Main Science and Technology Results/Foregrounds

The project SOLUTIONS has been designed in four subprojects called Concepts and Solutions (SP1), Tools (SP2), Models (SP3) and Cases (SP4), which are highly interactive and presented in Figure 1.

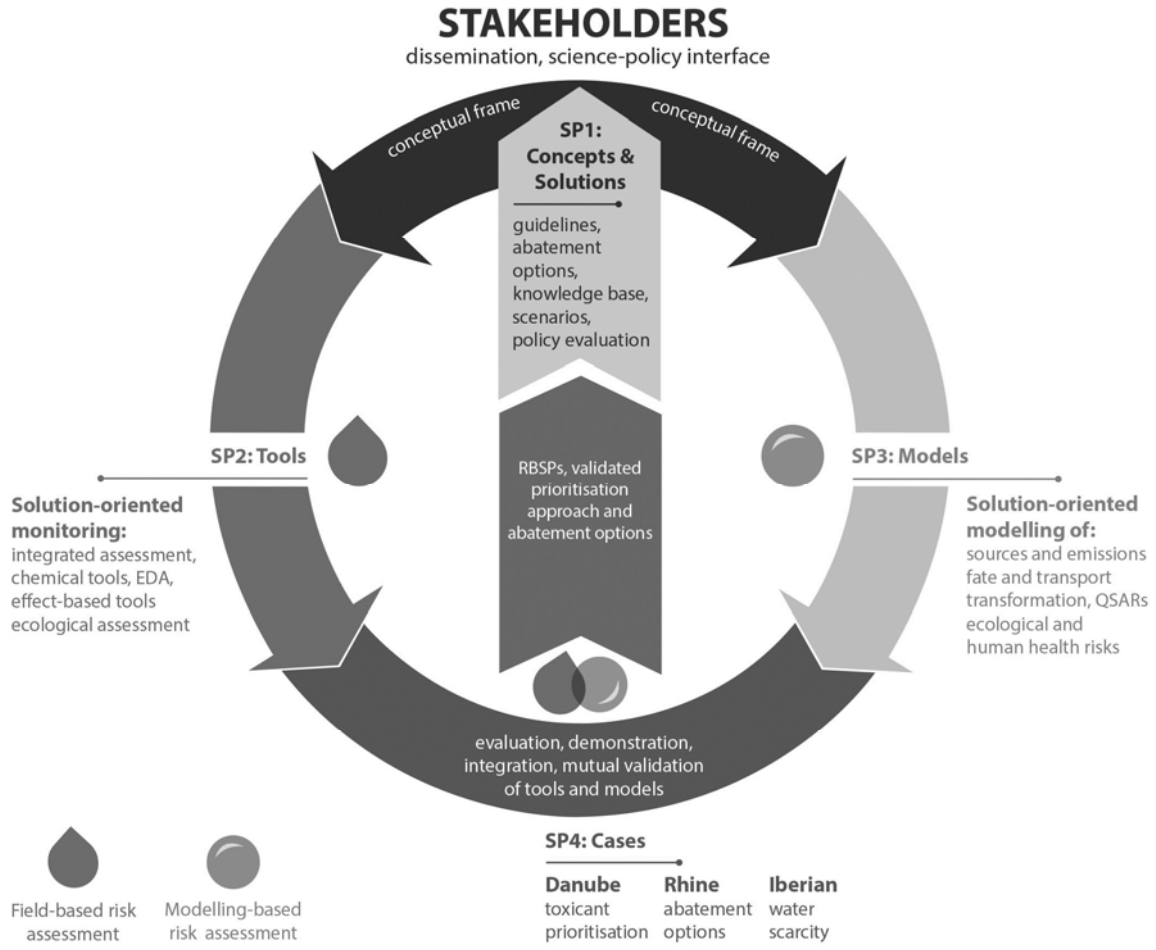

Figure 1: Structure of the project

SP1 comprises of a work package (WP1) providing the conceptual framework of SOLUTIONS together with several WPs delivering the final products based on this conceptual framework as well as on all the research that has been conducted in SPs 2, 3 and 4. The final products comprise an advanced methodology for the prioritization of contaminants, a database and guidance on abatement and innovative toxicants management, RiBaTox as a web-based tool providing SOLUTIONS tools and services in a user-friendly way to support monitoring, assessment and abatement as well as to address regulatory and societal questions on pollution, a toxicant knowledge base comprehensively compiling and providing SOLUTIONS data, trends and scenarios on future pollution and solutions to conflicts and gaps in policies.

