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BTO rapport

SOLUTIONS and BTO - Summary of results and applications for the drinking water sector

KWR

Bridging Science to Practice

SOLUTIONS and BTO - Summary of results and applications for the drinking water sector

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Summary

SOLUTIONS was a large FP7 research project of the European Union where 39 partners from academia, research institutes and industry researched solutions ("SOLUTIONS") for water cycle contaminants. The project has delivered various concepts, tools, models and case studies. The objective of the BTO research was to review the various results of the solutions project and select one result, in consultation with the Chemical Safety theme group, to pilot in relation to a specific issue from the drinking water sector.

Thirty-four results and products from the SOLUTIONS website were reviewed and scored by an expert review team consisting of Thomas ter Laak, Milou Dingemans, Andrea Brunner and Bas van der Grift. Each item was scored for its 'Technology Readiness Level', a measure of the maturity of a technology or system on a scale of one to nine, the relevance and the applicability for the drinking water sector. Results already in use at KWR were noted and not considered for the pilot study. Each reviewer was asked to put forward one or two results suitable for the pilot study. Priority was given to results where KWR could bring the result out of the prototype (TRL 5-6) to the demonstration stage (TRL 7-8).

Four pilot projects were presented to the Chemical Safety theme group in July 2019 and a vote chose the pilot project to develop a degradation rate database for emerging contaminants. The chosen result was a literature review of degradation rates of emerging contaminants in soil and groundwater. The aim of the review was to assess the uncertainty of the fate of emerging organic contaminants in hydrological models. From the literature, first order degradation rates were extracted or calculated based on the data presented. This data was compiled in an MS-Excel database.

The database was matched with AquaPriori, a tool being developed within KWR by Dirk de Vries and Martin Korevaar of the Drinking Water Treatment team. The tool can predict the removal efficiency for non-tested, priority substances in water treatment processes based on quantitative structural property relationships (QSPRs). The tool is being developed for two treatments processes, activated carbon and reverse osmosis. Adding the database of degradation rates from the chosen publications to AquaPriori was a good fit for both research projects. By combining the database and AquaPriori tool we were able to use the funds in the SOLUTIONS pilot project efficiently and add value to an existing tool. There was the ambition on the AquaPriori side to add additional treatment processes to the tool and the database of degradation rates can be used to evaluate the removal efficiency of treatment processes including soil or dune passage. In addition, similar substances were of interest to both databases, namely emerging contaminants and as yet untested substances. Finally, the underlying principle of QSPR can also be applies to, for example toxicological and biological processes. The biodegradability of substances also be linked to substance properties via quantitative structure biodegradability relationships (QSBRs).

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1 SOLUTIONS

1.1 Introduction

SOLUTIONS was a large FP7 research project of the European Union where 39 partners from academia, research institutes and industry researched solutions ("SOLUTIONS") for water cycle contaminants. The project has delivered various concepts, tools, models and case studies. The objective of the BTO research was to review the various results of the solutions project and select one result, in consultation with the Chemical Safety theme group (Themagroep Chemische Veiligheid), to pilot in relation to a specific issue from the drinking water sector.

1.2 Methodology

The SOLUTIONS project resulted in many publications, (public) deliverables, reports, databases and tools (Figure 1). Within this research, only the outputs highlighted in the 'Results' and 'Products' section of the SOLUTIONS website were reviewed. It would have been prohibitively time consuming to review each of the 182 publications and we reasoned that the publications, tools and databases highlighted specifically in the 'Results' and 'Products' section were likely the most significant of the research output.

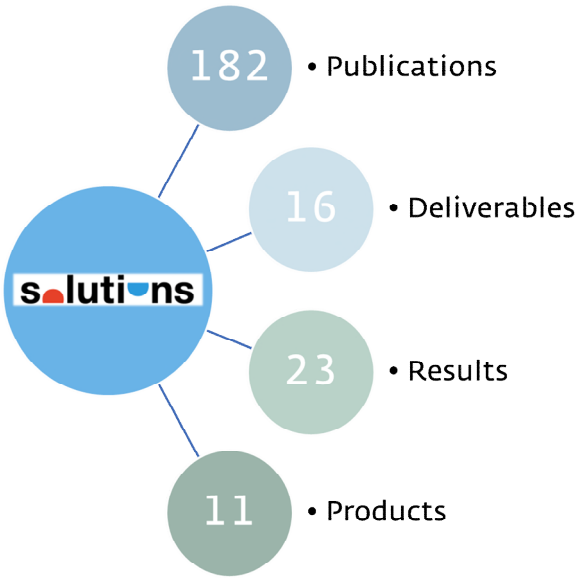


Figure 1 Summary of output from the SOLUTIONS project at the time of the review

The results were grouped into four themes;

1. Monitoring tools
2. Modelling tools
3. Abatement, Prioritization and Policy recommendations
4. Webtools and Databases

Each of the results were numbered and input to a table which summarizes the result. See Table 1 for an explanation of the summary table. Each results was reviewed and scored by an expert in the field (Figure 2). Reviewers scored each results for the "Technology Readiness Level" (Figure 3), relevance of the result and the applicability for the drinking water sector. Results already in use at KWR were noted and not considered for the

pilot study. Each reviewer was asked to put forward one or two results suitable for the pilot study. Priority was given to results with a TRL of 5-6, where KWR could bring the result out of the prototype to the demonstration stage (Figure 3).

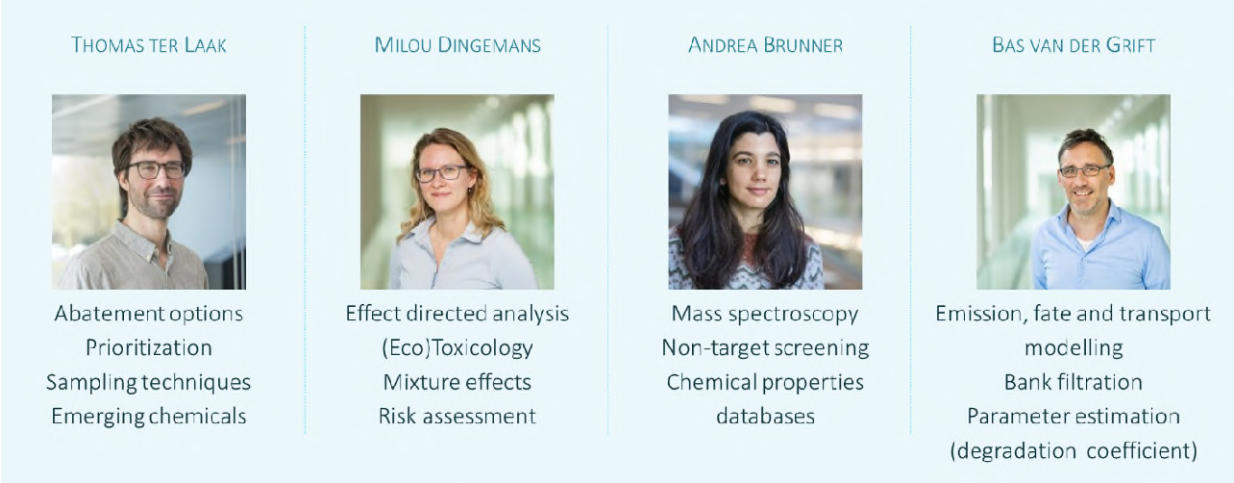


Figure 2 Expert reviewers and area of expertise

Figure 3 Explanation of the Technology Readiness Level

1.3 Proposed Pilot Studies

Four projects were proposed to the Chemical Safety theme group (Figure 4), click the links below to go to the summary of each the results and explanation of proposed pilot studies;

- R1 - Integrating Chemical Analysis and Bioanalysis to Evaluate the Contribution of Wastewater Effluent on the Micropollutant Burden in Small Streams
- R6 - Effect-Directed Analysis Supporting Monitoring of Aquatic Environments — An in-Depth Overview
- R7 - Multicriteria Approach to Select Polyaromatic River Mutagen Candidates
- R17 - The Uncertainty of Biodegradation Rate Constants of Emerging Organic Compounds in Soil and Groundwater – A Compilation of Literature Values for 82 Substances

In the July meeting the Chemical Safety theme group voted to go forward with the pilot study for R17 – degradation rate database.

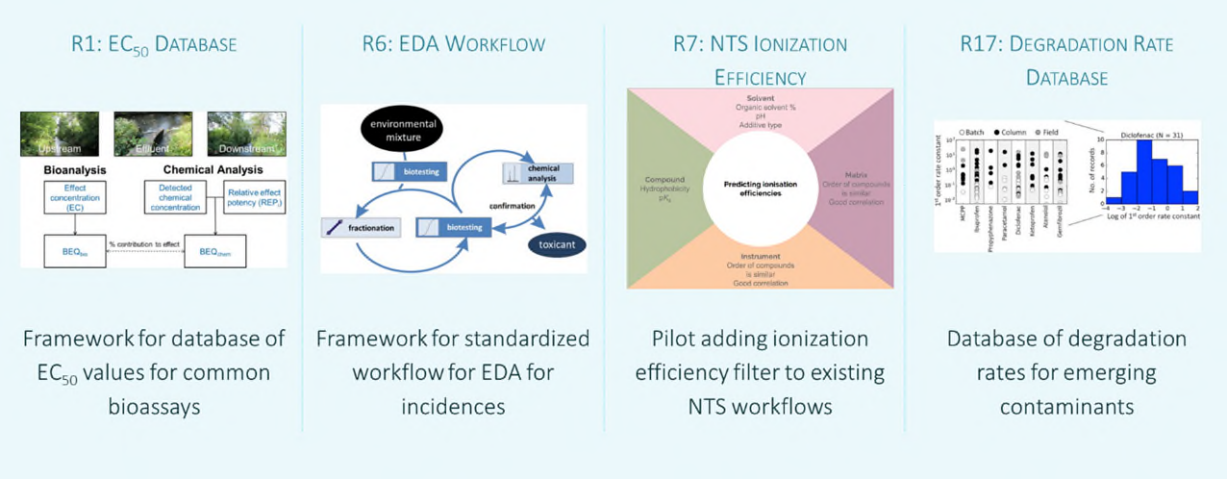


Figure 4 Four results proposed to the Chemical Safety theme group for a pilot study

1.4 Pilot Study

Publication

The publication from J. Greskowiak et al. (2017) was a literature review of degradation rates of emerging contaminants in soil and groundwater. The aim of the review was to assess the uncertainty of the fate of emerging organic contaminants in hydrological models. From the literature, first order degradation rates were extracted or calculated based on the data presented. This data was compiled in an excel database which was accessible via the supplementary information on the journal site. However, an alternative copy of the database was obtained directly from the authors to avoid any issues of copyright regarding the published database. The database itself contains 519 data points from 48 publications on 82 emerging contaminants. There are a range of experimental scales included (bench/column/field), redox conditions, a variety of source waters (e.g. surface water groundwater, tap water, wastewater), and sediment types (e.g. soil, river bed, technical sand, glass beads). The database is being incorporated into a tool currently being developed at KWR – AquaPriori.

AquaPriori

AquaPriori is a being developed at KWR within the Drinking Water Treatment team by Dirk de Vries and Martin Korevaar. The tool can determine the removal efficiency for non-tested, priority substances in water treatment

processes (Vries et al., 2017). Studies into the effectiveness of water treatments processes can be costly and are related to specific conditions including the type of treatment, substances present and specific process conditions. If sufficient data are available about the removal of certain substances, the expected removal rate can be statistically related to molecular properties of the substances. This is known as quantitative structure activity relationships (QSAR) or quantitative structural property relationships (QSPR). These relationships, in combination with knowledge about the removal process, can be used to statistically predict the removal efficiency for new, emerging or unknown substances (Vries et al., 2017).

The tool is currently being developed for two processes, activated carbon and reverse osmosis. A demo tool was developed in a previous project which is able to determine the removal efficiency for a, as yet untested, substance using QSPR and process properties (Figure 5). The application is also able to show similar substances for which there is known data and the uncertainty of the QSPR (Vries et al., 2017).

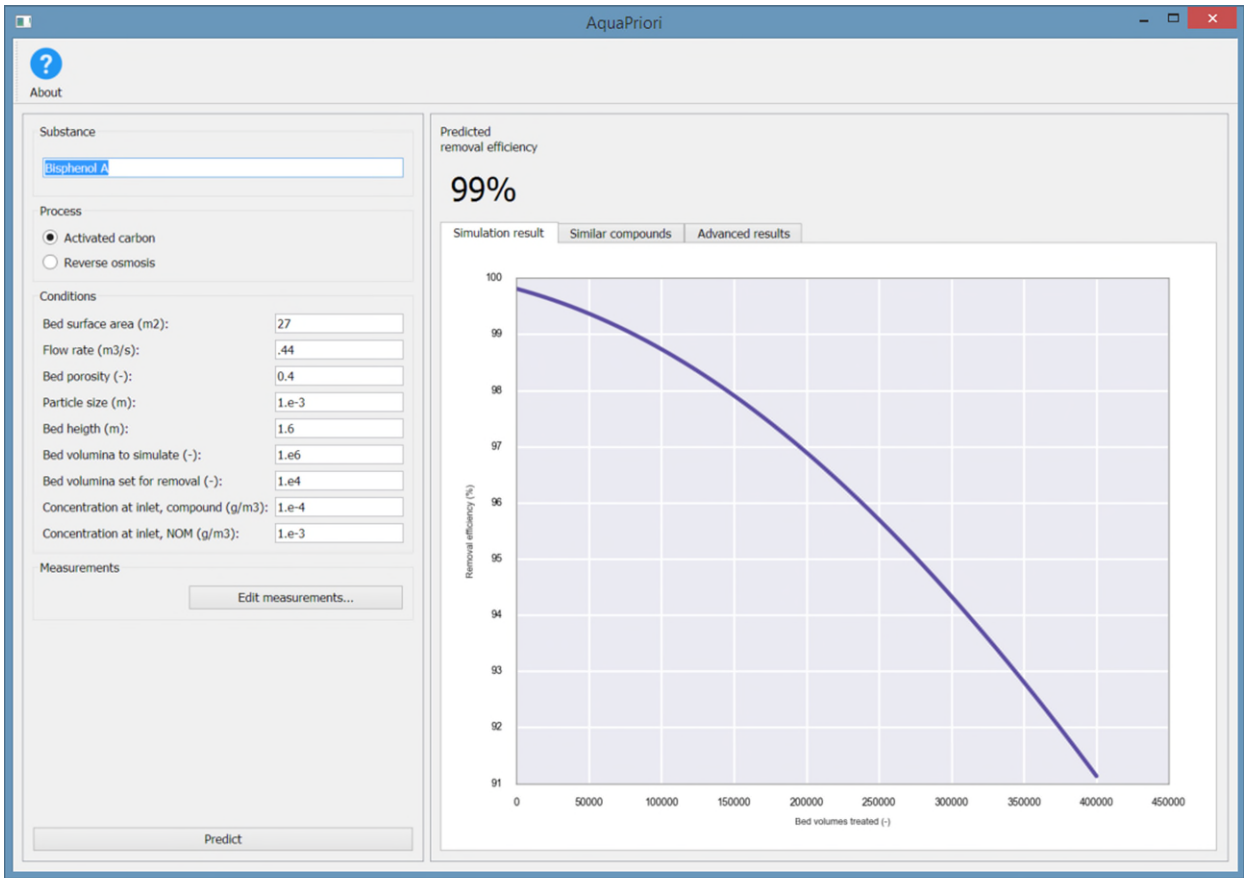


Figure 5 Screenshot from previously developed AquaPriori demo-tool showing the removal efficiency of bisphenol A by activated carbon as a function of the bed volume, which is a measured of the amount of treated water passed through the activated carbon (Vries et al., 2017)

AquaPriori and SOLUTIONS

Adding the database of degradation rates from the SOLUTIONS results to the AquaPriori tool is good fit for both projects for a number of reasons.

- As the AquaPriori tool is still in the development stage, the provided degradation rate data are able to be incorporated from the start. This ensures proper integration of the data within the tool.

- Within this pilot project there would not have been the funds to develop a functioning database from the excel file, let alone a working tool to access the data, while this is possible by coupling the data to AquaPriori.

- AquaPriori is focused on the removal of substances which have not been previously tested – these substances match well with the data from the publication on emerging organic contaminants.

- The underlying principle of QSPR is also applicable to biological processes, where the biodegradability of substances also be linked to substance properties via quantitative structure biodegradability relationships (QSBRs) (Vries et al., 2017).

- There was also the ambition from AquaPriori's side to incorporate more treatment processes into the tool and this database fulfills that wish – the data provided can be used to evaluate the removal efficiency of processes such as soil or dune passage.

