L., 2015. Effect-based trigger values for in vitro bioassays: reading across from existing water quality guideline values. *Water Res.* 81, 137–148.
- Escher, B.I., van Daele, C., Dutt, M., Tang, J.Y.M., Altenburger, R., 2013. Most oxidative stress response in water samples comes from unknown chemicals: the need for effect-based water quality trigger values. *Environ. Sci. Technol.* 47, 7002–7011.
- European Chemicals Agency, 2014. Guidance on Information Requirements and Chemical Safety Assessment Chapter R.7b: Endpoint Specific Guidance.
- European Medicines Agency, 2006. Guideline on the Environmental Risk Assessment of Medicinal Products for Human Use. Committee for Medicinal Products for Human Use. EMEA/CHMP/SWP/4447/00 corr2¹.
- European Medicines Agency, 2008. Guideline on Environmental Impact Assessment for Veterinary Medicinal Products Phase II. Committee for Medicinal Products for Veterinary Use (CVMP). CVMP/VICH/790/03-FINAL.
- European Union, 1986. Council Directive of 12 June 1986 on the Protection of the Environment, and in Particular of the Soil, when Sewage Sludge is Used in Agriculture (86/278/EEC). p. 6 OJ L 181, 4.7.86, 6.
- European Union, 1998. Council Directive 98/83/EC of 3 November 1998 on the quality of water intended for human consumption OJ L330. 5.12.1998, 32.
- European Union, 2000. Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 Establishing a Framework for Community Action in the Field of Water Policy. p. 1 OJ L 327, 22.12.2000, 1.
- European Union, 2003a. Common Implementation Strategy for the Water Framework Directive (2000/60/EC). Guidance Document No 7. Monitoring under the Water Framework Directive.
- European Union, 2003b. Directive 2002/95/EC of the European Parliament and of the Council of 27 January 2003 on the restriction of the use of certain hazardous substances in electrical and electronic equipment. p. 19 OJ L13.2.2003.
- European Union, 2006. Directive 2006/118/EC of the European Parliament and of the Council of 12 December 2006 on the protection of groundwater against pollution and deterioration. *Off. J. Eur. Union* 2006, 19 OJ L372. 27.12.2006, 19.
- European Union, 2008a. Directive 2008/56/EC of the European Parliament and of the Council of 17 June 2008 Establishing a Framework for Community Action in the Field of Marine Environmental Policy (Marine Strategy Framework Directive). p. 19 OJ L164. 25.6.2008, 19.
- European Union, 2008b. Directive 2008/105/EC of the European Parliament and of the Council on Environmental Quality Standards in the Field of Water Policy, Amending and Subsequently Repealing Directives 82/176/EEC, 83/513/EEC, 84/156/EEC, 84/491/EEC and 86/280/EEC, and amending Directive 2000/60/EC. p. 84 OJ L 348. 24.12.2008, 84.
- European Union, 2009a. Commission Directive 2009/90/EC of 31 July 2009 Laying Down, Pursuant to Directive 2000/60/EC of the European Parliament and of the Council, Technical Specifications for Chemical Analysis and Monitoring of Water Status OJ L201. p. 36 1.8.2009, 36.
- European Union, 2009b. Directive 2009/128/EC of the European Parliament and of the Council Establishing a Framework for Community Action to Achieve the Sustainable Use of Pesticides. OJ L309. p. 71 24.11.2009, 71.
- European Union, 2010b. Directive 2010/75/EU of the European Parliament and of the Council of 24 November 2010 on industrial emissions (integrated pollution prevention and control) (Recast). OJ L334. p. 17 (17.12.2010).
- European Union, 2010c. Directive 2010/84/EU of the European Parliament and of the Council Amending, as Regards Pharmacovigilance, Directive 2001/83/EC on the Community Code Relating to Medicinal Products for Human Use, OJ L348, 31.12.2010; Regulation (EU) No 1235/2010 of the European Parliament and of the Council Amending, as Regards Pharmacovigilance of Medicinal Products for Human Use, Regulation (EC) No 726/2004 Laying Down Community Procedures for the Authorization and Supervision of Medicinal Products for Human and Veterinary Use and Establishing a European Medicines Agency, and Regulation (EC) No 1394/2007 on Advanced Therapy Medicinal Products, OJ L348, 31/12/2010. p. 74.