1. SP1: Concepts and SOLUTIONS

1.1 WP1: Conceptual framework and integration of concepts and solutions

The overall objective of the project SOLUTIONS was to provide solutions for monitoring, assessment and abatement of the complex mixtures of chemicals that can be detected in European water

resources and thus approaches and tools to assess the “likelihood that surface water bodies will fail to meet the environmental quality objectives” due to chemical mixtures. Although there was a specific focus on emerging substances, the conceptual framework of SOLUTIONS has been designed in a way that it is able to address the whole universe of chemicals including those that may be considered as legacy chemicals, presently used substances and even future compounds. Having in mind that current monitoring and assessment based on a small set of Priority Substances often does neither provide a clear link to the Ecological Status nor suggest and prioritize abatement options, a solutions-oriented approach was the focal point of the conceptual framework (Figure 2). In agreement with stakeholders’ questions and requirements the SOLUTIONS conceptual framework has several entry points including

(a) Environmental observations (called “environment” in the scheme) such as a not good Ecological Status or measurable toxicity in environmental compartments. This may trigger the need to identify and prioritize chemicals, mixtures and sources thereof as well as the requirement to select efficient abatement options. Both questions are intensively addressed in SOLUTIONS particularly in the SPs on tools and cases.
(b) Given chemicals and the need to predict exposure and risks from a water body up to the European scale. This requirement has been successfully addressed particularly in the SP on models and validated in close interaction with SP cases. At the same time upcoming chemicals due to societal changes have been modeled in order to predict, prioritize and minimize future risks
(c) Societal developments (called “society” in the scheme) where scenarios and trends have been analyzed by the SOLUTIONS think tank in WP6 focusing on urbanisation, food supply, health care and new technologies. Since legal and policy instruments are an important tool to implement societal needs and to decide on abatement options, legal frameworks have been investigated for synergies in WP 7.
(d) Abatement options. Prioritizing most efficient abatement options is a key question under limited available resources. SOLUTIONS contributed to this task with an extensive database on abatement options and their efficiency for emerging chemicals together with prioritization approaches involving specific subjects of protection such as drinking water abstraction and valuable ecosystems, exposure and risk modeling and chemical footprints.

The SOLUTIONS conceptual framework has been provided and discussed in Deliverable 1.1 as well as in two scientific publications [1, 2]. The conceptual framework has been directly translated to the on-line tool RiBaTox (WP 4) as one of the major SOLUTIONS products supporting the dissemination of the SOLUTIONS tools and services and supporting practitioners in selecting appropriate and efficient tools to answer their questions.