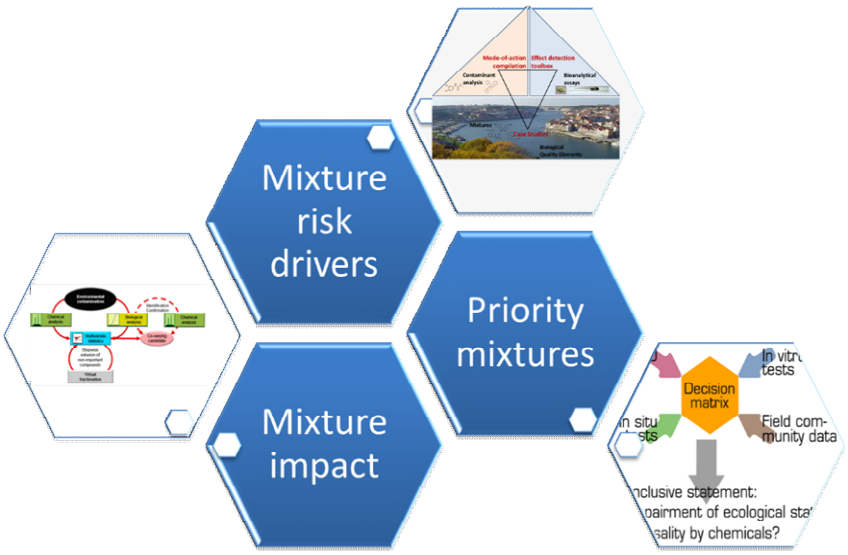
For more information about the development of AquaPriori please contact Dirk de Vries (dirk.vries@kwrwater.nl) and Martin Korevaar (martin.korevaar@kwrwater.nl).

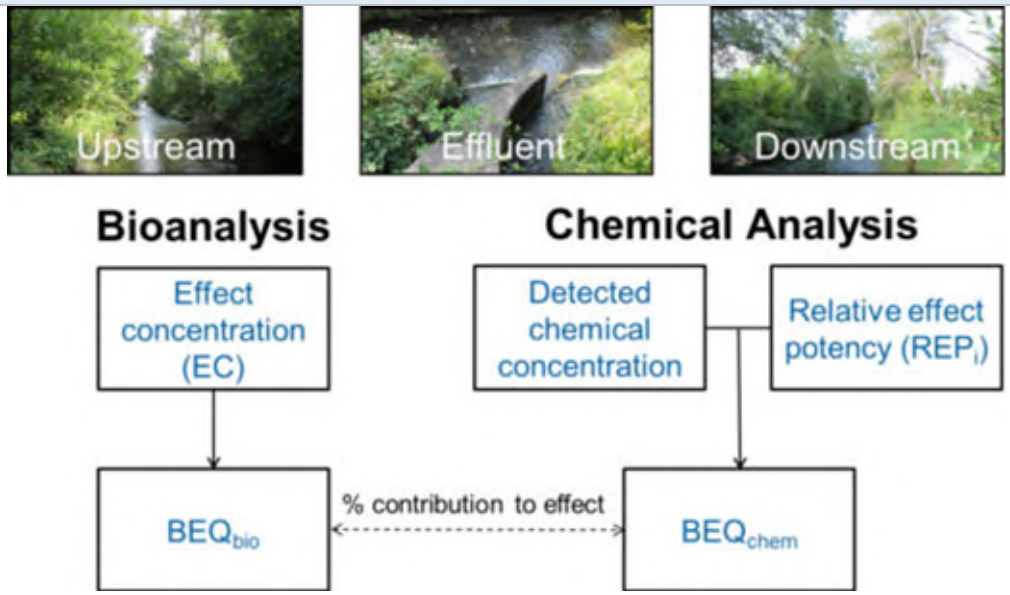
2 Summary of results and products

Table 1 Explanation of the summary table for the results

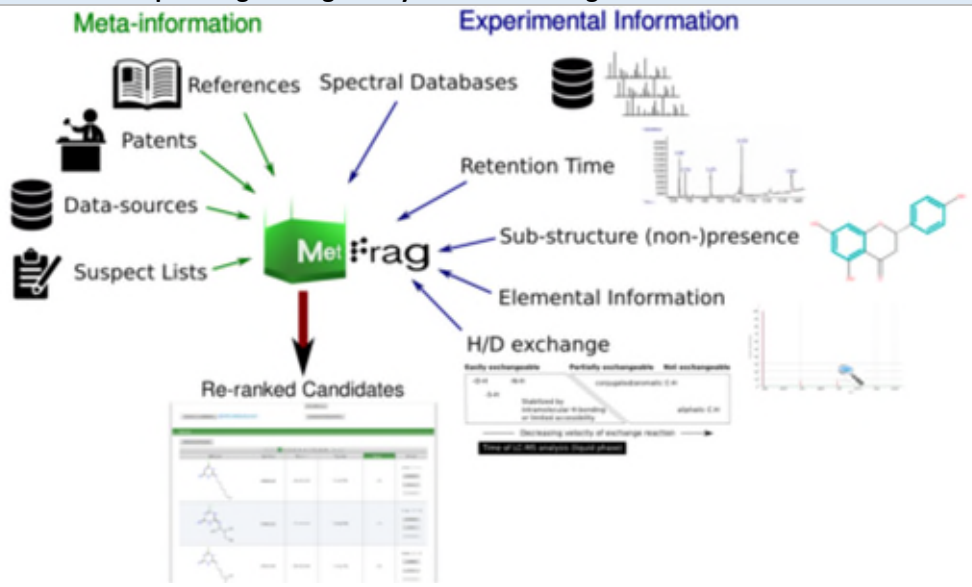
R# (result number) - Title of the Result	
Graphic	*Graphical abstract, if given*
Description (from website)	*Description of the result from the SOLUTIONS website, https://www.solutions-project.eu/*
Abstract (Paper)	*Abstract of the journal article or summary of the deliverable/working paper*
Source	*What kind of result (journal article, working paper, deliverable)*
Link	*Link to the result*
Citation	*Citation of the result*
Tool Type	*The type of tool (e.g. model, framework, sampling technique etc)*
Technology	*What the tool/technology does*
Summary	*Short, 1-2 sentence highlight of the result*
Reviewer	*Expert reviewer of the tool*
Use	*Possible use by KWR, drinking water companies or other partners of the tool*
TRL	*Technology readiness level of the result, from 1-9*
	Reasoning for score given for the TRL
Relevance	*Relevance of the result/tool for KWR, drinking water company or partner organization*
	Reasoning for the score given for relevance, other notes about the tool
Applicability	*Score for the applicability of the tool for the Dutch drinking water sector*
	[add possible applications of the tool for the Dutch drinking water sector]

2.1 Monitoring Tools

Graphic	
Description (from website)	Water quality monitoring is challenged with providing the basis for safeguarding the environment against adverse biological effects of anthropogenic chemical contamination. This requires advanced experimental techniques for sampling, chemical and biological analytics, as well as strategies of how to employ tools for specific monitoring purposes. This product describes three routes to link the occurrence of chemical mixtures to the assessment of adverse biological effects. 1. Advanced sampling, multi-residue target and non-target screening techniques covering a broader range of chemicals co-occurring in the environment. By improving sensitivity and detection limits for known bioactive compounds of concern, new analytical chemistry data can be used to identify river-basin specific pollutants. 2. Bioanalytical tools explored to provide aggregate measures integrating all components that produce adverse outcomes even for mixtures of varying compositions and thus allow comprehensive impact assessment. 3. Effect-directed analysis (EDA) advanced to identify major drivers of mixture toxicity by improving cause-effect relationships. The approaches suggested were explored in studies at Danube and Rhine basins, and also in rivers of the Iberian Peninsula. Guidance for use of specific monitoring tools is also provided through the SOLUTIONS RiBaTox software.

R1 - Integrating Chemical Analysis and Bioanalysis to Evaluate the Contribution of Wastewater Effluent on the Micropollutant Burden in Small Streams	
Graphic	
Description (from website)	SOLUTIONS applied chemical and biological analyses to assess the micropollutant burden during low flow conditions up- and down-stream of three wastewater treatment plants discharging into small streams in the Swiss Rhine catchment Neale, Munz et al., 2017. Chemical analysis included 405 organic substances, while the applied bioassays comprised 13 different endpoints, representing different stages of cellular toxicity pathways including xenobiotic metabolism, receptor-mediated effects and adaptive stress responses, as well as whole organism effects. As expected, chemical and bio-analyses showed higher chemical concentrations and effects for effluent samples, with the lowest chemical concentrations and effects in most assays for the upstream sites. While chemical analysis showed differences in the chemical pollution profiles at the different sampling locations, bioanalysis provided information about the mixture effects of additional chemicals in the samples. Mixture toxicity modeling was performed to assess the contribution of detected chemicals to the observed effect. For most bioassays, very little of the observed effects could be explained by the detected chemicals which emphasizes the importance of combining bioanalysis with chemical analysis to provide a more complete picture of the micropollutant burden. However, the lack of effect data for the detected micropollutants in the different assays was a major limitation and more data is needed for a significant improvement of the mixture modeling. Further, both chemical and bio-analyses showed relevant contribution of diffuse sources from upstream during low flow conditions – besides the significant contribution of wastewater effluents to the micropollutant burden downstream - uggesting that improved wastewater treatment technology will not completely reduce the micropollutant burden, which renders additional source control measures also necessary.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0048969716323312
Citation	Neale, P. A.; Munz, N. A.; Aït-Aïssa, S.; Altenburger, R.; Brion, F.; Busch, W.; Escher, B. I.; Hilscherová, K.; Kienle, C.; Novák, J.; et al. Integrating Chemical Analysis and

	Bioanalysis to Evaluate the Contribution of Wastewater Effluent on the Micropollutant Burden in Small Streams. *Sci. Total Environ.* **2017**, *576*, 785–795. https://doi.org/10.1016/j.scitotenv.2016.10.141.
Tool	Chemical analysis support
Technology	Mass balance model
Summary	Mixture toxicity modelling to determine what percent of a chemical analysis can explain the bioassay response.
Reviewer	Milou Dingemans
Use	Integrate chemical and bioassay results for water quality monitoring
TRL	5
	First application of the mass balance model from chemical analysis to bioassays
Relevance	8
	There is interest in quantifying what chemicals are responsible for bioassay responses in water quality monitoring already. If bioassay responses are observed that cannot be explained by the chemicals measured, further research is needed to identify the unknown emerging chemicals can be responsible for the observed effect.
Applicability	9
	This method can be used to evaluate whether the observed effects in bioassay can be explained by measured target chemicals, which if not, can point towards a source (emission) of emerging chemicals that induce effects. However, this method requires toxicity information (EC50 values in the applied bioassay) for the individual chemicals of which concentrations are measured using chemical methods. This information can be collected from the ToxCast database, although not every bioassay commonly used in water quality monitoring is included here. That information needs to be harvested from literature. It is recommended to collect this information in a (NORMAN) database.
Proposed Pilot Study	The pilot study would compile a database of EC_{50} values for commonly applied bioassays in water quality monitoring. Often, toxicity data is lacking and it is difficult to find the data in the literature. A database would collect the information in an easily accessible way to streamline effect based analyses.

R2 - MetFrag Relaunched: Incorporating Strategies beyond in Silico Fragmentation	
Graphic	
Description (from website)	MetFrag is a freely available software for the annotation of accurate tandem mass spectra of small molecules such as metabolites and substances of environmental interest. Annotation is a first and critical step for the identification of a molecular structure. Candidate molecules from various databases are fragmented in silico and matched against mass to charge values. A score calculated using the fragment peak matches indicates the quality of the candidate spectrum assignment. MetFrag, launched in 2010, was one of the first approaches combining compound database searching and fragmentation prediction for the identification of small molecules from tandem mass spectrometry data. Since then many new approaches have evolved, including MetFrag itself within SOLUTIONS. Ruttkies et al. 2016 details the latest developments to MetFrag and its use in small molecule identification since the original publication. A great benefit is the addition of different information sources, beyond in silico fragmentation, into the identification workflow, reducing user workloads and improving the structure elucidation process.
Abstract	The in silico fragmenter MetFrag, launched in 2010, was one of the first approaches combining compound database searching and fragmentation prediction for small molecule identification from tandem mass spectrometry data. Since then many new approaches have evolved, as has MetFrag itself. This article details the latest developments to MetFrag and its use in small molecule identification since the original publication. MetFrag has gone through algorithmic and scoring refinements. New features include the retrieval of reference, data source and patent information via ChemSpider and PubChem web services, as well as InChIKey filtering to reduce candidate redundancy due to stereoisomerism. Candidates can be filtered or scored differently based on criteria like occurrence of certain elements and/or substructures prior to fragmentation, or presence in so-called “suspect lists”. Retention time information can now be calculated either within MetFrag with a sufficient amount of user-provided retention times, or incorporated separately as “user-defined scores” to be included in candidate ranking. The changes to MetFrag were evaluated on the original dataset as well as a dataset of 473 merged high resolution tandem mass spectra (HR-MS/MS) and compared with another open

	source in silico fragmenter, CFM-ID. Using HR-MS/MS information only, MetFrag2.2 and CFM-ID had 30 and 43 Top 1 ranks, respectively, using PubChem as a database. Including reference and retention information in MetFrag2.2 improved this to 420 and 336 Top 1 ranks with ChemSpider and PubChem (89 and 71 %), respectively, and even up to 343 Top 1 ranks (PubChem) when combining with CFM-ID. The optimal parameters and weights were verified using three additional datasets of 824 merged HR-MS/MS spectra in total. Further examples are given to demonstrate flexibility of the enhanced features. In many cases additional information is available from the experimental context to add to small molecule identification, which is especially useful where the mass spectrum alone is not sufficient for candidate selection from a large number of candidates. The results achieved with MetFrag2.2 clearly show the benefit of considering this additional information. The new functions greatly enhance the chance of identification success and have been incorporated into a command line interface in a flexible way designed to be integrated into high throughput workflows. Feedback on the command line version of MetFrag2.2 available at http://c-ruttkies.github.io/MetFrag/ is welcome.
Source	Journal Paper
Link	https://jcheminf.biomedcentral.com/articles/10.1186/s13321-016-0115-9
Citation	Neumann, S.; Ruttkies, C.; Hollender, J.; Schymanski, E. L.; Wolf, S. MetFrag Relaunched: Incorporating Strategies beyond in Silico Fragmentation. *J. Cheminform.* **2016**, *8* (1), 1–16. https://doi.org/10.1186/s13321-016-0115-9.
Tool Type	Chemical analysis support
Technology	Open source software for annotating mass spectra of small molecules from non-target screening
Summary	In-silico fragmentation of candidates to identify unknown small molecules from chemical analysis (suspect screening)
Reviewer	Andrea Mizzi Brunner
Use	Used for non-target/suspect screening for water quality monitoring, finding metabolite and other small molecules
TRL	9
	Software in use already since 2009, this is a release of new updates to the program
Relevance	10
	Already in use at KWR, HWL, Vitens, WLN
Applicability	Already in use at KWR, both web based GUI and R package
	Implementation at the drinking water laboratories: MetFrag introduction and tutorial was part of a workshop on non-target screening KWR organized in December 2017 within the BTO project "Mass Spectrometry: tools for unknown IDs" (BTO 2017.073); implementation of MetFrag in R was presented and applied in a non-target screening data analysis workshop KWR organized in March 2019 within the

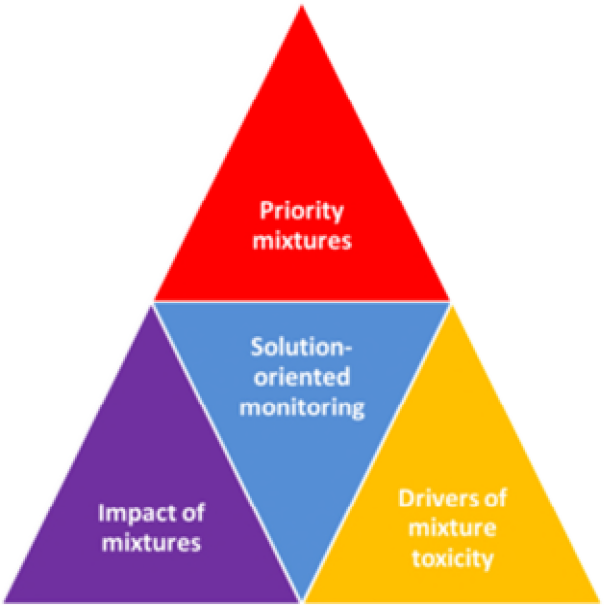
BTO project “Non-target screening to identify unknowns: Automation and increasing confidence” (BTO 2019.032).