- European Union, 2011a. Commission Implementing Regulation (EU) No 540/2011 of 25 May 2011 implementing Regulation (EC) No 1107/2009 of the European Parliament and of the Council as Regards the List of Approved Active Substances. 2011R540-EN-03.09.2015–021.001-1.
- European Union, 2011b. WFD-CIS guidance document no. 27 technical guidance on deriving environmental quality standards. Technical Report 2011-055.
- European Union, 2012a. The Combination Effects of Chemicals – Chemical mixtures. Communication from the Commission to the Council, COM(2012) 252 Final, Brussels, 31.5.2012.
- European Union, 2012b. Directive 2012/19/EU of the Parliament and of the Council of 4 July 2012 on Waste Electrical and Electronic Equipment (WEEE). OJ L197, 24.7.2012, p. 38.
- European Union, 2012c. Regulation (EU) No 528/2012 of the European Parliament and the Council of 22 May 2012 Concerning the Making Available on the Market and Use of Biocidal Products. OJ L167, 27.6.2012, p. 1.
- European Union, 2013a. Decision No 1386/2013/EU of the European Parliament and the Council of 20 November 2013 on a General Union Environment Action Programme to 2020 “Living Well, Within the Limits of Our Planet”. OJ L345, 28.12.2013, p. 171.
- European Union, 2013b. Directive 2013/39/EU of the European Parliament and the Council of 12 August 2013 Amending Directives 2000/60/EC and 2008/105/EC as Regards Priority Substances in the Field of water policy. OJ L226, 24.8.2013, p. 1.
- European Union, 2014a. Commission Directive 2014/80/EU of 20 June 2014 Amending Annex II to Directive 2006/118/EC of the European Parliament and the Council on the Protection of Groundwater Against Pollution and Deterioration. OJ L182, 21.6.2014, p. 52.
- European Union, 2014b. Technical report on aquatic effect-based monitoring. Technical Report – 2014 – 077 <http://dx.doi.org/10.2779/7260>.
- European Union, 2014c. Commission Regulation (EU) No 589/2014 of 2 June 2014 Laying Down Methods of Sampling and Analysis for the Control of Levels of Dioxins, Dioxin-like PCBs and Non-dioxin-like PCBs in Certain Foodstuffs and Repealing Regulation (EU) No 252/2012. OJ L164, 3.6.2014, p. 18.
- European Union, 2015a. Commission Implementing Decision (EU) 2015/495 of 20 March 2015. OJ L78, 24.3.2015, p. 40.
- European Union, 2015b. Common Implementation Strategy for the Water Framework Directive (2000/60/EC) and the Floods Directive (2007/60/EC). Work Programme 2016–2018 as Agreed by Water Directors at Their Meeting in Luxembourg on 25 November 2015.
- European Union, 2015c. Evaluation and Fitness Check (FC) Roadmap. http://ec.europa.eu/smart-regulation/roadmaps/docs/2015_grow_050_refit_chemicals_outside_reach_en.pdf.
- European Union, 2016. Consultation on the Regulatory Fitness of Chemicals Legislation (Excluding REACH). http://ec.europa.eu/growth/tools-databases/newsroom/cf/itemdetail.cfm?item_id=8695.
- European Union Joint Research Centre, 2014. Best Available Techniques (BAT) Reference Document for Common Waste Water and Waste Gas Treatment/management Systems in the Chemical Sector. Industrial Emissions Directive 2010/75/EU (Integrated Pollution Prevention and Control). http://eippcb.jrc.ec.europa.eu/reference/BREF/CWW_Final_Draft_07_2014.pdf.
- Fang, K., Heijungs, R., de Snoo, G.R., 2014. Theoretical exploration for the combination of the ecological, energy, carbon, and water footprints: overview of a footprint family. *Ecol. Indic.* 36, 508–518.