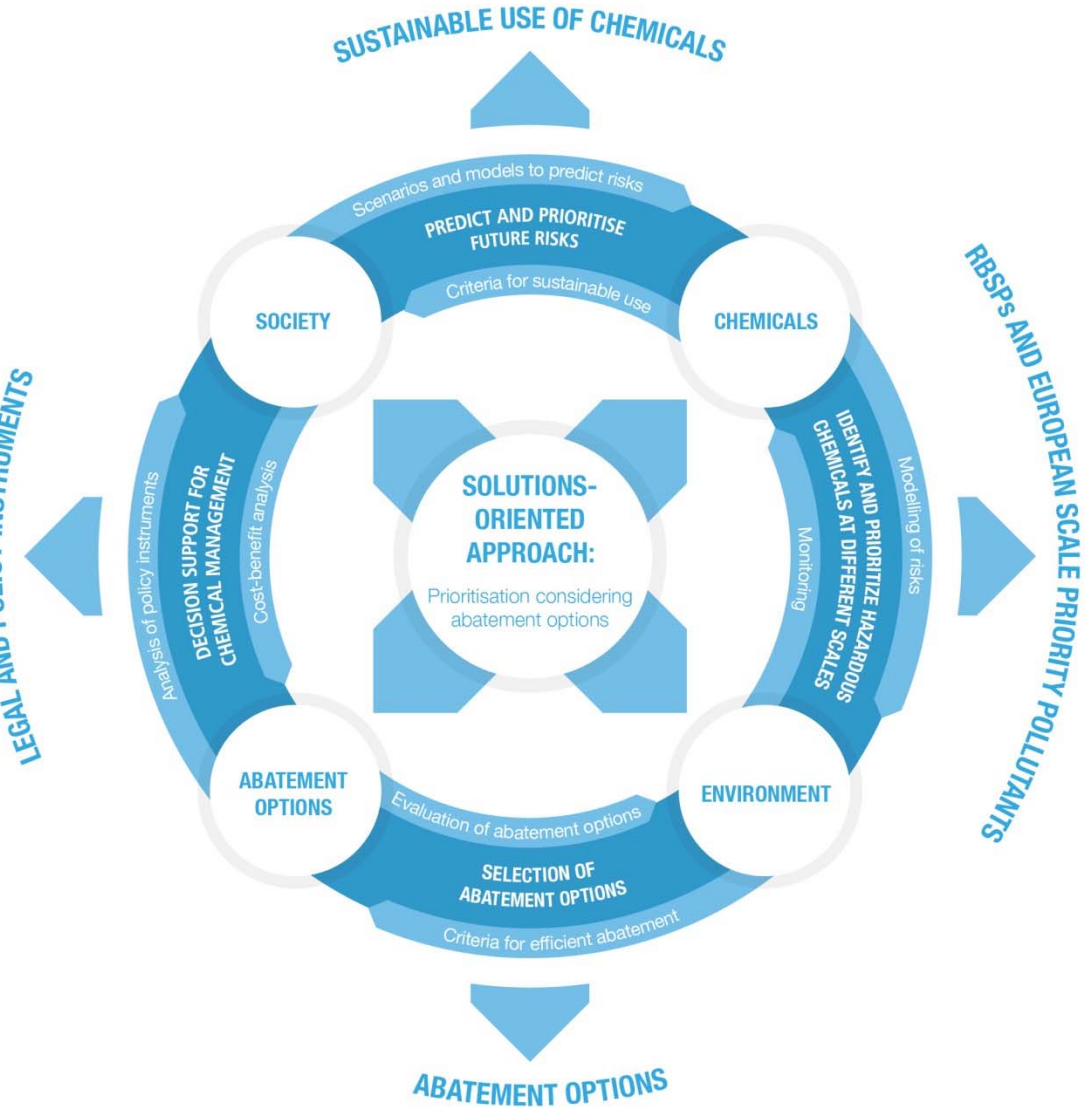

Figure 2: Conceptual Framework of SOLUTIONS

1.2 WP2: Advanced methodology for the prioritization of contaminants

The prioritization of contaminants and contaminant mixtures is one of the key issues of solutions-oriented monitoring and assessment of chemical contamination. The proposal for advanced prioritization of contaminants aims to tackle the major shortcomings of current prioritization procedures under the WFD. These include (a) the fact that the high demands for a conclusive risk assessment cannot be met and risks of emerging pollutants remain undetected due to the lack of monitoring data and missing knowledge on exposure and effects, and (b) the focus on individual pollutants rather than appreciating the fact that chemicals never occur in isolation but always as complex mixtures. Existing concepts and methods for prioritization have been carefully reviewed. Since none of them provides a comprehensive solution for the complex problem, a novel framework has been suggested which integrates all available lines of evidence on significant risks (Figure 3). This includes evidences from (a) modelling of co-exposure and resulting mixture risks, (b) chemical monitoring of a broad range of chemicals together with component-based approaches for mixture risk assessment and driver identification, (c) effect-based monitoring together with effect-directed

analysis for the identification of causative pollutants, compound groups and mixtures and (d) ecological monitoring and indications on drivers of ecological deterioration.