R3 - Assessment of a Novel Device for Onsite Integrative Large-Volume Solid Phase Extraction of Water Samples to Enable a Comprehensive Chemical and Effect-Based Analysis	
Abstract	The implementation of targeted and non-targeted chemical screening analysis in combination with in vitro and organism-level bioassays is a prerequisite for a more holistic monitoring of water quality in the future. For chemical analysis, little or no sample enrichment is often sufficient, while bioanalysis often requires larger sample volumes at a certain enrichment factor for conducting comprehensive bioassays on different endpoints or further effect-directed analysis (EDA). To avoid logistic and technical issues related to the storage and transport of large volumes of water, sampling would benefit greatly from onsite extraction. This study presents a novel onsite large volume solid phase extraction (LVSPE) device tailored to fulfill the requirements for the successful effect-based and chemical screening of water resources and complies with available international standards for automated sampling devices. Laboratory recovery experiments using 251 organic compounds in the log D range from − 3.6 to 9.4 (at pH 7.0) spiked into pristine water resulted in acceptable recoveries and from 60 to 123% for 159 out of 251 substances. Within a European-wide demonstration program, the LVSPE was able to enrich compounds in concentration ranges over three orders of magnitude (1 ng L− 1 to 2400 ng L− 1). It was possible to discriminate responsive samples from samples with no or only low effects in a set of six different bioassays (i.e. acetylcholinesterase and algal growth inhibition, androgenicity, estrogenicity, fish embryo toxicity, glucocorticoid activity). The LVSPE thus proved applicable for onsite extraction of sufficient amounts of water to investigate water quality thoroughly by means of chemical analysis and effect-based tools without the common limitations due to small sample volumes.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0048969716328303
Citation	Schulze, T.; Ahel, M.; Ahlheim, J.; Aït-Aïssa, S.; Brion, F.; Di Paolo, C.; Froment, J.; Hidasi, A. O.; Hollender, J.; Hollert, H.; et al. Assessment of a Novel Device for Onsite Integrative Large-Volume Solid Phase Extraction of Water Samples to Enable a Comprehensive Chemical and Effect-Based Analysis. *Sci. Total Environ.* **2017**, *581–582* (December 2016), 350–358. https://doi.org/10.1016/j.scitotenv.2016.12.140.
Tool Type	Sampling Technique
Technology	Large volume solid phase extraction
Summary	LVSPE for up to 50L which is able to extract and enrich samples on site, suitable for chemical and bioassay analysis
Reviewer	Thomas ter Laak
Use	Environmental sampling for polar and /or low concentration (CEC, micropollutants) substances
TRL	6 Machine is a prototype with limited field and laboratory testing, current regular application for drinking water companies requires a further developed tool. Tool is interesting for research purposes.

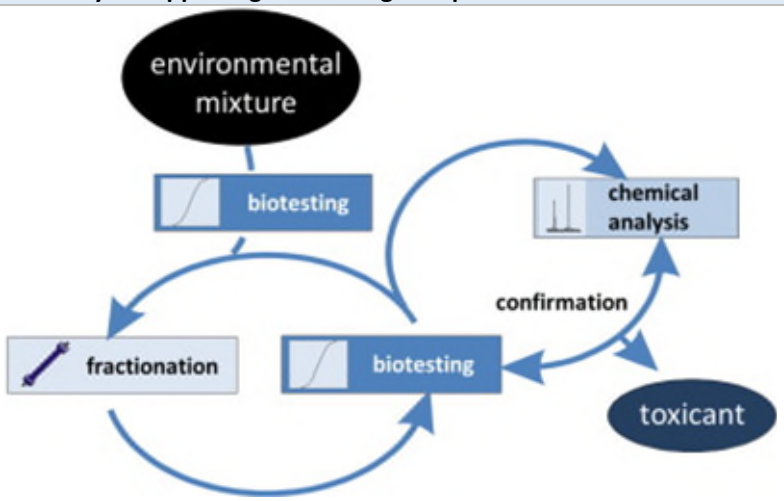
	Additionally, part of the knowledge is (applied sorbents, tested range of chemicals) is very valuable fit testing in laboratories as well.
Relevance	8
	What the current alternative methods comparison with cost? For the more polar substances, sampling water and extraction *ex situ* fulfills most needs for DW companies. For chemical analysis direct injection generally meets the requirements, The applicability for groundwater or along treatment trains is currently not tested and might require additional studies for implementation. All in all, there is no direct urge to apply this tool as it was designed. For bioassays, sample concentration is required. *Ex situ* extractions hold some advantages such as controllable conditions that can improve accuracy as well as application range, considering properties of chemicals. However, such an *in situ* tool might in future be very valuable to retrospectively monitor peaks of contaminants in sources (mainly surface waters since these have a more dynamic character) to see the evolution of contaminants in the source and drinking water treatment train after a potential contamination-event. These application probably need a tool that has a bit higher TRL.
Applicability	6
	Such an *is situ* tool might in future be very valuable to retrospectively monitor peaks of contaminants in sources / intake water (mainly surface waters since these have a more dynamic character) to see the evolution of contaminants in the source and drinking water treatment train after a potential contamination-event. Probably, the implementation can be integrated with available water transport and pressure, to no active pumping installation but only the extraction cartridges can be applied and stored after a given exposure time window. This allows to collect a library of chemical water quality parameters that can be assessed/studied either as a monitoring activity or initiated by specific (contamination) events. It allows to evaluate water quality continuously, even though it will always have a retrospective character, as the quality of the water tested is sampled / extracted in a time window before the actual analysis. These proposed applications need a tool that has a bit higher TRL and customization to the drinking water treatment schemes. Subsequently, evaluation of extraction efficiency in relation to *in situ* concentrations and concentration-profiles (e.g. sampling kinetics, saturation, competition aspects) as well as technical implementation and validation of the whole system is required before application in the DW sector as a monitoring tool.

R4 – Solutions for Present and Future Emerging Pollutants in Land and Water Resources Management: Guidelines Describing Passive Sampling and Analytical Aspects of the Procedure for Relevant Compounds	
Abstract	Passive sampling is a powerful tool that can conveniently be used for monitoring of organic compounds in water and other environmental compartments. It has been designed to provide estimates of freely dissolved concentrations which have been shown to be in many cases most appropriate to explain exposure and adverse effects in biota. Partition based passive sampling also allows direct comparison of measured water concentrations with concentrations in diverse compartments (e.g. water, sediment, biota), based on the assessment of chemical activity in those matrices. The time-integrating character of sampling 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. Thus, it is suitable for assessment of pollutant trends in water bodies. This internal deliverable of the SOLUTIONS project provides a practical guidance on the use of passive samplers for monitoring organic pollutants in water. Two categories of passive samplers are addressed. The first category comprises partition-based samplers for the measurement of non-polar contaminants, and the guidance sets focus on silicone rubber based samplers, which have been widely applied in the SOLUTIONS project. The second category encompasses adsorption passive samplers for monitoring more polar aquatic contaminants; the typically applied samplers are based on the use of sorbents designed for solid-phase extraction. This guidance should assist users of passive samplers, who wish to implement passive sampling methods in their research or monitoring work, as well as more experienced users in the use of the available methods according to the state-of-the art. The guideline addresses principles of passive sampling, sampler preparation, field deployment, laboratory processing, chemical analysis, calculation of aqueous concentrations and associated uncertainty considerations. Aspects of quality assurance are also addressed. Finally, practical examples of sampler operation and sample processing procedures are provided, which have been developed and applied within the SOLUTIONS project.
Source	Report Guideline
Link	http://www.solutions-project.eu/wp-content/uploads/2017/01/SOLUTIONS_Guidelines_Passive_Sampling.pdf
Citation	Vrana, B.; Smedes, F.; Hilscherová, K.; Rusina, T.; Okonski, K.; Novák, J. *Solutions for Present and Future Emerging Pollutants in Land and Water Resources Management: Guidelines Describing Passive Sampling and Analytical Aspects of the Procedure for Relevant Compounds*; 2017.
Tool Type	Sampling Technique
Technology	Passive sampling guide
Summary	Practical guideline for using passive samplers for monitoring organic pollutants in water
Reviewer	Thomas ter Laak

Use	Reference guide for using passive samplers, check current procedures for use of passive samples and/or monitoring of organic micropollutants against guidelines for new ideas/validation (state of the art)
TRL	9*
	*for passive samplers themselves (commercially available, widely used) but possible that specific kinds of samplers suitable for more polar substances are <9
Relevance	7
	Passive sampling has been applied in the drinking water sector and in groundwater monitoring on a limited scale (Bäuerlein, Mansell et al. 2011, de Jonge and Rothenberg 2005). Passive sampling is a very powerful tool in studying presence and concentrations of the more hydrophobic chemicals in low concentrations, but quantification of more polar and ionic chemicals turns out to be more complicated and very circumstantial. Rendering an (currently) more qualitative than qualitative tool. It is worth wile explore possibilities of these tools for the drinking water sector but as stated in R3, this will initially have a very experimental character. Furthermore it should be focused on the advantage of time integrated sampling rather than being an alternative of common sampling of water, as the benefits are in the time integrated character rather than in the mere *in situ*" application, since this comes with benefits and drawbacks. Often the drawbacks might be considered more important than the advantages.
Applicability	Reference guide for using passive samplers, check current procedures for use of passive samples and/or monitoring of organic micropollutants against guidelines for new ideas/validation (state of the art)
	9*

R5 - Future Water Quality Monitoring: Improving the Balance between Exposure and Toxicity Assessments of Real-World Pollutant Mixtures	
Graphic	
Abstract	Environmental quality monitoring of water resources is challenged with providing the basis for safeguarding the environment against adverse biological effects of anthropogenic chemical contamination from diffuse and point sources. While current regulatory efforts focus on monitoring and assessing a few legacy chemicals, many more anthropogenic chemicals can be detected simultaneously in our aquatic resources. However, exposure to chemical mixtures does not necessarily translate into adverse biological effects nor clearly shows whether mitigation measures are needed. Thus, the question which mixtures are present and which have associated combined effects becomes central for defining adequate monitoring and assessment strategies. Here we describe the vision of the international, EU-funded project SOLUTIONS, where three routes are explored to link the occurrence of chemical mixtures at specific sites to the assessment of adverse biological combination effects. First of all, multi-residue target and non-target screening techniques covering a broader range of anticipated chemicals co-occurring in the environment are being developed. By improving sensitivity and detection limits for known bioactive compounds of concern, new analytical chemistry data for multiple components can be obtained and used to characterize priority mixtures. This information on chemical occurrence will be used to predict mixture toxicity and to derive combined effect estimates suitable for advancing environmental quality standards. Secondly, bioanalytical tools will be explored to provide aggregate bioactivity measures integrating all components that produce common (adverse) outcomes even for mixtures of varying compositions. The ambition is to provide comprehensive arrays of effect-based tools and trait-based field observations that link multiple chemical exposures to various environmental protection goals more directly and to provide improved in situ observations for impact assessment of mixtures. Thirdly, effect-directed analysis (EDA) will be applied to identify major drivers of mixture toxicity. Refinements of EDA include the use of statistical approaches with monitoring information for guidance of experimental EDA studies. These three approaches will be explored using case studies at the Danube and Rhine river basins as well as rivers of the Iberian

	Peninsula. The synthesis of findings will be organised to provide guidance for future solution-oriented environmental monitoring and explore more systematic ways to assess mixture exposures and combination effects in future water quality monitoring.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0048969714017598
Citation	Altenburger, R.; Brack, W.; Burgess, R. M.; Busch, W.; Escher, B. I.; Focks, A.; Mark Hewitt, L.; Jacobsen, B. N.; de Alda, M. L.; Ait-Aissa, S.; et al. Future Water Quality Monitoring: Improving the Balance between Exposure and Toxicity Assessments of Real-World Pollutant Mixtures. *Environ. Sci. Eur.* **2019**, *31* (1), 12. https://doi.org/10.1186/s12302-019-0193-1.
Tool Type	Sampling Technique; Bioanalytical Tool; Effect Directed Analysis
Technology	Guide for integrating chemical and effect-based monitoring
Summary	Assessing monitoring results benefits substantially from obtaining and linking information on the occurrence of both chemicals and potentially adverse biological effects. (1) identify, (2) asses impact on aquatic ecosystem, (3) quantify cause-effect relationships between contaminants and adverse effects
Reviewer	Milou Dingemans
Use	Better integration in water quality monitoring of chemical and biological (effect based) qualities
TRL	6/7
	A few case studies (separate papers) for the framework, but not yet widely applied
Relevance	8
	There is interest in integrating chemical and biological analyses in water quality monitoring
Applicability	4 (policy brief with overview of SOLUTIONS developments and recommendations)
	This is a policy brief giving an overview of sampling and innovative monitoring methods (chemical target, suspect and non-target analyses). 'Major improvements for broader applicability include tailored sampling techniques, screening and identification techniques for a broader and more diverse set of chemicals, higher detection sensitivity, standardized protocols for chemical, toxicological, and ecological assessments combined with systematic evidence evaluation techniques.' This document provides a very good overview and 'suggests systematic ways to deal with mixture exposures and combined effects in a more balanced way, and thus provides guidance for future tailored environmental monitoring.'

R6 - Effect-Directed Analysis Supporting Monitoring of Aquatic Environments — An in-Depth Overview	
Graphic	
Abstract	Aquatic environments are often contaminated with complex mixtures of chemicals that may pose a risk to ecosystems and human health. This contamination cannot be addressed with target analysis alone but tools are required to reduce this complexity and identify those chemicals that might cause adverse effects. Effect-directed analysis (EDA) is designed to meet this challenge and faces increasing interest in water and sediment quality monitoring. Thus, the present paper summarizes current experience with the EDA approach and the tools required, and provides practical advice on their application. The paper highlights the need for proper problem formulation and gives general advice for study design. As the EDA approach is directed by toxicity, basic principles for the selection of bioassays are given as well as a comprehensive compilation of appropriate assays, including their strengths and weaknesses. A specific focus is given to strategies for sampling, extraction and bioassay dosing since they strongly impact prioritization of toxicants in EDA. Reduction of sample complexity mainly relies on fractionation procedures, which are discussed in this paper, including quality assurance and quality control. Automated combinations of fractionation, biotesting and chemical analysis using so-called hyphenated tools can enhance the throughput and might reduce the risk of artifacts in laboratory work. The key to determining the chemical structures causing effects is analytical toxicant identification. The latest approaches, tools, software and databases for target-, suspect and non-target screening as well as unknown identification are discussed together with analytical and toxicological confirmation approaches. A better understanding of optimal use and combination of EDA tools will help to design efficient and successful toxicant identification studies in the context of quality monitoring in multiply stressed environments.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0048969715310834
Citation	Brack, W.; Hollert, H.; De Aragão Umbuzeiro, G.; Kool, J.; Lamoree, M.; Seiler, T.-B.; Krauss, M.; Schymanski, E. L.; Mark Hewitt, L.; Muschket, M.; et al. Effect-Directed Analysis Supporting Monitoring of Aquatic Environments — An in-Depth Overview. Sci. Total Environ. 2016, 544, 1073–1118. https://doi.org/10.1016/j.scitotenv.2015.11.102.

Tool Type	Effect Directed Analysis
Technology	Best practice for Effect directed analysis testing (framework)
Summary	Effect Directed Analysis: structural identification of bioactive chemicals and assessment of their contribution to overall endpoint-specific activity. Combines biological testing and physio-chemical separation procedures to isolate toxic fractions and compounds followed by chemical analysis (e.g. GC-MS)
Reviewer	Milou Dingemans
Use	Application of EDA on water samples, improve identification of toxic substances in mixtures. Creation of new EDA sampling programs.
TRL	7
	This is a framework for applying many well established techniques (bioassays, chemical analysis, chemical preparation techniques) all together in an integrated manner
Relevance	8
	There is interest in integrating chemical and biological analyses in water quality monitoring
Applicability	9
	For mitigation purposes it is needed to identify the unknown emerging chemical(s) that may be responsible for bioassay effects and potentially associated adverse outcomes. This can be done by Effect-Directed Analysis (EDA), which involves making fractions of the complex mixtures. Identifying the active fraction allows better chemical analyses to track the culprit chemical. In the Dutch drinking water sector a standardized workflow can be developed. Such a workflow [fractionation, testing in fast effect-based assays and (non-target) chemical methods] could also be used in in case of incidents.
Proposed Pilot Study	Often, when incidences or crises occur, swift action is needed to identify contamination. This cannot necessarily be addressed using targeted analysis alone. EDA is designed to meet this challenge. However, a workflow is needed which can be implemented swiftly. The pilot study would develop a standardized workflow for EDA implementation at KWR. A workflow is also being developed at HWL, however KWR's role would be more focused on implementation in the case of incidents or crises.