- Faust, M., Altenburger, R., Backhaus, T., Blanck, H., Boedeker, W., Gramatica, P., et al., 2003. Joint algal toxicity of 16 dissimilarly acting chemicals is predictable by the concept of independent action. *Aquat. Toxicol.* 63, 43–63.
- Faust, M., Backhaus, T., 2015. In response: prioritization and standard setting for pollutant mixtures in the aquatic environment: a business consultant’s perspective. *Environ. Toxicol. Chem.* 34, 2185–2187.
- Finkel, A.M., 2011. “Solution-focused risk assessment”: a proposal for the fusion of environmental analysis and action. *Hum. Ecol. Risk Assess. Int. J.* 17, 754–787.
- Focks, A., Luttik, R., Zorn, M., Brock, T., Roex, E., Van der Linden, T., et al., 2014a. A simulation study on effects of exposure to a combination of pesticides used in an orchard and tuber crop on the recovery time of a vulnerable aquatic invertebrate. *Environ. Toxicol. Chem.* 33, 1489–1498.
- Focks, A., ter Horst, M., van den Berg, E., Baveco, H., van den Brink, P.J., 2014b. Integrating chemical fate and population-level effect models for pesticides at landscape scale: new options for risk assessment. *Ecol. Model.* 280, 102–116.
- Förstner, U., Hollert, H., Brinkmann, M., Eichbaum, K., Weber, R., Salomons, W., 2016. Dioxin in the Elbe river basin: policy and science under the water framework directive 2000–2015 and toward 2021. *Environ. Sci. Eur.* 28.
- Gartiser, S., Hafner, C., Oeking, S., Paschke, A., 2009. Results of a “whole effluent assessment” study from different industrial sectors in Germany according to OSPAR’s WEA strategy. *J. Environ. Monit.* 11, 359–369.
- Ghosh, U., Kane Driscoll, S., Burgess, R.M., Jonker, M.T., Reible, D., Gobas, F., et al., 2014. Passive sampling methods for contaminated sediments: practical guidance for selection, calibration, and implementation. *Integr. Environ. Assess. Manag.* 10, 210–223.
- Government of Canada, 2014. Overview of the Chemicals Management Plan. <http://www.chemicalsubstanceschimiques.gc.ca/fact-fait/chemveng-eng.php>.
- Hamers, T., Legler, J., Blaha, L., Hylland, K., Marigomez, I., Schipper, C.A., et al., 2013. Expert opinion on toxicity profiling—report from a NORMAN expert group meeting. *Integr. Environ. Assess. Manag.* 9, 185–191.
- Hecker, M., Hollert, H., 2011. Endocrine disruptor screening: regulatory perspectives and needs. *Environ. Sci. Eur.* 23.
- Heiss, C., Küster, A., 2015. In response: a regulatory perspective on prioritization of emerging pollutants in the context of the water framework directive. *Environ. Toxicol. Chem.* 34, 2181–2183.
- Hering, D., Carvalho, L., Argillier, C., Bekkioglu, M., Borja, A., Cardoso, A.C., et al., 2015. Managing aquatic ecosystems and water resources under multiple stress - an introduction to the MARS project. *Sci. Total Environ.* 503, 10–21.
- Hernández, F., Ibáñez, M., Portolés, T., Cervera, M.I., Sancho, J.V., López, F.J., 2015. Advancing towards universal screening for organic pollutants in waters. *J. Hazard. Mater.* 282, 86–95.
- Hewitt, L.M., Kovacs, T.G., Dubé, M.G., MacLachy, D.L., Martel, P.H., McMaster, M.E., et al., 2008. Altered reproduction in fish exposed to pulp and paper mill effluents: roles of individual compounds and mill operating conditions. *Environ. Toxicol. Chem.* 27, 682–697.
- Hewitt, L.M., Marvin, C.H., 2005. Analytical methods in environmental effects-directed investigations of effluents. *Mut. Res. Rev. Mut. Res.* 589, 208–232.