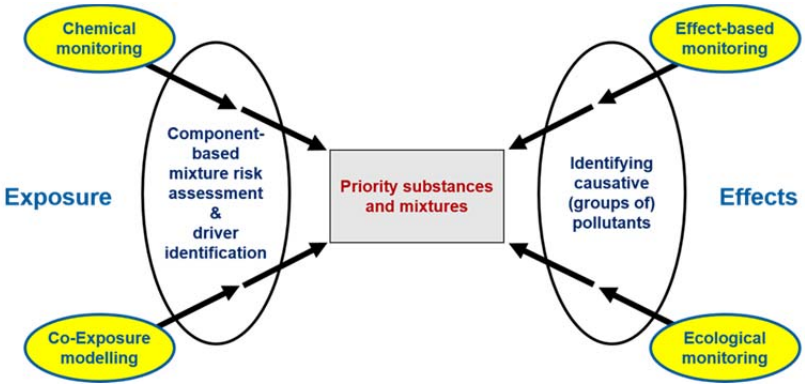

Figure 3: Multiple lines of evidence approach for prioritization of chemicals and mixtures

The prioritization approach is the result of three workshops in Paris (2014) establishing of the state-of-the-art in prioritization, in Gothenburg (2017) focusing on the identification of priority mixtures, the identification of risk drivers and the establishment of Environmental Quality Standards for priority mixtures, and again in Gothenburg (2018) on the final design of the methodological framework.

The results of this WP are presented in detail in Deliverable D2.1.

1.3 WP3: Abatement and innovative toxicants management

Technical and non-technical abatement options as well as efficient concepts to prioritize them are keys for a solutions-oriented assessment as highlighted in the SOLUTIONS conceptual framework. As a first step the perspectives of water cycle and the chemical life cycle were connected and possible abatement options were reviewed [3]. The requirement for and the added value of a mitigation database to assess effectiveness of interventions by coupling them to regional or global hydrological models has been explored. Modeling the impact of pollution sources such as municipal and industrial WWTPs on susceptible functions of water resources allows for a spatially smart implementation of abatement options. This has been demonstrated for the example of Dutch WWTPs impacting on drinking water abstraction and on Natura 2000 areas [4] (Figure 4).

A similar approach has been used to prioritize industrial WWTPs for their impact on Dutch surface water quality and drinking water production (Deliverable D3.1). The results indicated that 32% of the abstracted water for drinking water production is affected by industrial WWTPs and several of them could be prioritized for their impact.