R7 - Multicriteria Approach to Select Polyaromatic River Mutagen Candidates	
Abstract	The identification of unknown compounds remains one of the most challenging tasks to link observed toxic effects in complex environmental mixtures to responsible toxicants in effect-directed analysis (EDA). Here, a workflow is presented based on non-target liquid chromatography-high resolution mass spectrometry (LC-HRMS) starting with molecular formulas determined in a previous study. A compound database search (ChemSpider) was performed to retrieve candidates for each formula. Subsequently, the number of candidates was reduced by applying MS-, physical-chemical, and chromatography-based selection criteria including HRMS/MS fragmentation and plausibility, ionization efficiency with different ion sources and detection modes, acid/base behavior, octanol/water partitioning, retention time prediction and finally toxic effects (mutagenicity caused by aromatic amines). The workflow strongly decreased the number of possible candidates and resulted in the tentative identification of possible mutagens and the positive identification of the non-mutagen benzyl(diphenyl) phosphine oxide in a mutagenic fraction. The positive identification of mutagens was hampered by a lack of commercially available standards. The workflow is an innovative and promising approach and forms an excellent basis for possible further advancements.
Source	Journal Paper
Link	https://pubs.acs.org/doi/abs/10.1021/es503640k
Citation	Gallampois, C. M. J.; Schymanski, E. L.; Krauss, M.; Ulrich, N.; Bataineh, M.; Brack, W. Multicriteria Approach to Select Polyaromatic River Mutagen Candidates. *Environ. Sci. Technol.* **2015**, *49* (5), 2959–2968. https://doi.org/10.1021/es503640k.
Tool Type	Bioanalytical Tool
Technology	Workflow for non-target LC-HRMS from chemical formulas from a database (ChemSpider)
Summary	Workflow decreased the number of possible candidates and resulted in tentative identification of possible mutagens. Candidates were screened by applying MS-, physical-chemical and chromatography based selection criteria, including HRMS/MS fragmentation, acid-base behavior, octanol-water partitioning, retention time prediction and final toxic effects (mutagenicity from aromatic amines)
Reviewer	Andrea Mizzi Brunner
Use	Extensive refinements of compound database searches to allow for quicker candidate selection based on optimized use of the analytical and toxicological information available
TRL	4
	The paper presents a defined strategy, but not an actual workflow, i.e. no software, or R package. Implementation requires information of the various steps such as ionization efficiency, fragmentation interpretation, and retention time data, to be retrieved and an automated workflow to be generated.
Relevance	8

	To date the high number of features, i.e. unique combinations of accurate mass and retention time, resulting from NTS renders structural identification virtually impossible and prioritization is required. In particular, the implementation of retention time prediction, ionization behavior and exclusion of candidate toxicants can support prioritization and ultimately identification. The presented strategy is therefore of high relevance for the field of chemical water quality monitoring.
Applicability	8
	The strategy presented by Gallampois et al is tailored to polyaromatic hydrocarbons that might be mutagenic. However, parts of the strategy are already outdated, for example novel retention time prediction models are available. We recommend modular implementation of parts of the (updated) strategy for a more generic approach. 1. Metfrag score cut-off Implementation of an automatic cutoff where the distribution shows a clear break between the top candidates and the next candidates. 2. Retention time prediction and Ionization behavior / ionization efficiency prediction for quantification BTO 2020 project proposal "Improved monitoring of chemical water quality through hydroinformatics" for the thematic research group Chemical Safety proposes implementation of these steps into existing non-target screening workflows. 3. Quantitative structure activity relationships (QSARs) and structural alerts for exclusion of candidate toxicants: DPWE project proposal "Identification and risk assessment of transformation products formed through drinking water treatment" proposed implementation of QSARs and structural alerts for toxicological risk assessment of transformation products. However, structural alerts can not only be used for candidate exclusion, but also for more in depth fragmentation and thus structural elucidation of candidates. This potential is currently being addressed in BTO project "Improved non-target screening based identification through MS online prioritization" part 1" Improved identification of toxic compounds in drinking water sources through HRMS based intelligent acquisition".
Proposed Pilot Study	The pilot study would add filtering of suspects by ionization efficiency to the existing NTS workflows. This is currently done on a case-by-case basis using manual evaluation of the candidate list. However, the SOLUTIONS result reviewed included ionization behavior in the criterion for candidate selection. This would allows for quicker candidate selection and quantification. Translating signal intensities to concentrations will be key for the successful implementation of NTS in the drinking water sector, in particular for risk based monitoring strategies. The results of the pilot could already be applicable in the BTO 2020 project "Non-target screening op tijd en kwantitatief"

R8 - Metabolic Transformation as a Diagnostic Tool for the Selection of Candidate Promutagens in Effect-Directed Analysis	
Abstract	To implement metabolic activation by S9 rat liver homogenate in the selection of candidate promutagens in effect-directed analysis, we critically assessed the capability of LC-HRMS measurements to detect depletion and formation of metabolites by S9 exposure. The exposure of a reference mixture to S9 led to a depletion by >70% for most compounds. Other processes than metabolism were excluded as significant contribution to compound depletion. Metabolites formed by S9 exposure were identified and S9 metabolism was incorporated in the identification of candidate promutagens in a wastewater treatment plant (WWTP) effluent with mutagenic activity only after metabolic activation by S9. The metabolism by S9 in the WWTP effluent was confirmed. Based on a candidate exclusion of all peaks not depleted, thus not activated by the S9 mix, the number of candidate promutagens was reduced by 40%. Selected remaining candidates were evaluated and identified, but could not be confirmed as promutagens.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0269749114004023
Citation	Hug, C.; Krauss, M.; Nüsser, L.; Hollert, H.; Brack, W. Metabolic Transformation as a Diagnostic Tool for the Selection of Candidate Promutagens in Effect-Directed Analysis. *Environ. Pollut.* **2015**, *196*, 114–124. https://doi.org/10.1016/j.envpol.2014.10.003.
Tool Type	Bioanalytical Tool
Technology	Using metabolic transformation as a diagnosis tool for selecting pro-mutagens
Summary	The depletion of compounds by S9 was used to exclude candidates for the identification of promutagens in WWTP effluent fractions, this reduced the possible candidates by 40%. Formation of peaks by metabolites also considered for genotoxic effects
Reviewer	Milou Dingemans
Use	Coupling biological and chemical methods to increase efficiency in non-target screening
TRL	6/7
	novel idea, do not mention other studies which have tried this, not yet able to identify parent-metabolite compounds in complex mixes
Relevance	8
	There is interest in coupling chemical and biological analyses in water quality monitoring
Applicability	8
	This method can be used to predict or identify the presence in (waste)water of members of a specific class of chemicals, i.e. chemicals that become mutagenic

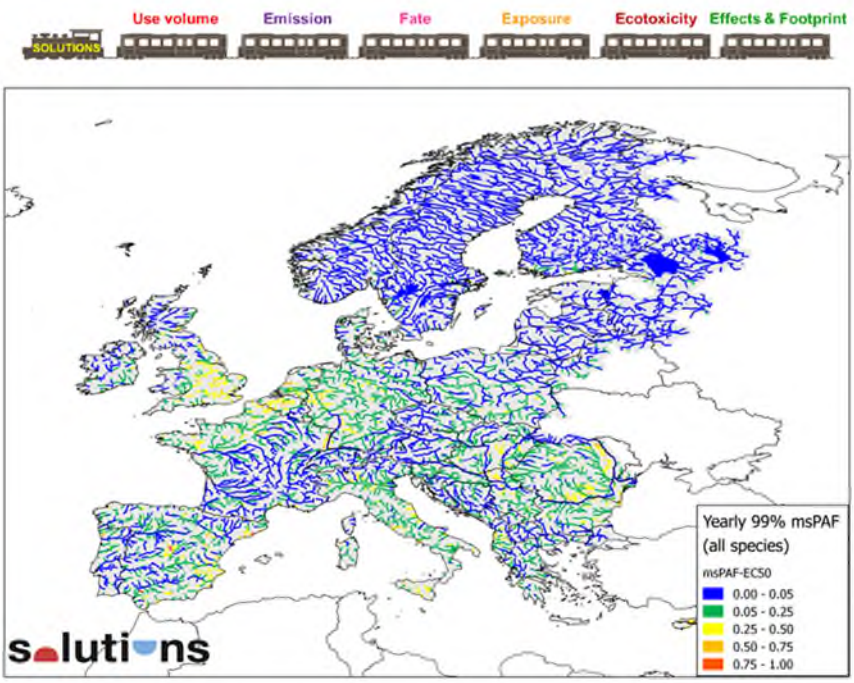
	after metabolic activation *in vivo*. Could be used to expand risk-based monitoring programs.

R9 - High-Resolution Mass Spectrometry in the Effect-Directed Analysis of Water Resources	
Note:	*No access to article*
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0166526X16300101
Citation	Krauss, M. (2016). High-Resolution Mass Spectrometry in the Effect-Directed Analysis of Water Resources. *Comprehensive Analytical Chemistry*, *71*, 433–457. https://doi.org/10.1016/BS.COAC.2016.01.010
Tool Type	Bioanalytical Tool
Reviewer	Andrea Mizzi Brunner
Use	N/A – this is a review on different effect directed analysis and mass spectrometry techniques, does not present new information.
TRL	N/A
Relevance	N/A
Applicability	N/A

R10 - Linking Mutagenic Activity to Micropollutant Concentrations in Wastewater Samples by Partial Least Square Regression and Subsequent Identification of Variables	
Abstract	We deployed multivariate regression to identify compounds co-varying with the mutagenic activity of complex environmental samples. Wastewater treatment plant (WWTP) effluents with a large share of industrial input of different sampling dates were evaluated for mutagenic activity by the Ames Fluctuation Test and chemically characterized by a screening for suspected pro-mutagens and non-targeted software-based peak detection in full scan data. Areas of automatically detected peaks were used as predictor matrix for partial least squares projections to latent structures (PLS) in combination with measured mutagenic activity. Detected peaks were successively reduced by the exclusion of all peaks with lowest variable importance until the best model (high R2 and Q2) was reached. Peaks in the best model co-varying with the observed mutagenicity showed increased chlorine, bromine, sulfur, and nitrogen abundance compared to original peak set indicating a preferential selection of anthropogenic compounds. The PLS regression revealed four tentatively identified compounds, newly identified 4-(dimethylamino)-pyridine, and three known micropollutants present in domestic wastewater as co-varying with the mutagenic activity. Co-variance between compounds stemming from industrial wastewater and mutagenic activity supported the application of “virtual” EDA as a statistical tool to separate toxicologically relevant from less relevant compounds.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0045653515005354
Citation	Hug, C.; Sievers, M.; Ottermanns, R.; Hollert, H.; Brack, W.; Krauss, M. Linking Mutagenic Activity to Micropollutant Concentrations in Wastewater Samples by Partial Least Square Regression and Subsequent Identification of Variables. *Chemosphere* **2015**, *138*, 176–182. https://doi.org/10.1016/j.chemosphere.2015.05.072.
Tool Type	Effect Directed Analysis
Technology	Using virtual EDA as a statistical tool to separate toxicologically relevant from less-relevant compounds
Summary	uses large number of samples to correlate effects with chemical analytical signals using multivariate statistics to reduce the complexity of environmental contamination
Reviewer	Milou Dingemans
Use	Given large data set of/samples from which (water companies) could apply virtual EDA as less costly and less time-consuming technique which can be applied at a larger scale. EDA is currently limited to small number of samples
TRL	5
	listed as a proof of concept study
Relevance	8

	Requires large dataset to work, could possibly be applied when doing large sampling campaign
Applicability	8
	This hydroinformatics approach (multivariate regression) can be used to evaluate which chemicals correlate to responses observed in bioassays. This can be used to enrich risk-based monitoring programs. Adequately large numbers of samples are needed.

2.2 Theme 2 – Modelling Tools

Graphic	
Description (from website)	SOLUTIONS developed an integrated sequence of interlinked models. This "model train" aims to estimate the risk of a (new) emerging pollutant based on very limited information only: the use volume and category, and the molecular structure. The model train consists of four major components: 1 a generic emissions model; 2 a spatially and temporally explicit fate and transport model STREAM-EU, 3 a sequence of models to estimate substance properties and 4 models to calculate risk for human health and ecology. The components have been developed and are in the final stage of evaluation, by comparison to field data from the SOLUTIONS Case Studies (Danube, Rhine and Spanish Case Studies). The model train has been run for about 1,800 chemicals for the whole of Europe (see Figure). The results demonstrated that the model train is a suitable tool to better understand the risks associated to emerging pollutants on a European scale. They provide a continuous picture in time and space that cannot be derived from field data. They allow quantitative risk assessments for "data poor" emerging chemicals. Moreover, they allow to perform "what if" scenarios, and to investigate abatement options and the pollutants of tomorrow. A series of such applications has been produced and is now being analyzed and published.

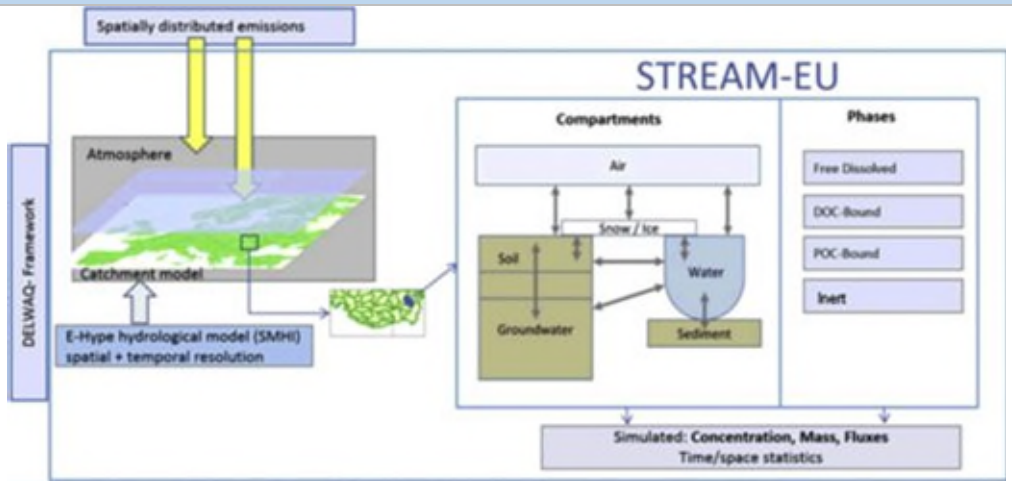
Emission Models	
Graphic	
Description (from website)	In addition to generic approaches to estimate emissions of organic chemicals, SOLUTIONS scientists have been developing techniques to estimate emissions for specific substances or substances groups in case studies. Lindim et al. 2015 (R11) estimated the emissions of perfluorooctane sulfonic acid PFOS, and perfluorooctanoic acid PFOA to surface waters and used an application of STREAM-EU (R15) to the Danube River catchment to verify the accuracy of estimates. Results obtained showed that the best estimates for PFOS and PFOA emissions in the Danube region are obtained by considering the combined contributions of human population, wealth (based on local gross domestic product GDP) and wastewater treatment. Human population alone cannot explain the levels of PFOS and PFOA found in the Danube catchment waters. Introducing wealth distribution information in the form of local GDPs improves emission estimates markedly, likely by better representing emissions resulting from consumer trends, industrial and commercial sources. The largest source of PFOS and PFOA to freshwater are wastewater treatment plants. Lindim et al. 2016 (R12) completed an emissions inventory for 54 top consumed human pharmaceuticals in Sweden was done based on national consumption data, human metabolic rates and wastewater treatment removal rates. The highest emissions to water were found for Metformin, Furosemide, Gabapentin, Atenolol and Tramadol.

R11 - Estimating Emissions of PFOS and PFOA to the Danube River Catchment and Evaluating Them Using a Catchment-Scale Chemical Transport and Fate Model	
Abstract	Novel approaches for estimating the emissions of perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) to surface waters are explored. The Danube River catchment is used to investigate emissions contributing to riverine loads of PFOS and PFOA and to verify the accuracy of estimates using a catchment-scale dynamic fugacity-based chemical transport and fate model (STREAM-EU; Spatially and Temporally Resolved Exposure Assessment Model for European basins). Model accuracy evaluation performed by comparing STREAM-EU predicted concentrations and monitoring data for the Danube and its tributaries shows that the best estimates for PFOS and PFOA emissions in the Danube region are obtained by considering the combined contributions of human population, wealth (based on local gross domestic product (GDP)) and wastewater treatment. Human population alone cannot explain the levels of PFOS and PFOA found in the Danube catchment waters. Introducing wealth distribution information in the form of local GDPs improves emission estimates markedly, likely by better representing emissions resulting from consumer trends, industrial and commercial sources. For compounds such as PFOS and PFOA, whose main sink and transport media is the aquatic

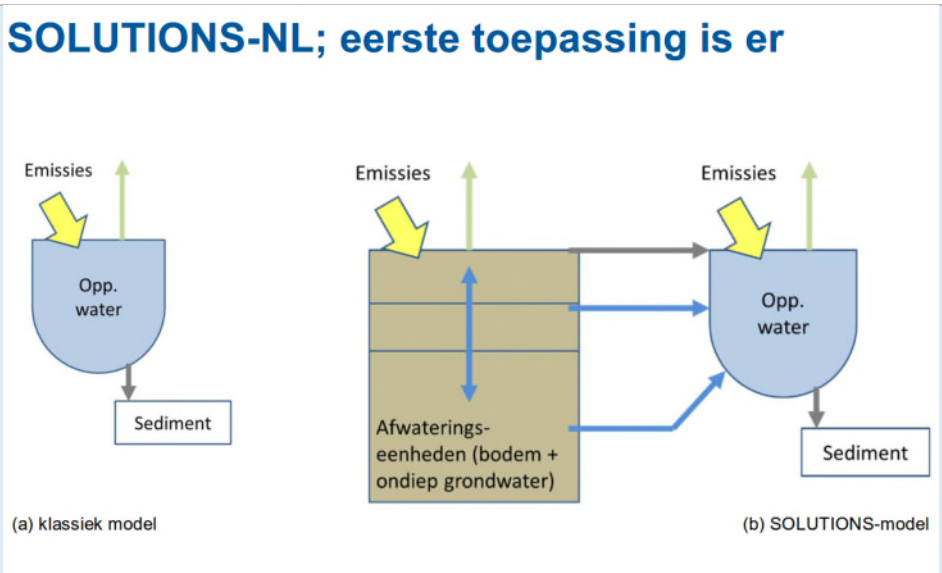
	compartment, a major source to freshwater are wastewater treatment plants. Introducing wastewater treatment information in the emission estimations also further improves emission estimates.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0269749115300440
Citation	Lindim, C.; Cousins, I. T.; Vangils, J. 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.* **2015**, *207*, 97–106. https://doi.org/10.1016/j.envpol.2015.08.050.
Tool Type	Emission model
Technology	STREAM-EU, Model taking into account human population, wealth, and WWT
Summary	Improvements in predicting PFOS and PFOA by introducing local GDP and wastewater treatment plant data
Reviewer	Bas van der Grift
Use	Apply these modelling approaches to the NLs catchment for estimating PFOS/PFOA emissions contributing to riverine loads
TRL	6
	first study published using this approach, applied in 11 catchments
Relevance	8
	PFOS a popular topic and similar emission modeling efforts already in use at KWR (e.g. VO waterkwaliteitskaart)
Applicability	7
	The PRTR (Pollutant Release and Transfer Register; emissieregistratie.nl) is the framework developed to estimates emissions to surface water in the Netherlands. The Technology Readiness Level of the PRTR is higher than the work presented here. However, at the moment PFOS and PFOA are not incorporated in the in the water emissions in the PRTR. The incorporation of PFOS and PFOA in PRTR is under development. Data used in this study might be useful for this work. An applications like this tool build for the Rhine and Meus catchment is useful to estimate transboundary riverine PFOS and PFOA load. This can be used as boundary conditions for the SOLUTIONS-NL tool.