- Hrachowitz, M., Benettin, P., van Breukelen, B.M., Fovet, O., Howden, N.J.K., R. L., et al., 2016. Transit times—the link between hydrology and water quality at the catchment scale. *WIREs Water* <http://dx.doi.org/10.1002/wat2.1155>.

- Huckins, J.N., Manuweera, G.K., Petty, J.D., Mackay, D., Lebo, J.A., 1993. Lipid-containing semipermeable membrane devices for monitoring organic contaminants in water. *Environ. Sci. Technol.* 27, 2489–2496.
- Hug, C., Sievers, M., Ottermanns, R., Hollert, H., Brack, W., Krauss, M., 2015. Linking mutagenic activity to micropollutant concentrations in wastewater samples by partial least square regression and subsequent identification of variables. *Chemosphere* 138, 176–182.
- Institut National de l'Environnement Industriel et des Risques, International Office for Water, 2009q. Implementations of Requirements on Priority Substances Within the Context of the Water Framework Directive. Prioritisation process: Monitoring-based ranking. European Commission Directorate-General Environment, Directorate D – Water, Chemicals and Cohesion. ENV.D2 – Protection of Water and Marine Environment.
- Jahnke, A., Mayer, P., Schäfer, S., Witt, G., Haase, N., Escher, B.I., 2016. Strategies for transferring mixtures of organic contaminants from aquatic environments into bioassays. *Environ. Sci. Technol.* 50, 5424–5431.
- Kapo, K.E., Holmes, C.M., Dyer, S.D., de Zwart, D., Posthuma, L., 2014. Developing a foundation for eco-epidemiological assessment of aquatic ecological status over large geographic regions utilizing existing data resources and models. *Environ. Toxicol. Chem.* 33, 1665–1677.
- Kase, R., 2016. Effect-based and Chemical Analytical Monitoring for the Steroidal Estrogens. <http://www.ecotoxcentre.ch/projects/aquatic-ecotoxicology/monitoring-of-steroidal-estrogens/>.
- KEMI Swedish Chemical Agency, 2014. SPIN, Substances in Preparations in Nordic Countries. 2014.
- Kienle, C., Vermeirssen, E., Kunz, P., Werner, I., 2015. Grobbeurteilung der Wasserqualität von abwasserbelasteten Gewässern anhand von ökotoxikologischen Biotests. In: SZfAÖE-E. O. (Ed.), Studie im Auftrag desw Bundesamtes für Umwelt (BAFU). In.
- Kool, J., Heus, F., de Kloe, G., Lingeman, H., Smit, A.B., Leurs, R., et al., 2011. High-resolution bioactivity profiling of mixtures toward the acetylcholine binding protein using a nanofractionation spotter technology. *J. Biomol. Screen.* 16, 917–924.
- Kunz, P.Y., Kienle, C., Carere, M., Homazava, N., Kase, R., 2015. In vitro bioassays to screen for endocrine active pharmaceuticals in surface and waste waters. *J. Pharm. Biomed. Anal.* 106, 107–115.
- Lindim, C., Cousins, I.T., van Gils, J., 2015. Estimating emissions of PFOS and PFOA to the Danube River catchment and evaluating them using a catchment-scale chemical transport and fate model. *Environ. Pollut.* 207, 97–106.
- Lindim, C., van Gils, J., Cousins, I.T., 2016a. Europe-wide estuarine export and surface water concentrations of PFOS and PFOA. *Water Res.* 103, 124–132.
- Lindim, C., van Gils, J., Cousins, I.T., 2016b. A large-scale model for simulating the fate and transport of organic contaminants in river basins. *Chemosphere* 144, 803–810.
- Lohmann, R., Burgess, R.M., Cantwell, M.G., Ryba, S.A., MacFarlane, J.K., Gschwend, P.M., 2004. Dependency of polychlorinated biphenyl and polycyclic aromatic hydrocarbon bioaccumulation in *Mya arenaria* on both water column and sediment bed chemical activities. *Environ. Toxicol. Chem.* 23, 2551–2562.