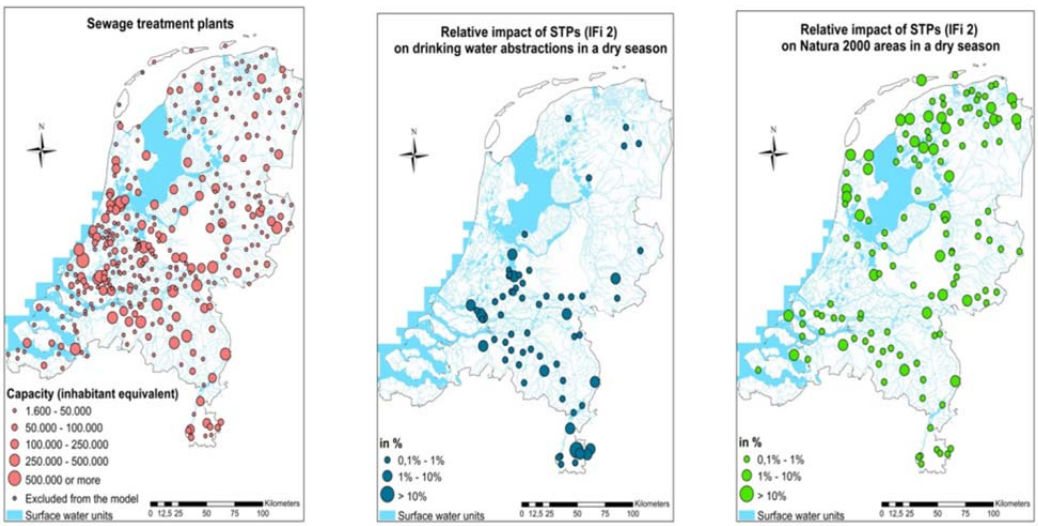

Figure 4: Overview of all Dutch WWTPs and their relative impact on drinking water abstraction and Natura 2000 areas [4]

Based on the concept of impact boundaries from the global to the regional scale Chemical Footprints have been explored and are recommended as a large-scale indicator the priority of abatement summarizing the volume of water needed to dilute the chemical mixture of a water body to a safe level in comparison with the available water amount. The SOLUTIONS approach allows for calculating Chemical Footprints for all water bodies in a region separately and provides the opportunity to explore how chemical pollution in upstream regions influence downstream water bodies. Regional chemical footprints can be mapped support management decisions (Figure 5).

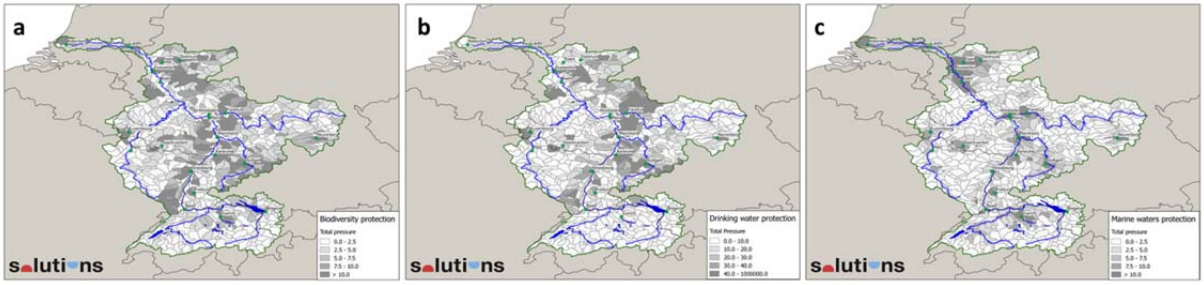

Figure 5: Chemical Footprints of Rhine catchment for biodiversity (a), for drinking water (a) and for marine environment protection (c)

After prioritization of regions and sources for spatially smart abatement typically effective water treatment technologies need to be selected which is hampered by a lack of a homogenous approach for testing water treatment technologies. SOLUTIONS filled this gap by developing a data evaluation framework to be used by stakeholders and by defining criteria for reliability and relevance of data together with extensive guidance for data evaluation (D3.1). In addition, a database on treatment technologies and their efficiency for major pollutants has been provided (D3.1).

1.4 WP4: RiBaTox Web-based Decision Support System

As discussed in 1.1, the SOLUTIONS Conceptual Framework has been translated in close dialogue with our stakeholders to a user-friendly tool called RiBaTox, which is designed to provide structured

access to the knowledge gathered in the project to support policy makers, technical staff and water managers in selecting appropriate models and tools to address their questions. RiBaTox is freely accessible via the SOLUTIONS website or directly under https://solutions.marvin.vito.be/ and has been extensively described in D4.1. RiBaTox is designed as a systematic tree providing valuable information on a branch, twig and leave level in a comprehensive format of 94 factsheets. On the branch level users can select between monitoring, modelling, prioritization, abatement and policy strategies as well as access databases and case studies. On a twig level these categories are further broken down detailing monitoring strategies to strategies for sampling, chemical analysis, effect-based monitoring, toxicant identification and ecological assessment which then guide users to specific methodologies. All fact sheets can be accessed via this systematic tree approach as well as via the entry points and questions that are highlighted in the conceptual framework including "chemicals", "environment", "abatement options" and "society". The factsheets have a consistent format, explain the objectives that can be addressed with the approach, describe the methodology, give examples of application and interpretation and provide references and contact information. They are highly interactive and provide numerous links to related factsheets. All factsheets can be also downloaded as D4.1 from the SOLUTIONS website and used as a hardcopy. RiBaTox also provides direct links to all relevant databases produced in SOLUTIONS.