R12 - Evaluation of Human Pharmaceutical Emissions and Concentrations in Swedish River Basins	
Abstract	An emissions inventory for top consumed human pharmaceuticals in Sweden was done based on national consumption data, human metabolic rates and wastewater treatment removal rates. Concentrations of pharmaceuticals in surface waters in Swedish river basins were predicted using estimated emissions from the inventory and river discharges. Our findings indicate that the top ten emitted pharmaceuticals in our study set of 54 substances are all emitted in amounts above 0.5 ton/y to both surface waters and soils. The highest emissions to water were in decreasing order for Metformin, Furosemide, Gabapentin, Atenolol and Tramadol. Predicted emissions to soils calculated with the knowledge that in Sweden sludge is mostly disposed to soil, point to the highest emissions among the studied drugs coming from, in decreasing order, Metformin, Paracetamol, Ibuprofen, Gabapentin and Atenolol. Surface water concentrations in Sweden's largest rivers, all located in low density population zones, were found to be below 10 ng/L for all substances studied. In contrast, concentrations in surface waters in Stockholm's metropolitan area, the most populous in Sweden, surpassed 100 ng/L for four substances: Atenolol, Metformin, Furosemide and Gabapentin.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0048969716317673
Citation	Lindim, C.; van Gils, J.; Georgieva, D.; Mekenyan, O.; Cousins, I. T. Evaluation of Human Pharmaceutical Emissions and Concentrations in Swedish River Basins. *Sci. Total Environ.* **2016**, *572*, 508–519. https://doi.org/10.1016/j.scitotenv.2016.08.074.
Tool Type	Emission model; Spatial/temporal fate and transport model
Technology	Estimating emissions and predicting environmental concentrations of pharmaceuticals in Swedish river basins from consumption data, human metabolic rates and removal rates in urban wastewater treatment plants
Summary	First estimate of environmental concentrations of pharmaceuticals in Swedish waters
Reviewer	Bas van der Grift
Use	5
TRL	first application
	8
Relevance	Pharmaceutical release a popular topic and similar emission modeling efforts already in use at KWR (e.g. VO waterkwaliteitskaart)
	7
Applicability	As above for tool R11. The value of this tool is mainly the generic method to estimate emission of substances to surface water. Improvement in emission of substances should be incorporated in the PRTR. The results of emission models are not directly usable for the drinking water sector but only after incorporation into surface water quality models. Results of surface water quality models are useful for the sector on short

	and longer time horizons. This accounts for drinking water companies that use surface water as source but also for companies that abstract groundwater. Infiltration of surface water can be a potential source of contaminants in groundwater.
	5

Spatially and temporally resolved exposure assessment model for European basins (STREAM-EU) and Case Studies	
Graphic	
Description (from website)	SOLUTIONS scientists developed a novel dynamic mass balance model for predicting the environmental fate of organic contaminants in river basins Lindim et al. 2015 (R15). It is based on a pre-existing open source water quality modelling framework Delft3D-WAQ and has been linked to the Europe wide hydrology model E-Hype by SMHI. STREAM-EU goes beyond the current state-of-the-science in that it can simulate spatially and temporally-resolved contaminant concentrations in all relevant environmental media (surface water, groundwater, snow, soil and sediments) at the river basin scale. The model can currently be applied to multiple organic contaminants in any river basin in Europe. The Spatially and Temporally Resolved Exposure Assessment Model for European basins STREAM-EU model has already seen three published applications (R11, R13, R14). Lindim et al. 2015 (R11) simulate the environmental fate of perfluoroctanesulfonic acid PFOS, and perfluorooctanoic acid PFOA in the Danube River basin and compare model predictions to recent monitoring data. The model predicts PFOS and PFOA concentrations that agree well with measured concentrations for large stretches of the river. This was later up-scaled (R13) to the eleven most populated European river catchments to provide a European-wide perspective on the contamination with PFOS and PFOA. STREAM-EU model was used to predict the water concentrations, estuarine export and retention of these substances. Emissions of PFOS and PFOA to those catchments were calculated based on a previously published method. The simulation results are in reasonable agreement with field data, and indicate widespread exceedance of the surface water Environmental Quality Standards for PFOS. A third application (R14) provides an exposure assessment for 54 pharmaceuticals in Swedish surface waters. Again, the water concentrations, estuarine export and retention of these substances were quantified. In an on-going effort these results are being used to estimate effects on Swedish river ecosystems.

For applications of the STREAM-EU model see case studies in R11, R13 and R14	
R15- A Large-Scale Model for Simulating the Fate & Transport of Organic Contaminants in River Basins	
Abstract	We present STREAM-EU (Spatially and Temporally Resolved Exposure Assessment Model for EUropean basins), a novel dynamic mass balance model for predicting the environmental fate of organic contaminants in river basins. STREAM-EU goes beyond the current state-of-the-science in that it can simulate spatially and temporally-resolved contaminant concentrations in all relevant environmental media (surface water, groundwater, snow, soil and sediments) at the river basin scale. The model can currently be applied to multiple organic contaminants in any river basin in Europe, but the model framework is adaptable to any river basin in any continent. We simulate the environmental fate of perfluoroctanesulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) in the Danube River basin and compare model predictions to recent monitoring data. The model predicts PFOS and PFOA concentrations that agree well with measured concentrations for large stretches of the river. Disagreements between the model predictions and measurements in some river sections are shown to be useful indicators of unknown contamination sources to the river basin.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0045653515301387
Citation	Lindim, C.; van Gils, J.; Cousins, I. T. A Large-Scale Model for Simulating the Fate & Transport of Organic Contaminants in River Basins. *Chemosphere* **2016**, *144*, 803–810. https://doi.org/10.1016/j.chemosphere.2015.09.051.
Tool Type	Spatial/temporal fate and transport
Technology	STREAM-EU modelling approach implemented in Deft3D-WAQ
Summary	Model implemented in open source framework Delft3D-WAQ, numerical solution of the mass balance equations in a temporally and spatially explicit way. Does not include hydrodynamic or hydrology modelling. Model describes the unsteady-state behavior of a chemical in the environment and the mass balance is represented by a set of ordinary differential equations. See article section 2 for detailed explanation of the model
Reviewer	Bas van der Grift
Use	Apply similar models using the STREAM-EU modelling approach for pharmaceuticals, PFOS or other emerging contaminants
TRL	6
	Applied in a number of catchments, but not yet by other researchers. As spinoff from the SOLUTIONS project there is a “SOLUTIONS-NL” project to improve the surface water quality modelling for wide range of substances in the Netherlands. This application is developed in close collaboration with the PRTR. Although a number of improvements still have to be made this is a promising development with the research field of surface water quality modelling.



Relevance	8
	Surface water quality models the can predict future development in concentrations of many organic compounds are highly relevant for the Dutch drinking water sector. These kind of models can help to take measures and develop policy to improve water quality in river basins.
Applicability	8
	The Dutch drinking water sector will benefit from models that can predict the concentrations of substances in surface water bodies on different spatial and temporal scales. The main improvement from this tool in comparison with earlier developed models is the wide range of substances that it can handle from domestic, agricultural and industrial sources. The direct value of the STREAM-EU models for the Dutch drinking water sector is that the results can be used as boundary conditions for the SOLUTION-NL models that are under development. Data and knowledge behind the STREAM-EU model can be used further development of the SOLUTION-NL models. Estimations of emission of substances is still a topic of further research.

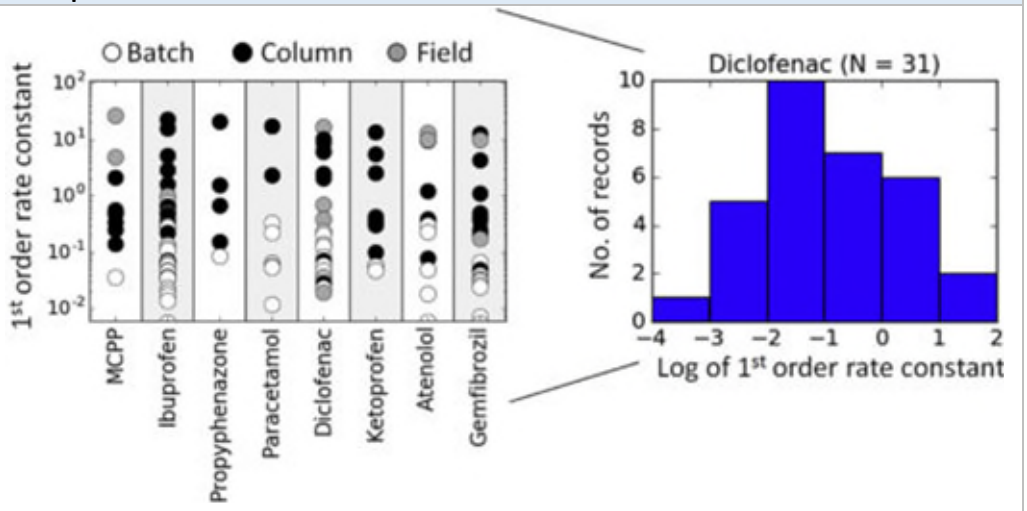
R13 and R14 are case studies using STREAM-EU and are therefore not evaluated as separate technologies	
R13 - Europe-Wide Estuarine Export and Surface Water Concentrations of PFOS and PFOA	
Abstract	The STREAM-EU model was used to predict the water concentrations, estuarine export and retention of perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) in the eleven most populated European river catchments to provide a European-wide perspective on the contamination by these substances. Emissions of PFOS and PFOA to those catchments were calculated based on population, wealth and wastewater treatment plant (WWTP) coverage and efficiency using a previously published method and used as model input. Our estimated emissions showed the lowest values for the Thames catchment (PFOS: 0.4 ton/y; PFOA: 0.2 ton/y) and the highest values for the Rhine for PFOS (1.6 ton/y) and for the Dnieper for PFOA (1.7 ton/y). The model predicted concentrations agreed reasonable well with the existing range of measurements, apart from for PFOA in the River Po, where there is a known historical industrial contamination, and PFOS in the Rhone River, where results were much higher than the few measurements available. It was concerning that the model predicted that the surface water EQS for PFOS (0.65 ng/L) was exceeded by a wide margin in all the eleven studied European river catchments. The total calculated riverine export to the seas from the eleven catchments was 4.5 ton/y of PFOS and 3.7 ton/y of PFOA with highest exported quantities from the Rhine (PFOS: 1.0 ton/y; PFOA: 1.0 ton/y) and Danube estuaries (PFOS: 0.9 ton/y; PFOA: 0.7 ton/y). For the seas where the rivers discharge, riverine discharge of PFOS was estimated to be 2.5–30 times more important as an input than atmospheric deposition, whereas for PFOA the opposite was true (atmospheric deposition was 2–10 times more important) except for very small seas.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0043135416305280
Citation	Lindim, C.; van Gils, J.; Cousins, I. T. Europe-Wide Estuarine Export and Surface Water Concentrations of PFOS and PFOA. *Water Res.* **2016**, *103*, 124–132. https://doi.org/10.1016/j.watres.2016.07.024.
Tool Type	STREAM-EU Case Study
Technology	STREAM-EU model applied to 11 catchments in Europe to estimate the PFOS emission to surface waters
Summary	Europe-wide prediction of PFOS contamination
R14 - Model-Predicted Occurrence of Multiple Pharmaceuticals in Swedish Surface Waters and Their Flushing to the Baltic Sea	
Abstract	An exposure assessment for multiple pharmaceuticals in Swedish surface waters was made using the STREAM-EU model. Results indicate that Metformin (27 ton/y), Paracetamol (6.9 ton/y) and Ibuprofen (2.33 ton/y) were the drugs with higher amounts reaching the Baltic Sea in 2011. 35 of the studied substances had more than 1 kg/y of predicted flush to the sea. Exposure potential given by the ratio amount of

	the drug exported to the sea/amount emitted to the environment was higher than 50% for 7 drugs (Piperacillin, Lorazepam, Metformin, Hydroxycarbamide, Hydrochlorothiazide, Furosemide and Cetirizine), implying that a high proportion of them will reach the sea, and below 10% for 27 drugs, implying high catchment attenuation. Exposure potentials were found to be dependent of persistency and hydrophobicity of the drugs. Chemicals with Log D > 2 had exposure potentials <10% regardless of their persistence. Chemicals with Log D < −2 had exposure potentials >35% with higher ratios typically achieved for longer half-lives. For Stockholm urban area, 17 of the 54 pharmaceuticals studied had calculated concentrations higher than 10 ng/L. Model agreement with monitored values had an r^2 = 0.62 for predicted concentrations and an r^2 = 0.95 for predicted disposed amounts to sea.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0269749116323089
Citation	Lindim, C.; van Gils, J.; Cousins, I. T.; Kühne, R.; Georgieva, D.; Kutsarova, S.; Mekenyan, O. Model-Predicted Occurrence of Multiple Pharmaceuticals in Swedish Surface Waters and Their Flushing to the Baltic Sea. *Environ. Pollut.* **2017**, *223*, 595–604. https://doi.org/10.1016/j.envpol.2017.01.062.
Tool Type	Spatial/temporal fate and transport
Technology	STREAM-EU model applied pharmaceutical concentrations in Swedish surface water and flushing to Baltic sea
Summary	exposure potential for pharmaceuticals were related to their distribution coefficient (non-dissociated fraction*octanol water partitioning coefficient)

Chemical Footprints	
Graphic	
Description (from website)	Freshwater environments are contaminated with complex mixtures of chemicals posing risks to ecosystems & human health. One core goal of the European Environmental Action plan 2020 is to reach a non-toxic environment. Chemical footprints represent the amount of water in a country or a city that is required to dilute all emissions to concentrations that do neither pose a risk to ecosystems nor to human health. Thus, chemical footprints as applied by Zijp et al. 2014 are a valuable tool to assess toxic impacts against safe boundaries for a specific regions and help to prioritize abatement options.