- Loos, R., 2012. Analytical methods relevant to the European Commission's 2012 proposal on priority substances under the Water Framework Directive. JRC Scientific and Policy Reports. European Commission. Joint Research Centre. Institute for Environment and Sustainability, Luxembourg.
- Loos, R., Gawlik, B.M., Locoro, G., Rimaviciute, E., Contini, S., Bidoglio, G., 2009. EU-wide survey of polar organic persistent pollutants in European river waters. *Environ. Pollut.* 157, 561–568.
- Lübcke-von Varel, U., Bataineh, M., Lohrmann, S., Löffler, I., Schulze, T., Flückiger-Isler, S., et al., 2012. Identification and quantitative confirmation of dinitropyrenes and 3-nitrobenzanthrone as major mutagens in contaminated sediments. *Environ. Int.* 44, 31–39.
- Lübcke-von Varel, U., Löffler, I., Streck, G., Machala, M., Ciganek, M., Neca, J., et al., 2011. Polar compounds dominate in vitro effects of sediment extracts. *Environ. Sci. Technol.* 45, 2384.
- Malaj, E., von der Ohe, P.C., Grote, M., Kühne, R., Mondy, C.P., Usseglio-Polatera, P., et al., 2014. Organic chemicals jeopardize freshwater ecosystems health on the continental scale. *Proc. Natl. Acad. Sci.* 111, 9549–9554.
- Martel, P.H., Kovacs, T.G., O'Connor, B.L., Semeniuk, S., Hewitt, L.M., Maclatchy, D.L., et al., 2011. Effluent monitoring at a bleached kraft mill: directions for best management practices for eliminating effects on fish reproduction. *J. Environ. Sci. Health A Tox. Hazard. Subst. Environ. Eng.* 46, 833–843.
- Mayer, P., Parkerton, T.F., Adams, R.G., Cargill, J.G., Gan, J., Gouin, T., et al., 2014. Passive sampling methods for contaminated sediments: scientific rationale supporting use of freely dissolved concentrations. *Integr. Environ. Assess. Manag.* 10, 197–209.
- Mayer, P., Tolls, J., Hermens, L., Mackay, D., 2003. Equilibrium sampling devices. *Environ. Sci. Technol.* 37, 184A–191A.
- Miège, C., Mazzella, N., Allan, I., Dulio, V., Smedes, F., Tixier, C., et al., 2015. Position paper on passive sampling techniques for the monitoring of contaminants in the aquatic environment – achievements to date and perspectives. *Trends Environ. Anal. Chem.* 8, 20–26.
- Moermond, C.T.A., Kase, R., Korkaric, M., Agerstrand, M., 2016. CRED: criteria for reporting and evaluating ecotoxicity data. *Environ. Toxicol. Chem.* 35, 1297–1309.
- Molander, L., Breitholtz, M., Andersson, P.L., Rybacka, A., Ruden, C., 2012. Are chemicals in articles an obstacle for reaching environmental goals? - missing links in EU chemical management. *Sci. Total Environ.* 435, 280–289.
- Moschet, C., Wittmer, I., Simovic, J., Junghans, M., Piazzoli, A., Singer, H., et al., 2014. How a complete pesticide screening changes the assessment of surface water quality. *Environ. Sci. Technol.* 48, 5423–5432.
- Mottes, C., Lesueur-Jannoyer, M., Le Bail, M., Malezieux, E., 2014. Pesticide transfer models in crop and watershed systems: a review. *Agron. Sustain. Dev.* 34, 229–250.
- Munkittrick, K.R., Arens, C.J., Lowell, R.B., Kaminski, G.P., 2009. A review of potential methods of determining critical effect size for designing environmental monitoring programs. *Environ. Toxicol. Chem.* 28, 1361–1371.
- Neale, P.A., Ait-Aissa, S., Brack, W., Creusot, N., Denison, M.S., Deutschmann, B., et al., 2015. Linking in vitro effects and detected organic micropollutants in surface water using mixture-toxicity modeling. *Environ. Sci. Technol.* 49, 14614–14624.
- Posthuma, L., Bjorn, A., Zijp, M.C., Birkved, M., Diamond, M.L., Hauschild, M.Z., et al., 2014. Beyond safe operating space: finding chemical Footprinting feasible. *Environ. Sci. Technol.* 48, 6057–6059.
- Posthuma, L., de Zwart, D., 2012. Predicted mixture toxic pressure relates to observed fraction of benthic macrofauna species impacted by contaminant mixtures. *Environ. Toxicol. Chem.* 31, 2175–2188.
- Posthuma, L., De Zwart, D., Keijzers, R., Postma, J., 2016. Water Systems Analysis with the Ecological Key Factor 'Toxicity'. Part 2. Calibration. Toxic Pressure and Ecological Effects on Macrofauna in the Netherlands. STOWA, Amersfoort, the Netherlands.
- Posthuma, L., Dyer, S.D., de Zwart, D., Kapo, K., Holmes, C.M., Burton Jr., G.A., 2016. Eco-epidemiology of aquatic ecosystems: separating chemicals from multiple stressors. *Sci. Total Environ.* 573, 1303–1319.
- Poulier, G., Lissalde, S., Charriau, A., Buzier, R., Delmas, F., Gery, K., et al., 2014. Can POCIS be used in Water Framework Directive (2000/60/EC) monitoring networks? A study focusing on pesticides in a French agricultural watershed. *Sci. Total Environ.* 497–498, 282–292.
- Redshaw, C.H., Stahl-Timmins, W.M., Fleming, L.E., Davidson, I., Depledge, M.H., 2013. Potential changes in disease patterns and pharmaceutical use in response to climate change. *J. Toxicol. Environ. Health B Crit. Rev.* 16, 285–320.
- Reichenberg, F., Mayer, P., 2006. Two complementary sides of bioavailability: accessibility and chemical activity of organic contaminants in sediments and soils. *Environ. Toxicol. Chem.* 25, 1239–1245.
- Reichert, P., Langhans, S.D., Lienert, J., Schuwirth, N., 2015. The conceptual foundation of environmental decision support. *J. Environ. Manag.* 154, 316–332.
- Reyjol, Y., Argillier, C., Bonne, W., Borja, A., Buijse, A.D., Cardoso, A.C., et al., 2014. Assessing the ecological status in the context of the European Water Framework Directive: where do we go now? *Sci. Total Environ.* 497, 332–344.
- Rico, A., Van den Brink, P.J., 2015. Evaluating aquatic invertebrate vulnerability to insecticides based on intrinsic sensitivity, biological traits, and toxic mode of action. *Environ. Toxicol. Chem.* 34, 1907–1917.
- Rockström, J., Steffen, W., Noone, K., Persson, Å., Chapin, F.S., Lambin, E.F., et al., 2009b. A safe operating space for humanity. *Nature* 461, 472–475.
- Rockström, J., Steffen, W., Noone, K., Persson, Å., Chapin, F.S., Lambin, E., et al., 2009a. Planetary boundaries: exploring the safe operating space for humanity. *Ecol. Soc.* 14, 32.
- Schäfer, R.B., von der Ohe, P.C., Kuehne, R., Schueuermann, G., Liess, M., 2011. Occurrence and toxicity of 331 organic pollutants in large rivers of north Germany over a decade (1994 to 2004). *Environ. Sci. Technol.* 45, 6167–6174.
- Scheidleder, A., 2012. In: Austria, E.A. (Ed.), Groundwater threshold values. In-depth assessment of the differences in groundwater threshold values established by Member States. http://ec.europa.eu/environment/archives/water/imp/rep/2007/pdf/In-depth_assessment_GW_TV-FinalReport.pdf.
- Schuwirth, N., Reichert, P., 2013. Bridging the gap between theoretical ecology and real ecosystems: modeling invertebrate community composition in streams. *Ecology* 94, 368–379.