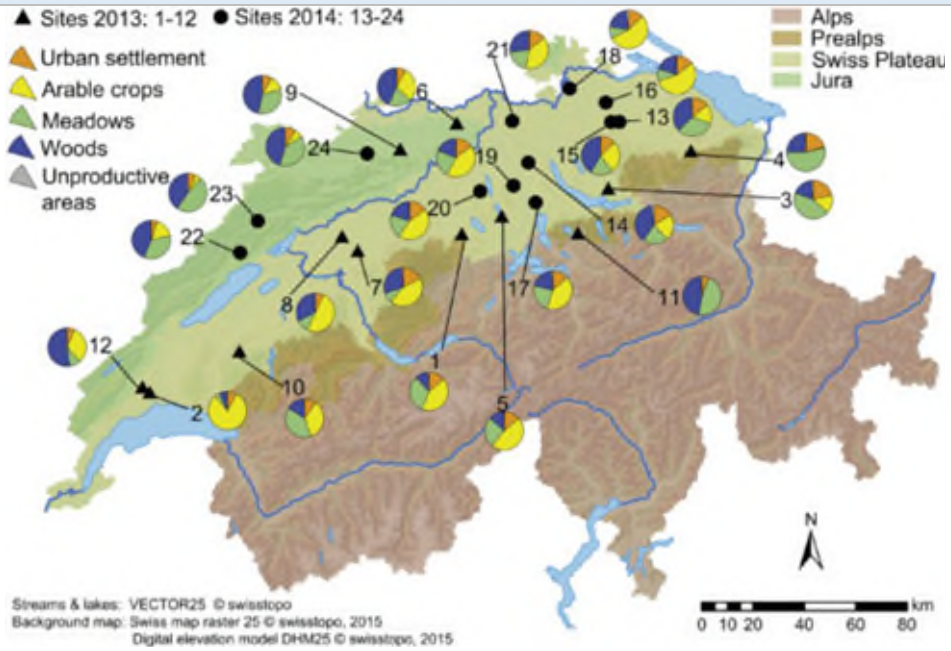
R16 - Definition and Applications of a Versatile Chemical Pollution Footprint Methodology	
Abstract	Because of the great variety in behavior and modes of action of chemicals, impact assessment of multiple substances is complex, as is the communication of its results. Given calls for cumulative impact assessments, we developed a methodology that is aimed at expressing the expected cumulative impacts of mixtures of chemicals on aquatic ecosystems for a region and subsequently allows to present these results as a chemical pollution footprint, in short: a chemical footprint. Setting and using a boundary for chemical pollution is part of the methodology. Two case studies were executed to test and illustrate the methodology. The first case illustrates that the production and use of organic substances in Europe, judged with the European water volume, stays within the currently set policy boundaries for chemical pollution. The second case shows that the use of pesticides in Northwestern Europe, judged with the regional water volume, has exceeded the set boundaries, while showing a declining trend over time. The impact of mixtures of substances in the environment could be expressed as a chemical footprint, and the relative contribution of substances to that footprint could be evaluated. These features are a novel type of information to support risk management, by helping prioritization of management among chemicals and environmental compartments.
Source	Journal Paper
Link	https://pubs.acs.org/doi/abs/10.1021/es500629f

Citation	Zijp, M. C.; Posthuma, L.; Van De Meent, D. Definition and Applications of a Versatile Chemical Pollution Footprint Methodology. *Environ. Sci. Technol.* **2014**, *48* (18), 10588–10597. https://doi.org/10.1021/es500629f.
Tool Type	Calculate risk for human and ecological health
Technology	Chemical Footprint; Risk Assessment
Summary	Determines the 'chemical footprint' of a region and effects on biodiversity based on the cumulative impacts of chemical pollution. Versatile method to express the expected eco-toxicological impact of a mixture of substances
Reviewer	Milou Dingemans
Use	apply similar methods
TRL	5
	first application
Relevance	7
	This approach can be used to prioritize locations for mitigation measures. The chemical footprint is based on potential effects on aquatic ecosystems that differ from but may be used as a proxy for human health. It is unknown whether this is a conservative approach or can be used for an early-prediction for potential human health effects.
Applicability	7
	This methods is developed further in the Kennisimpuls Waterkwaliteit.

Water Quality Assessments	
R17 - The Uncertainty of Biodegradation Rate Constants of Emerging Organic Compounds in Soil and Groundwater – A Compilation of Literature Values for 82 Substances	
Graphic	
Description (from website)	This study assesses the uncertainty with respect to 1st-order biodegradation rate constants of emerging organic compounds (EOCs) for soil and groundwater reported in the literature, as these values are needed to predict fate of EOCs in the environment. For the majority of compounds, the reported degradation rate constants vary over more than three orders of magnitude. Correlation to factors that are well known to affect the degradation rate, such as temperature or redox condition was weak. No correlation at all was found with results from available quantitative structure-activity relationship models. This suggests that many unknown site specific or experimentally specific factors influence the degradation behavior of EOCs in the environment. Thus, local and catchment scale predictive models to estimate EOC concentration at receptors e.g. receiving waters or drinking water wells, need to consider the large uncertainty in 1st-order rate constants. As a consequence, applying rate constants that were derived from one experiment or field site investigation to other experiments or field sites should be done with extreme caution.
Abstract	The present study reports on biodegradation rate constants of emerging organic compounds (EOCs) in soil and groundwater available in the literature. The major aim of this compilation was to provide an assessment of the uncertainty of hydrological models with respect to the fate of EOCs. The literature search identified a total number of 82 EOCs for which 1st-order rate constants could be derived. It was found that for the majority of compounds degradation rate constants vary over more than three orders of magnitude. Correlation to factors that are well known to affect the degradation rate, such as temperature or redox condition was weak. No correlation at all was found with results from available quantitative structure-activity relationship models. This suggests that many unknown site specific or experimentally specific factors influence the degradation behavior of EOCs in the environment. Thus, local and catchment scale predictive models to estimate EOC concentration at receptors, e.g., receiving waters or drinking water wells, need to consider the large uncertainty in 1st-order rate constants. As a consequence, applying rate constants that were derived from one

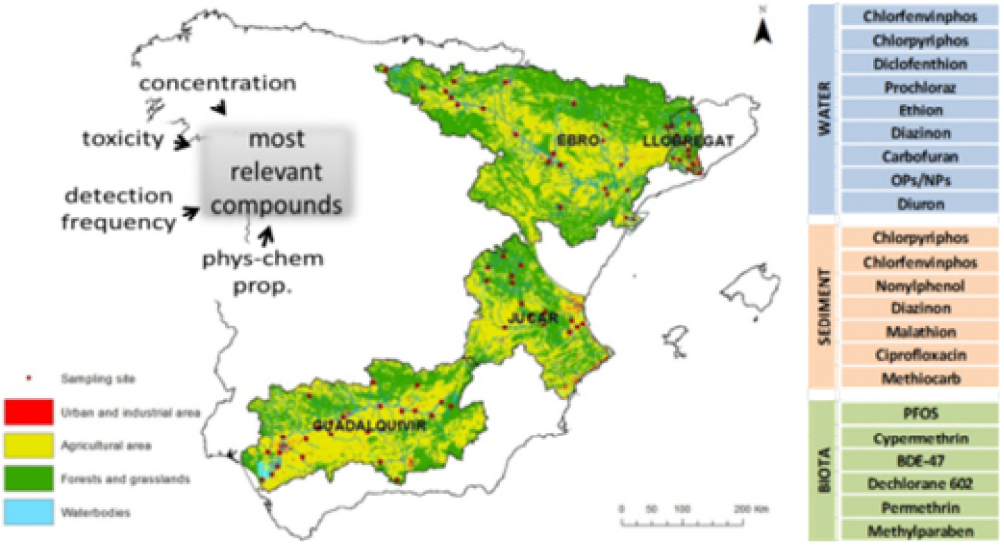
	experiment or field site investigation to other experiments or field sites should be done with extreme caution.
Citation	Greskowiak, J.; Hamann, E.; Burke, V.; Massmann, G. The Uncertainty of Biodegradation Rate Constants of Emerging Organic Compounds in Soil and Groundwater – A Compilation of Literature Values for 82 Substances. *Water Res.* **2017**, *126*, 122–133. https://doi.org/10.1016/j.watres.2017.09.017.
Tool Type	Model parameter estimation
Technology	Correlation between degradation rates of emerging organic compounds in soil and groundwater studies
Summary	Found no correlation between degradation rate and QSAR model, suggesting site-specific and environmental factors influence the degradation behavior of EOCs in the environment. Applying rate constants from literature to other experimental or field studies should be done with extreme caution
Reviewer	Bas van der Grift
Use	Good to know going forward in field and laboratory studies about emerging contaminants and trying to apply degradation rates. Only a few of the 82 substances had more than 10 experimentally tested degradation rates, therefore it could help to study more and contribute to the statistical analysis of degradation rates in porous media (create a database)
TRL	5
	Additional experimental data is required
Relevance	8
	Data on degradation rates is essential for predicting or modelling the behavior of emerging contaminants in the soil/groundwater domain. Therefore, this work is highly relevant for the Dutch drinking water sector. The paper did not show relationship between degradation rates and temperature or redox conditions, no concrete ways to fix this. This indicates that there are still manly unknowns. For the majority of the considered substances there is clearly not enough experimental data available to extract reliable statistical information on degradation rate constants in natural porous media.
Applicability	7
	This paper gives the state-of-the-art of knowledge on degradation rates of 82 Emerging Organic Compounds. From this paper, it becomes clear that there are still a lot of unknowns. However, an up-to-date database with measured degradation rates under different environmental setting is very useful for the drinking water sector. The data in this paper can be added to such a database.
Proposed Pilot Study	The pilot study would use and build on the collected degradation rates of emerging contaminants in soil and groundwater. Ideally, the database of degradation rates would be incorporated into a larger database or tool in development at KWR, so as to increase the functionality and use of the data. Possible uses for the data include predicting and modelling behavior of emerging contaminants during dune/soil

	passage (water treatment), risk assessment for emerging contaminants, database of removal efficiencies for various treatment technologies.

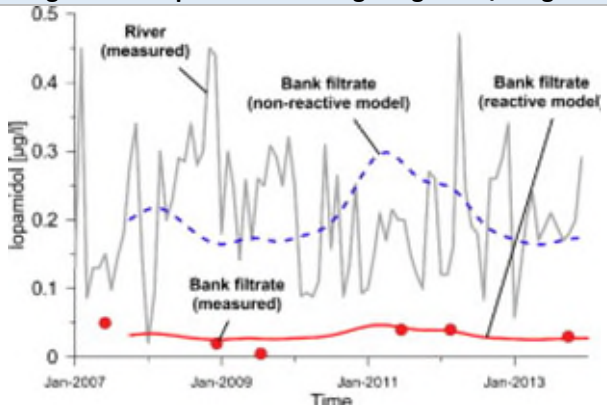
R18 - Pesticides Drive Risk of Micropollutants in Wastewater-Impacted Streams during Low Flow Conditions	
Graphic	
Description (from website)	In collaboration with Ecoimpact, SOLUTIONS assessed the chemical exposure and the concentration patterns of organic micropollutants upstream, downstream and at effluents of 24 Swiss wastewater treatment plants Munz et al., 2017. The aim was to determine whether the risk for aquatic organisms living in wastewater-impacted streams is mainly driven by higher concentrations of pharmaceuticals and other typical household chemicals, or if pesticides play an important role also when released during low flow conditions. The streams were located across independent catchments with different land uses and were grab sampled during low flow conditions at eight time points. SOLUTIONS observed regular detections of micropollutants over all sites. While pharmaceuticals and other typical household chemicals constituted the highest loads, many pesticides were detected only during episodic events. Nevertheless, occasional concentration peaks were observed for pesticides, and the toxic pressure was mainly driven by a few pesticides and the anti-inflammatory drug diclofenac. The comparison with macroinvertebrate data underlined the importance of pesticides in wastewater-impacted streams. This relevance of pesticides also during low flow conditions seems to be typical for catchments where urban and agricultural land use co-occur as it is the case for many European countries.
Abstract	Micropollutants enter surface waters through various pathways, of which wastewater treatment plants (WWTPs) are a major source. The large diversity of micropollutants and their many modes of toxic action pose a challenge for assessing environmental risks. In this study, we investigated the potential impact of WWTPs on receiving ecosystems by describing concentration patterns of micropollutants, predicting acute risks for aquatic organisms and validating these results with macroinvertebrate biomonitoring data. Grab samples were taken upstream, downstream and at the effluent of 24 Swiss WWTPs during low flow conditions across independent catchments with different land uses. Using liquid chromatography high resolution tandem mass spectrometry, a comprehensive target screening of almost 400 organic substances, focusing mainly on pesticides

	and pharmaceuticals, was conducted at two time points, and complemented with the analysis of a priority mixture of 57 substances over eight time points. Acute toxic pressure was predicted using the risk assessment approach of the multi-substance potentially affected fraction, first applying concentration addition for substances with the same toxic mode of action and subsequently response addition for the calculation of the risk of the total mixture. This toxic pressure was compared to macroinvertebrate sensitivity to pesticides (SPEAR index) upstream and downstream of the WWTPs. The concentrations were, as expected, especially for pharmaceuticals and other household chemicals higher downstream than upstream, with the detection frequency of plant protection products upstream correlating with the fraction of arable land in the catchments. While the concentration sums downstream were clearly dominated by pharmaceuticals or other household chemicals, the acute toxic pressure was mainly driven by pesticides, often caused by the episodic occurrence of these compounds even during low flow conditions. In general, five single substances explained much of the total risk, with diclofenac, diazinon and clothianidin as the main drivers. Despite the low predicted acute risk of 0%–2.1% for affected species, a significant positive correlation with macroinvertebrate sensitivity to pesticides was observed. However, more effect data for pharmaceuticals and a better quantification of episodic pesticide pollution events are needed for a more comprehensive risk assessment.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0043135416308466
Citation	Munz, N. A.; Burdon, F. J.; de Zwart, D.; Junghans, M.; Melo, L.; Reyes, M.; Schönenberger, U.; Singer, H. P.; Spycher, B.; Hollender, J.; et al. Pesticides Drive Risk of Micropollutants in Wastewater-Impacted Streams during Low Flow Conditions. *Water Res.* **2017**, *110*, 366–377. https://doi.org/10.1016/j.watres.2016.11.001.
Tool Type	Risk Assessment
Technology	Calculate risk for human and ecological health
Summary	Measurements of micropollutants (pharmaceuticals and WWTP contaminants, pesticides), want to determine if pharmaceuticals of pesticides are drivers of risk for aquatic organisms. Pesticides dominate the risk, but are mainly discharges during episodic events and therefore poorly captures when using grab samples only - though toxicity of pharmaceuticals if limited due to the paucity of toxicity data available
Reviewer	Thomas ter Laak
Use	Do a similar study in NL streams and compare to Swiss study
TRL	*NA*
	Measurement campaign, not a technology
Relevance	6
	The assessment focuses on ecotoxicological impact. Since the Swiss situation is different than NL, this approach can be applied more easily than in a delta setting (European Commission 1998, Baken, Sjerps et al. 2018).

Applicability	6
	Estimate impact of point sources to contamination in drinking water sources. Concept is interesting but it is not an actual tool, so not applicable for going forward with a case study

R19 - Ecotoxicological Risk Assessment of Chemical Pollution in Four Iberian River Basins and Its Relationship with the Aquatic Macroinvertebrate Community Status.	
Graphic	
Description (from website)	Mediterranean rivers are different from Northern & Central European in terms of hydrological regime, climate conditions, socio-economics; all leading to differences in the nature and relative importance of existing environmental stressors. To identify the most relevant organic pollutants in this kind of scenarios, characterized by frequent water scarcity episodes and heavy human pressure, over 200 organic priority and emerging pollutants were comprehensively monitored in water, sediment and biota from 4 river basins and further prioritized on the basis of their occurrence, toxicity, and physical-chemical data. We provide a prioritization of contaminants relevant to Iberian rivers to support water authorities with respect to the set up of River Basin Management Plans.
Abstract	Ecotoxicological risk assessment of chemical pollution in four Iberian river basins (Llobregat, Ebro, Júcar and Guadalquivir) was performed. The data set included more than 200 emerging and priority compounds measured at 77 sampling sites along four river basins studied. The toxic units (TU) approach was used to assess the risk of individual compounds and the concentration addition model (CA) to assess the site specific risk. Link between chemical pollution and aquatic macroinvertebrate communities in situ was examined by using four biological indexes; SPEAR ("Species at Risk Index") as the indicator of decline of sensitive species in relation to general organic (SPEARorganic) and pesticides (SPEARpesticides) pollution; and Shannon and Margalef biodiversity indexes. The results of the study suggested that organic chemicals posed the risk of acute effects at 42% of the sampling sites and the risk of chronic effects at all the sites. Metals posed the acute risk at 44% of the sites. The main drivers of the risk were mainly pesticides and metals. However, several emerging contaminants (e.g. the antidepressant drug sertraline and the disinfectant triclosan) were contributing to the chronic effects risk. When risk associated with metals and organic chemicals was compared, the latter dominated in 2010, mainly due to the presence of highly toxic pesticides, while metals did in 2011. Compounds that are not regulated on the European level were posing the risk of chronic effects at 23% of the sites. The decline of sensitive macroinvertebrate taxa expressed in terms of SPEAR index was correlated with the increase of toxic stress related to

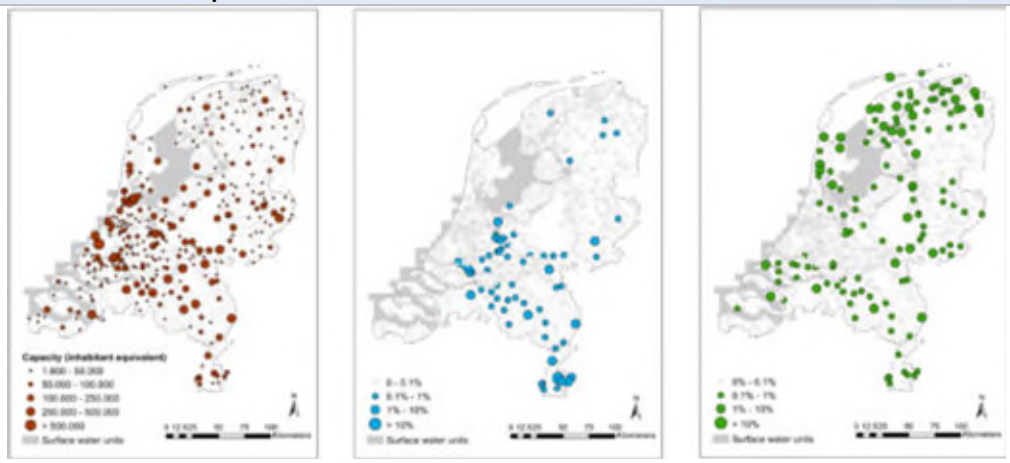
	organic compounds Biodiversity indexes were negatively correlated with the metals and the urban land use type in the catchment.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0048969715303089?via%3Dihub
Citation	Kuzmanović, M.; López-Doval, J. C.; De Castro-Català, N.; Guasch, H.; Petrović, M.; Muñoz, I.; Ginebreda, A.; Barceló, D. Ecotoxicological Risk Assessment of Chemical Pollution in Four Iberian River Basins and Its Relationship with the Aquatic Macroinvertebrate Community Status. *Sci. Total Environ.* **2016**, *540*, 324–333. https://doi.org/10.1016/j.scitotenv.2015.06.112.
Tool Type	Risk Assessment
Technology	Calculate risk for human and ecological health
Summary	Measurements of emerging and priority pollutants in river basins in Iberian River systems. Metals and pesticides pose acute risks at ¬40% of sites, and several emerging contaminants contribute to chronic effects
Reviewer	Milou Dingemans
Use	Do similar study in NL streams and compare to study
TRL	*NA*
	Measurement campaign, not a technology. The researchers use existing methodologies (diversity indexes for biological status and the TU approach)
Relevance	6
	Mediterranean region less similar to NL context than other studies from North and Central Europe
Applicability	4
	There are no new methods presented.