- Slobodnik, J., Mrafkova, L., Carere, M., Ferrara, F., Pennelli, B., Schüttormann, G., et al., 2012. Identification of river basin specific pollutants and derivation of environmental quality standards: a case study in the Slovak Republic. *TrAC Trends Anal. Chem.* 41, 133–145.
- Smital, T., Terzic, S., Loncar, J., Senta, I., Zaja, R., Popovic, M., et al., 2013. Prioritisation of organic contaminants in a river basin using chemical analyses and bioassays. *Environ. Sci. Pollut. Res.* 20, 1384–1395.
- Sobek, A., Bejgarn, S., Ruden, C., Breitholtz, M., 2016. The dilemma in prioritizing chemicals for environmental analysis: known versus unknown hazards. *Environ. Sci. Process. Impacts*.
- Solheim, A.L., Austnes, K., Kristensen, P., Peterlin, M., Kodeš, V., Collins, R., Semerádová, S., Künitzer, A., Filippi, R., Prchalová, H., Spiteri, C., Prins, T., 2012. Ecological and chemical status and pressures in European waters. ETC/ICM Technical Report 1/2012. http://icm.eionet.europa.eu/ETC_Reports/EcoChemStatusPressInEurWaters_201211/Ecological_and_chemical_status_and_pressures_ETC_13112012_Published.pdf.
- Stachel, B., Jantzen, E., Knoth, W., Krüger, F., Lepom, P., Oetken, M., et al., 2005. The Elbe flood in august 2002 - organic contaminants in sediment samples taken after the flood event. *J. Environ. Sci. Health A* 40, 265–287.
- Steffen, W., Richardson, K., Rockstrom, J., Cornell, S.E., Fetzer, I., Bennett, E.M., et al., 2015. Planetary boundaries: guiding human development on a changing planet. *Science* 347.
- Stigliani, W.M., 1988. Changes in valued “capacities” of soils and sediments as indicators of nonlinear and time-delayed environmental effects. *Environ. Monit. Assess.* 10, 245–307.
- Stigliani, W.M., 1991. Chemical time bombs: definition, concepts, and examples. IASA Executive Reports. International Institute for Applied Systems Analysis, Laxenburg, Austria.
- Tang, J.Y.M., Escher, B.I., 2014. Realistic environmental mixtures of micropollutants in surface, drinking, and recycled water: herbicides dominate the mixture toxicity toward algae. *Environ. Toxicol. Chem.* 33, 1427–1436.
- Tang, J.Y.M., McCarty, S., Glenn, E., Neale, P.A., Warne, M.S.J., Escher, B.I., 2013. Mixture effects of organic micropollutants present in water: towards the development of effect-based water quality trigger values for baseline toxicity. *Water Res.* 47, 3300–3314.
- Ter Laak, T.L., Van der Aa, M., Houtman, C., Stoks, P.G.M., Van Zewel, A., 2009. Temporal and Spatial Trends of Pharmaceuticals in the Rhine. Association of River Waterworks - RIWA, The Netherlands.
- Thain, J.E., Vethaak, A.D., Hylland, K., 2008. Contaminants in marine ecosystems: developing an integrated indicator framework using biological-effect techniques. *ICES J. Mar. Sci. J. du Conseil* 65, 1508–1514.

- Traina, S.J., McAvoy, D.C., Versteeg, D.J., 1996. Association of linear alkylbenzenesulfonates with dissolved humic substances and its effect on bioavailability. *Environ. Sci. Technol.* 30, 1300–1309.
- Van der Aa, N.G.F.M., Kommer, G.J., van Montfoort, J.E., Versteegh, J.F.M., 2011. Demographic projections of future pharmaceutical consumption in the Netherlands. *Water Sci. Technol.* 63, 825–831.
- Van der Oost, R.G.S., Suarez, M.M., 2016. Watersysteemanalyse met de Ecologische Sleutelfactor Toxiciteit. Deel 5. In: STOWA A (Ed.), *Background document on Effect-Based Trigger Values for Environmental Water Quality*.
- Van Wezel, A., Ter Laak, T.L., Fischer, A., Bäuerlein, P.S., Munthe, J., Posthuma, L., 2016. Operationalising solutions-focused risk assessment: A discussion paper on mitigation options for chemicals of emerging concern in surface waters. *Crit. Rev. Environ. Sci. Technol.* (submitted).
- Vethaak, A.D., Davies, I.M., Thain, J.E., Gubbins, M.J., Martínez-Gómez, C., Robinson, C.D., et al., 2016. Integrated indicator framework and methodology for monitoring and assessment of hazardous substances and their effects in the marine environment. *Mar. Environ. Res.* (in press).
- Vignati, D.A.L., Valsecchi, S., Polesello, S., Patrolecco, L., Dominik, J., 2009. Pollutant partitioning for monitoring surface waters. *Trac-Trends Anal. Chem.* 28, 159–169.
- Von der Ohe, P.C., de Deckere, E., Prüß, A., Munoz, I., Wolfram, G., Villagrana, M., et al., 2009. Towards an integrated assessment of the ecological and chemical status of European River Basins. *Integr. Environ. Assess. Manag.* 5, 50–61.
- Von der Ohe, P.C., Dulio, V., Slobodnik, J., De Deckere, E., Kühne, R., Ebert, R.U., et al., 2011. A new risk assessment approach for the prioritization of 500 classical and emerging organic microcontaminants as potential river basin specific pollutants under the European Water Framework Directive. *Sci. Total Environ.* 409, 2064–2077.
- Von der Ohe, P.C., Goedkoop, W., 2013. Distinguishing the effects of habitat degradation and pesticide stress on benthic invertebrates using stressor-specific metrics. *Sci. Total Environ.* 444, 480–490.
- Vrana, B., Allan, I.J., Greenwood, R., Mills, G.A., Dominiak, E., Svensson, K., et al., 2005. Passive sampling techniques for monitoring pollutants in water. *TrAC Trends Anal. Chem.* 24, 845–868.
- Vrana, B., Smedes, F., Prokes, R., Loos, R., Mazzella, N., Miega, C., et al., 2016. NORMAN interlaboratory study (ILS) on passive sampling of emerging pollutants; EUR 27655 EN. JRC Technical Reports <http://dx.doi.org/10.2788/6757>.
- Water and Marine Directors of the European Union, Candidate and EFTA Countries, 2013t. Informal meeting of water and marine directors of the European Union, candidate and EFTA countries. Vilnius, 4th and 5th of December 2013. Final Synthesis . <https://circabc.europa.eu/faces/jsp/extension/wai/navigation/container.jsp>.
- Wernersson, A.S., Carere, M., Maggi, C., Tusil, P., Soldan, P., James, A., et al., 2015. The European technical report on aquatic effect-based monitoring tools under the water framework directive. *Environ. Sci. Eur.* 27, 1–11.
- WFD Navigation Task Group, 2011. The Case for Europe-wide vs. River Basin-specific Sediment EQS. A Position Paper Prepared by the WFD Navigation Task Group February 2011. <http://www.pianc.org/downloads/eu/wfd/Sediment%20EQS%20NAVI%20TC%20paper%20to%20COM%20v5%2015-2-11.pdf> (Accessed 13 May 2016).
- Zijp, M.C., Posthuma, L., van de Meent, D., 2014. Definition and applications of a versatile chemical pollution footprint methodology. *Environ. Sci. Technol.* 48, 10588–10597.
- Zijp, M.C., Posthuma, L., Wintersen, A., Devilee, J., Swartjes, F.A., 2016. Definition and use of solution-focused sustainability assessment: a novel approach to generate, explore and decide on sustainable solutions for wicked problems. *Environ. Int.* 91, 319–331.
- Zwart, N., Hamers, T., Jonker, W., de Boer, J., Kool, J., Lamoree, M., 2015. Development of a miniaturized AMES assay for high-throughput effect-directed analysis of water samples using microfractionation. Presentation at SETAC Europe 25th Annual Meeting, 3–7 May 2015, Barcelona. Abstract Book. SETAC Europe Office, Brussels, Belgium, p. 61.