R20 - The Fate of Organic Micropollutants during Long-Term/Long-Distance River Bank Filtration	
Graphic	
Description (from website)	River bank filtration RBF is a common technique for the pre-treatment of surface water for drinking water supply. During subsurface passage from the river towards extraction wells, undesired substances, such as pathogenic virus or contaminants shall be removed. While many river contaminants cannot be detected after bank filtration several emerging pollutants such as the pharmaceutical carbamazepine are fully persistent even after more than 3 years of transfer time. This study by Hamann et al. 2016 is one of very few reporting on the long-term field-scale behavior of organic micropollutants. It highlights the efficiency of RBF for water quality improvement as a pre-treatment step for drinking water production
Abstract	The fate of organic micropollutants during long-term/long-distance river bank filtration (RBF) at a temporal scale of several years was investigated along a row of monitoring wells perpendicular to the Lek River (the Netherlands). Out of 247 compounds, which were irregularly analyzed in the period 1999–2013, only 15 were detected in both the river and river bank observation wells. Out of these, 10 compounds (1,4-dioxan, 1,5-naphthalene disulfonate (1,5-NDS), 2-amino-1,5-NDS, 3-amino-1,5-NDS, AOX, carbamazepine, EDTA, MTBE, toluene and triphenylphosphine oxide) showed fully persistent behavior (showing no concentration decrease at all), even after 3.6 years transit time. The remaining 5 compounds (1,3,5-naphthalene trisulfonate (1,3,5-NTS), 1,3,6-NTS, diglyme, iopamidol, triglyme) were partially removed. Their reactive transport parameters (removal rate constants/half-lives, retardation coefficients) were inferred from numerical modeling. In addition, maximum half-lives for 14 of the fully removed compounds, for which the data availability was sufficient to deduce 100% removal during sub-surface passage, were approximated based on travel times to the nearest well. The study is one of very few reporting on the long-term field-scale behavior of organic micropollutants. It highlights the efficiency of RBF for water quality improvement as a pre-treatment step for drinking water production. However, it also shows the very persistent behavior of various compounds in groundwater.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0048969715312134
Citation	Hamann, E.; Stuyfzand, P. J.; Greskowiak, J.; Timmer, H.; Massmann, G. The Fate of Organic Micropollutants during Long-Term/Long-Distance River Bank Filtration. *Sci.*

	Total Environ. **2016**, *545–546*, 629–640. https://doi.org/10.1016/j.scitotenv.2015.12.057.
Tool Type	Spatial/temporal fate and transport model
Technology	Riverbank filtration, prioritizing chemicals in water quality monitoring
Summary	Assessed RBF capacity to remove organic and inorganic compounds over long term-long-distance study. Of the 254 compounds monitored, only 15 were fully persistent (no decline in concentration) and 5 only partially removed. Show the capacity of RBF to remove a large number of compounds as a pretreatment for drinking water production
Reviewer	Bas van der Grift
Use	Oasen was involved in the study, good basis for prioritizing monitoring of compounds based on what is known to be removed and not removed from RBF
TRL	9*
	*Riverbank filtration already widely applied but studies that quantify degradation and retardation of organic compounds during RBF are still relatively rare.
Relevance	9
	RBF already widely applied, may be relevant for prioritizing monitoring of chemicals though? This work is a nice benchmark of how the behavior of organic compounds during RBF can be assessed. There may be a growing interest in RBF in the coming decades. The pressure to lower the groundwater abstraction might increase. This can result in a growing interest in surface water for drinking water production. There is more than enough water flowing through the river Rhine and Meuse. The challenges with direct use of surface water such as temporal variations in water quality might be bypassed by using RBF. Knowledge of the behavior of compounds during RBF is therefore highly relevant.
Applicability	7
	The tool itself is site specific and therefore has limited value for other drinking water production locations. However, the knowledge behind the tool is valuable. This can be used to develop reactive transport models at other locations. In addition, the result of this tool can be used to develop monitoring strategies at other locations.

2.3 Theme 3 – Abatement, Prioritization & Policy Recommendations

Abatement

R21 - Towards Spatially Smart Abatement of Human Pharmaceuticals in Surface Waters: Defining Impact of Sewage Treatment Plants on Susceptible Functions	
Graphic	
Description (from website)	Pharmaceuticals are considered a risk for various functions of surface waters. Enhanced purification at sewage treatment plants (STPs) can present a solution. But which STPs should be upgraded first? Coppens et al. 2015 investigated to what degree individual treatment plants affect the water quality in receiving surface waters, by using mathematical modelling. The individual STPs were ranked with respect to their overall negative impact on receiving waters with certain functions, in particular a provision of raw drinking water, and b nature protection. This provided a clear ranking of 345 Dutch STPs, as shown in the figure (red dots are all STPs, blue dots are priority STPs for protecting drinking water resources and green dots are priority STPs for nature protection). SOLUTIONS scientists are in the process of up-scaling this approach for the whole Rhine catchment area, one of SOLUTIONS three case study areas.
Abstract	For human pharmaceuticals, sewage treatment plants (STPs) are a major point of entry to surface waters. The receiving waters provide vital functions. Modeling the impact of STPs on susceptible functions of the surface water system allows for a spatially smart implementation of abatement options at, or in the service area of, STPs. This study was performed on a nation-wide scale for the Netherlands. Point source emissions included were 345 Dutch STPs and nine rivers from neighboring countries. The Dutch surface waters were represented by 2511 surface water units. Modeling was performed for two extreme discharge conditions. Monitoring data of 7 locations along the rivers Rhine and Meuse fall mostly within the range of modeled concentrations. Half of the abstracted volumes of raw water for drinking water production, and a quarter of the Natura 2000 areas (European Union nature protection areas) hosted by the surface waters, are influenced by STPs at low

	discharge. The vast majority of the total impact of all Dutch STPs during both discharge conditions can be attributed to only 19% of the STPs with regard to the drinking water function, and to 39% of the STPs with regard to the Natura 2000 function. Attributing water treatment technologies to STPs as one of the possible measures to improve water quality and protect susceptible functions can be done in a spatially smart and cost-effective way, using consumption-based detailed hydrological and water quality modeling.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0043135415300452
Citation	Coppens, L. J. C.; van Gils, J. A. G.; ter Laak, T. L.; Raterman, B. W.; van Wezel, A. P. Towards Spatially Smart Abatement of Human Pharmaceuticals in Surface Waters: Defining Impact of Sewage Treatment Plants on Susceptible Functions. *Water Res.* **2015**, *81*, 356–365. https://doi.org/10.1016/j.watres.2015.05.061.
Tool Type	Model, Abatement
Technology	Modelling to prioritize abatement options at WWTP based on drinking water and environmental impacts
Summary	WWTP are a major source of entry to surface water for pharmaceuticals. Modelling allows for prioritization of WWTP which impact human (drinking water) and environmental zones
Reviewer	Thomas ter Laak
Use	WWTP which negatively impact DW production are now known and abatements options can be discussed
TRL	6
	First application of model
Relevance	8
	DWC want to know which waste water treatment plants (WWTP) and surface waters are important for drinking water production and what chemicals are relevant. This was done for NL WWTP and Industrial wastewater treatment plants (Coppens, Gils et al. 2015, van den Hurk 2016).
Applicability	8
	It is already applied in the Dutch drinking water sector.

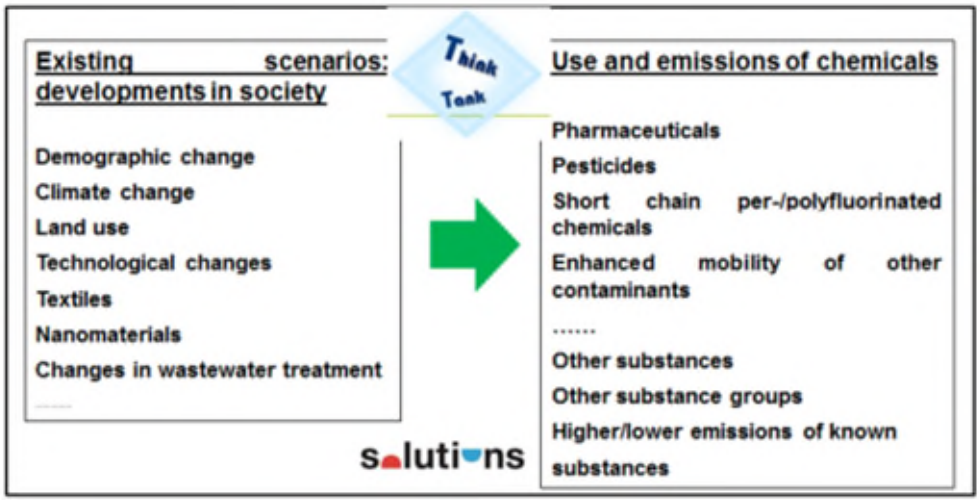
R22 - Mitigation Options for Chemicals of Emerging Concern in Surface Waters Operationalizing Solutions-Focused Risk Assessment	
Graphic	
Description (from website)	The water system provides fundamental services to society: industries, municipalities and agriculture withdraw, use and return water and demand water quality for intended purposes. As both water use and chemical emissions rise, increasing problems can be expected at the nexus of the chemical lifecycle and the water cycle. Currently, action on deterioration of water quality by chemicals is focused mostly on problem and risk analysis, while little attention is paid to mitigation options. Moreover, the intensification of current regulatory pathways presumably cannot yield a full solution to reach the policy goal of a non-toxic environment, so additional approaches seem warranted. This study by van Wezel et al. 2017 collates and evaluates mitigation options for chemical water quality improvement. These include mitigation options during the design, registration and authorization, production, use and waste phases, and ultimately technological interventions at the point of use, the point of environmental entry or at the point of a susceptible function of the water.
Abstract	The water system provides many services to society; industries, municipalities and agriculture all withdraw, use and return water and demand a water quality fit for the intended purposes. Both global production of chemicals and global water withdrawal grow faster than human population. This implies increased chemical threats to water, and creates a strong driver for mitigation to protect human health, ecosystem integrity and ecosystem services. Here we connect the perspectives of the water cycle and the chemical life cycle and review possible mitigation options. We categorize mitigation options in various stages of the chemicals' life cycle, taking various sectors and environmental pathways into account. More technologically oriented versus other types of mitigation options are discerned, and their relevance on spatial and temporal scale is discussed. We review various water treatment techniques in relation to physical–chemical properties of chemicals. Finally we discuss how a mitigation database can be used to assess the effectiveness of interventions, by coupling them to regional or global hydrological models. A solution-focused and systems-oriented perspective combined with a mitigation database offers a common perspective amongst actors on the effects for water quality of possible mitigation options throughout the chemical's life cycle, in various sectors and at various places in the water system. This can stimulate coherent implementation of effective mitigation options, cross-sectoral learning and further innovations to improve water quality.
Source	Journal Paper
Link	https://pubs.rsc.org/en/Content/ArticleLanding/2017/EW/C7EW00077D#!divAbstract

Citation	Van Wezel, A. P.; Ter Laak, T. L.; Fischer, A.; Bäuerlein, P. S.; Munthe, J.; Posthuma, L. Mitigation Options for Chemicals of Emerging Concern in Surface Waters Operationalising Solutions-Focused Risk Assessment. *Environ. Sci. Water Res. Technol.* **2017**, *3* (3), 403–414. https://doi.org/10.1039/c7ew00077d.
Tool Type	Abatement
Technology	Framework/Guidance Document
Summary	Mitigation options in various stages of the chemical life cycle are categorized. Framework for determining abatement options (or packages of abatement options)
Reviewer	Thomas ter Laak
Use	DWC can use framework to prioritize abatement options for different chemicals and for water coming from different industries (e.g. using different water sources)
TRL	6
	Framework well justified, first application
Relevance	8
	The (drinking) water sector has a strong technological focus on the solution to pollution. But this framework illustrates that the life cycle of a chemicals holds multiple steps from conception, design, production use, disposal and then emissions to drinking water sources and potential to contaminate drinking water. The framework illustrates the importance of the full life cycle and the relevance of looking for abatement options earlier in the life cycle. Currently, within the “Kennisimpuls Waterkwaliteit” the project “Ketenverkenner” is started to study these life cycles and the parties involved.
Applicability	8
	Within the “*ketenverkenner”* this subject is currently tackled.

R34 - AbatES	
Description (from website)	AbatES is a Decision Support System with information on emerging substances. This can be done in two ways: information per substance, or for up to 5 substances at a time by uploading monitoring data (Evaluate samples)
Source	Watershare Tool
Link	https://www.watershare.eu/tool/abates/
Citation	Van Wezel, A. P.; Ter Laak, T. L.; Fischer, A.; Bäuerlein, P. S.; Munthe, J.; Posthuma, L. Mitigation Options for Chemicals of Emerging Concern in Surface Waters Operationalising Solutions-Focused Risk Assessment. *Environ. Sci. Water Res. Technol.* **2017**, *3* (3), 403–414. https://doi.org/10.1039/c7ew00077d.
Tool Type	Decision support tool
Technology	Factsheets or uploading data and evaluation of samples
Summary	The tool gives structured information on emerging substances - see website for full explanation
Reviewer	Thomas ter Laak
Use	DWC can use when monitoring intake waters or water of interest. Tool provides a lot of data. Currently Abates is transformed to a “QCRA” tool within Watershare, partially developed within AquaNES (H2020) project. The new tool is user friendly and allows to combine treatment trains and see micropollutant behavior. At this moment only limited data are included in the tool. The tool can be applied to evaluate treatment efficiency of treatment steps and treatment trains for both wastewater treatment and drinking water treatment.
TRL	5-6
Relevance	7
Applicability	8
	When mature, the tool is a very user friendly way of evaluating treatment efficiency for scenario studies.

Prioritization and Future Chemicals of Concern

R24 - Developments in Society and Implications for Emerging Pollutants in the Aquatic Environment	
Abstract	Pollutant emissions in river basins change continuously. Management strategies should address such developments. Many scenarios are published which describe future changes in the environment and in society. Examples concern climate change, demographic change and urbanization. Based on these scenarios, specific trends can already be predicted (with uncertainties). Do these scenarios help to get a picture on future pollutants? The study presented here is based on the hypothesis that existing scenarios on developments in society may provide useful indications for future pollutants. The analysis of more than 30 reports on future scenarios shows that some developments are directly connected to consumption and the emission of specific substances. Secondly, it became evident that the effects of other development scenarios, such as those associated with climate change, are more complex. A precise quantitative evaluation of the implications of some scenarios on future pollutants can be particularly difficult for such scenarios. An important field of changes is technological developments. Frequently observed changes in this respect are substitutions of problematic substances with substances of similar structure.
Source	Working Paper
Link	https://www.oeko.de/en/publications/p-details/developments-in-society-and-implications-for-emerging-pollutants-in-the-aquatic-environment/
Citation	Moritz, S., Bunke, D., Brack, W., Herráez, D. L., & Posthuma, L. (2017). Developments in society and implications for emerging pollutants in the aquatic environment. Oeko-Institut Working Paper 1/2017.
Tool Type	Recommendations
Technology	Predicting future chemicals of concern
Summary	Paper about how societal trends can be used to predict/provide indications for future pollutants. PFCs, flame retardants, phthalates and nanomaterials identified as consequences of technological change.
Note: R24 and R25 are two papers on the same recommendations. Only one assessment of the relevance	

R25 - Pollution of Tomorrow: Solutions for Present and Future Emerging Pollutants in Land and Water Resources Management	
Graphic	
Description (from website)	How does the availability and use of water resources, population demography, agriculture, health care, climate and so on affect the patterns of global chemical pollution? Is it possible – at least to a certain degree – to predict future emerging pollutants? This SOLUTIONS discussion paper documents the work and the results of identifying and examining patterns and trends in current chemical pollution. Following this initial analysis, SOLUTIONS scientists have worked with external experts in dedicated workshops to discuss health care, economic, technological and demographic trends in society, in order to identify links with new and emerging pollutants. Finally, the obtained outcomes have been summarized in this freely available working paper by Moritz et al. 2017 (R24)
Abstract	Emerging pollutants (EPs) are monitored in surface waters since the nineties. With progress in analytical chemistry it is possible to analyze these substances in low concentrations. Which pollutants can be expected if future developments in society are taken into account? Such developments in society are described in a broad range of scenarios. Until now, implications of such developments for future pollutants have not been systematically discussed. This discussion paper addresses the question whether predictions of changes in society can be used as an information source for pollutants of tomorrow. In the first step, an overview about existing scenarios and their main findings on developments in society has been prepared. The second step assesses whether causal links can be seen between these societal and also technological development and future pollutants. 36 reports on developments in society (see Table 2 in chapter 6) have been analyzed regarding potential implications on future emerging pollutants. The analysis leads to the conclusions, that it is possible – at least to a certain degree – to predict future EPs by such an analysis: • The demographic change could impair EPs in a negative way. Due to the higher life expectancy in the next decades, the amount of pharmaceuticals circulating in sewage treatment plants and in the end in ecosystems will increase with high probability. • The world population growth and ongoing urbanization will lead to an increase of the distribution of EPs in the environment.

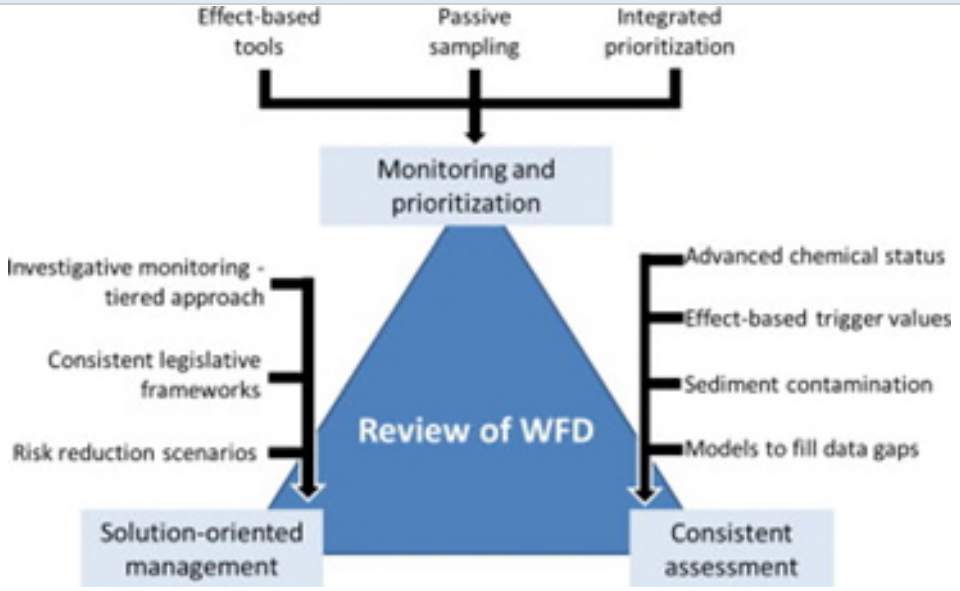
	• Legislation can induce the substitution of hazardous substances by others – sometimes with similar properties. The REACH candidate list shows which substances have been identified in Europe as substances of very high concern. It can be foreseen that for these substances substitutes The results indicate several connections between developments in technology and the increase of emerging pollutants, such as flame retardants, plasticiers and medium and short chain PFCs (per and polyfluorinated chemicals). New emerging pollutants can originate from well-known groups of chemicals. However, they can also come from unexpected new areas – such as Fracking or the development of key enabling technologies. Based on the findings presented in this discussion paper, four workshops organized within the project SOLUTIONS will focus on specific developments in society and related future pollutants.
Source	Internal Solutions Report
Link	http://www.solutions-project.eu/wp-content/uploads/2017/01/SOLUTIONS_Discussion_Paper_Pollution_Tomorrow.pdf
Citation	Bunke, D.; Moritz, S. Pollution of Tomorrow: Solutions for Present and Future Emerging Pollutants in Land and Water Resources Management; 2014.
Tool Type	Recommendations
Technology	Predicting future chemicals of concern
Summary	Broad predictions how emerging pollutants will impact society/water sector in the future. E.g. demographic changes, population growth, legislation, technological change, land use, textiles, nanomaterials, changes in WWT
Note: R24 and R25 are two papers on the same recommendations. Only one assessment of the relevance	
Reviewer	Thomas ter Laak
Use	Evaluating the new chemicals of emerging concern (CEC) is a challenge for the water sector. The recommendations are suitable to include in (location specific) evaluations of CEC in the (drinking) water cycle. Similar approaches are already done within ”verkennend onderzoek“ (VO)new substances and BTO project “verkenningen bronnen, gedrag en risico nieuwe stoffen” that is shared among the theme groups “Bronnen en Omgeving” and “Chemische Veiligheid”. The current paper is not a ready to use tool, but it can be seen as relevant literature for the projects mentioned above.
TRL	6
	Not a technology nor a model/framework, difficult to judge its readiness.
Relevance	7
	Directly applicable in the VO new substances project and *‘Verkenningen bronnen, gedrag en risico nieuwe stoffen’* project. However, the description only identifies generic groups of chemicals. So it does not allow to select specific –drinking water relevant- compounds.

Applicability	8 (as relevant literature / knowledge)
	Including this knowledge into the projects within “verkennend onderzoek” and “verkenningen bronnen, gedrag en risico nieuwe stoffen” project.

Policy Recommendations

R23 - Chemicals covered by regulatory frameworks of relevance for WFD	
Graphic	
Abstract	Chemical pollution and reducing risks to human health and the environment are in focus in a large number of European regulations and directives, but also as multilateral environmental agreements. Diverse international pieces of legislation and regulatory frameworks cover different parts of the chemical life-cycle which can be represented by five categories: Raw material extraction; Production; Trade; Use and End-of-life. An improved coordination and cooperation between the different regulatory frameworks aimed at reducing chemical risks to the environment and human health, can as well lead to an improved implementation of the Water Framework Directive across Europe. SOLUTIONS has developed this freely available on-line tool/database for the search of chemicals that are listed in directives, conventions and international agreements, and other initiatives of relevance for the fulfillment of the goals established by the WFD.
Source	Webtool
Link	http://apps.ivl.se/solutions
Tool Type	Policy recommendation
Technology	Database
Summary	Searchable database based on chemical name/CAS number/EC number. Excel exportable list of chemicals in a database or databases which list a chemical
Reviewer	Thomas ter Laak
Use	Checking which compounds are already covered in different legislation/regulation, e.g. when prioritizing emerging contaminations?
TRL	7
	Ready to use, not sure of application?
Relevance	7

	This database can help in evaluating which regulations cover specific chemicals that might (for instance) occur in the environment. On the one hand this reveals something about potential sources and on the other hand it might provide information on the hazard through toxicological information or classification.
Applicability	7
	Combining regulatory information with data on monitoring or occurrence data. Using the tool as information source when chemicals of interest pop up, either for evaluating the regulatory landscape of the particular chemical, its use and application or the potential quality criteria or toxicological information.

R26 - SOLUTIONS & NORMAN recommendations towards the review of WFD	
Graphic	
Description (from website)	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, nevertheless its practical implementation with regard to chemical pollution has faced certain challenges. SOLUTIONS and the monitoring network NORMAN have joined efforts in identifying several present-day challenges for monitoring, prioritizing, assessing, and managing risks posed by chemicals, and in evaluating the state-of-the-art of the science concerning those issues. In this article SOLUTIONS & NORMAN provide 10 recommendations to be addressed during the WFD review and updating processes in order to: i. improve monitoring and strengthen comprehensive prioritization; ii. foster consistent assessment; and iii. support solution-oriented management of surface waters
Abstract (Paper)	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.
Source	Journal Paper
Link	https://www.sciencedirect.com/science/article/pii/S0048969716322860
Citation	Brack, W.; Dulio, V.; Ågerstrand, M.; Allan, I.; Altenburger, R.; Brinkmann, M.; Bunke, D.; Burgess, R. M.; Cousins, I.; Escher, B. I.; et al. Towards the Review of the European Union Water Framework Management of Chemical Contamination in European Surface Water Resources. *Sci. Total Environ.* **2017**, *576*, 720–737. https://doi.org/10.1016/j.scitotenv.2016.10.104.
Tool Type	Recommendations
Technology	Framework/Guidelines
Summary	10 recommendations to improve monitoring and prioritization, consistent assessment and support solutions oriented management of surface waters
Reviewer	Milou Dingemans
Use	Use to inform monitoring programs at KWR and contribute to achieving the WFD
TRL	7
	Well thought through recommendations
Relevance	6
	Several of the SOLUTIONS recommendations are followed-up in the Kennisimpuls Waterkwaliteit
Applicability	4 (review paper on SOLUTIONS recommendations for the WFD)
	In this review paper, the SOLUTIONS consortium gives recommendations to 'improve monitoring and to strengthen comprehensive prioritization, to foster consistent assessment and to support solution-oriented management of surface waters'.

2.4 Theme 4 – Webtools and Databases

SOLUTIONS Toxicant Knowledge Base	
R27 – RiBaTox (Guide to Tools and Services for River Basin Toxicants)	
Graphic	RiBaTox
Description (from website)	RiBaTox (Guide to Tools and Services for River Basin Toxicants) is an online web-based service which supports the dissemination of the results of the SOLUTIONS project. It is intended for policy makers, their technical staff as well as water managers, but also for scientists and is also accessible to the public at large. New and improved models, tools, guidelines and databases are systematically documented and translated into SOLUTIONS "Tools and Services" designed to provide support to your challenges related to river basin toxicants. The output of RiBaTox are descriptions of SOLUTIONS Tools and Services in a so called Fact Sheet format, each downloadable as pdf. Please note that access to actual SOLUTIONS Tools and Services as such is not included in RiBaTox since it is not intended as a system where actual calculations are made or databases are directly consulted. For more detailed information or to receive and/or use the actual Tool or Service you are directed to references such as scientific publications, or may contact the developer(s) or supplier(s) of the Tool or Service directly based on the provided contact information. RiBaTox provides as options a Guide, an Overview and a Search function in order to help you find appropriate SOLUTIONS Tools and Services which may offer support to your challenge related to river basin toxicants. A RiBaTox manual with more information about the use of these options can be downloaded here. The full set of available Fact Sheets can be downloaded here.
Source	Webtool
Link	https://solutions.marvin.vito.be/
Tool Type	Decision support webtool
Technology	Decision support webtool for getting information about available strategies for a number of applications: abatement, case studies, communication, data, modelling, monitoring, policy and prioritization strategies.
Summary	By answering ~5 questions about the find of information/model/need one or several factsheets are suggested, which contain basic information and links to additional factsheets, publications or related resources
Reviewer	Thomas ter Laak
Use	Good starting point to find resources for a particular problem in water quality monitoring, sampling, abatement options etc.

TRL	7
	Ready to use It is a good starting point for issues regarding water quality.
Relevance	7
	Ready to use, but information in factsheets is very generic. Suitable as starting point for research on specific substances, or water quality issues. But does not include all relevant information from a research perspective.
Applicability	6
	The tool can be used as starting point, a road map for research on specific substances. The tool itself is too generic for in depth research needs.

R28 - Physio-chemical & Chemical data	
Source	Web Database
Link	https://www.normandata.eu/solutions/chemicalSearch.php
Tool Type	Web Database
Technology	Database of monitoring data from different countries and water sources
Summary	Provides monitoring/sampling data. Many different chemicals monitored in many European countries, classified by chemical, type of water matrix, sampling site, date, etc
Reviewer	Thomas ter Laak
Use	Could be used by Drinking water sector looking for data about a particular chemical or comparable data for a chemical in other countries/water types.
TRL	7
	It a bit cumbersome to use, not very user friendly
Relevance	7
	The database is very suitable to compare occurrence and concentrations of chemicals between countries. It is suitable to compare to monitoring data of drinking water companies and evaluating the monitoring program, this has been done in different studies. Additionally, the database and its predecessors have been applied in non-target screening to fill suspect lists. The database has been used in different occasions within BTO and other projects (ter Laak, Sjerps et al. 2015, Sjerps, Nugteren et al. 2016, Ter Laak and Kools 2016, ter Laak, Brunner et al. 2018). The current web based entrance form is not that user friendly, it is preferred to host the complete database in-house when used in research.
Applicability	8
	The database and its predecessors have been used in various occasions, and data of the drinking water companies is included in this database. It is a very useful repository for many purposes, ranging from evaluating and updating monitoring programs to suspect screening approaches in non-target data. Therefore, the filling

	of the database should be actively supported by various monitoring projects within the Drinking water sector, and additionally, the data should be applied within projects that study monitoring results or evaluate trends of chemicals of emerging concern in the water cycle. This is currently the case.

R29 - Bioassay Monitoring Data	
Source	Web Database
Link	https://www.normandata.eu/solutions/bioassaySearch.php
Tool Type	Web Database
Technology	Bioassay database
Summary	searchable data with bioassay data from surface water monitoring study
Reviewer	Milou Dingemans
Use	Can compare bioassay responses for own samples with database
TRL	5
	Currently it is not easy to export or view the data in a particularly useful way, this should be optimized.
Relevance	5
	Collecting (background) bioassay responses of different types of water can be helpful to interpret future datasets. In this version, several but not all commonly used bioassay are included.
Applicability	4
	This database should be developed further, ideally also including EC50 values for individual chemicals (see R1).

R30 - Passive Sampling	
Source	Web Database
Link	https://www.normandata.eu/solutions/passiveSearch.php
Tool Type	Web Database
Technology	Passive Sampling Database
Summary	Limited data (only Czech republic) of passive sampling results for surface waters
Reviewer	Thomas ter Laak
Use	If interested in passive sampling campaign for similar results obtained could compare to the limited dataset
TRL	5

	the web application is not really user friendly
Relevance	5
	Data set is currently too limited for proper use in the drinking water sector, especially when considering the more polar substances of interest.
Applicability	5
	Passive sampling data from the CZ republic is not that useful to the Dutch drinking water sector, however experiences, lessons learned and technical knowledge that is behind the acquisition of these data is very useful, when applying passive sampling in the Dutch situation.

R31 - Ecotoxicology	
Description (from website)	Ecotoxicology Database contains substances listed in the NORMAN substances with their Lowest PNEC, which were either predicted by QSAR or obtained experimentally. Experimental and predicted Lowest PNECs, which were voted by NORMAN ecotoxicology experts are addressed as 'verified'.
Source	Web Database
Link	https://www.normandata.eu/nds/ecotox/
Tool Type	Web Database
Technology	Norman Network Ecotoxicological Database
Summary	derivation of lowest predicted no-effect concentration
Reviewer	Milou Dingemans
Use	database with the lowest PNEC listed for ~40,000 compounds
TRL	6
	A bit difficult to use but does have nice exportable table
Relevance	7
	Depends on interest in future ecotoxicological data
Applicability	4
	Some ecotoxicological data could be predictive for human health relevant water quality but this is not clear.

R32 - Structure & Properties	
Source	Web Database
Link	https://www.normandata.eu/solutions/susdatSearch.php
Tool Type	Web Database

Technology	Chemical Properties Database
Summary	search for chemical properties and structure in a database from the Norman suspect exchange
Reviewer	Andrea Mizzi Brunner
Use	Already in use at KWR and Dutch drinking water laboratories
TRL	9
	Web based search GUI and downloadable suspect lists for integration into non-target screening workflows. At KWR, structures of >40000 SusDat compounds have been included into Compound Discoverer for non-target screening data analysis in collaboration with Thermo Fisher Scientific.
Relevance	9
	Database of choice for non-target screening data analysis when screening for environmentally relevant organic micropollutants.
Applicability	9
	Already in use at KWR and Dutch drinking water laboratories

R33 - Prioritization	
Source	Web Database
Link	https://www.normandata.eu/solutions/prioritisation.php
Summary	data base, but not clear how it works or prioritizes substances
Reviewer	Milou Dingemans
Use	?
TRL	4
	This database needs a manual to improve practical applicability, e.g. to compare parameters between chemicals.
Relevance	?
	Prioritization of environmental chemicals or suspects is very important, and this database needs to be further developed
Applicability	4
	This database needs to develop further and a manual should be included.

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