1.5 WP5: Toxicant knowledge base

The SOLUTIONS toxicant knowledge base provides compound- and structure-associated as well as site- and receptor-specific data and metadata of SOLUTIONS. It consists of different databases that are accessible via IDPS, the Integrated Data Portal for SOLUTIONS that includes five different modules including environmental modules, ecotoxicology, structure and properties, legislation and emission and abatement. One of the big advantages is the opportunity to search for different information on a specific chemical accessing all the modules at the same time. Searching a chemical by CAS, name, INChIKey or substructure, IDPS provides you with monitoring and ecotoxicity data for the compound of interest, structural information and physico-chemical properties, but also legislation, emission data and abatement information. Filtering options can be applied in order to restrict the search for example to a specific country, specific media or to distinct species. IDPS is linked to the European Information Platform for Chemical monitoring IPChem as well as to RiBaTox and accessible via the SOLUTIONS website.

1.6 WP6: Trends and scenarios

SOLUTIONS had the ambition to consider not only existing chemicals but also to provide first ideas of chemical pollution of tomorrow in order to provide options to act on future risks. The analysis of future perspectives on pollution trends was based on three major columns. The first column was the in-depth analysis of 34 publicly available studies on development in society by UNEP, EEA, McKinseys 2030 Water Resources Group, UNESCO, BMBF, OECD, EU Watch and many others including (a) scenarios for mid- and long-term developments in society, (b) developments in water use and water cycles, (c) developments in use and impact of chemicals, (d) climate change, (e) demographic change, (f) technological and economical changes, (g) development in food production, (h) nutrient scenarios and (i) further aspects such as precautionary principle, green economy, megatrends and scientific developments. The results are presented in D6.1. The second column was four workshops bringing together the SOLUTIONS think tank with external experts and addressing the topics public health 2030, food 2030, cities 2030 and technologies 2030. The third column was related to modelling of

future risks combining scenarios and the application of the SOLUTIONS model train (D14.2). This approach considered 2 different scenarios in relation to reference situation in 2018 including no specific action and responsible action on upcoming problems.

The approach resulted in 21 recommendations on how to include future emerging pollutants into the management of river basins, which are detailed in D6.1. A key message might be that future increase in pressure and changes in pollution patterns are expected that need to be addressed with more efforts than end-of-pipe technologies only but should rely on the design and production of more sustainable chemicals and products.

1.7 WP7: Solutions to conflicts and gaps in policies

Regulatory frameworks can be one of the key drivers towards a non-toxic environment as proposed by the European Commission. Thus, SOLUTIONS investigated 19 existing regulatory frameworks for chemicals including EU regulations on industrial chemicals (REACH), plat protection products (PPP), biocidal products (BPR), Cosmetics and medicinal products, EU directives on water (WFD), groundwater (GWD), marine environments (MSFD), dringking water (DWD), sewage sludge (SSD), industrial emission (IED), mining waste, hazardous substances in electric and electronic equipment (RoHS) and toy safety, and multilateral agreements such as the Stockholm Convention, the Convention on Long-Range Transboundary Pollution, the Protocol on Pollutant Release and Transfer and the Rotterdam Convention. As discussed in D7.1, the overview revealed a quite fragmented situation with the regulatory frameworks designed for specific groups of chemicals and for protecting different endpoints. Despite the existence of a large number of regulations, many chemicals are not regulated but represent a potential risk and are denoted as Chemicals of Emerging Concerns (CECs).

The studied regulatory frameworks all regulate chemicals, but with different objectives. They address different endpoints including human health, human health an the environment or only the environment. Many of the frameworks only regulate emissions and/or occurrence in one receiving media but also consider only specific stages in the life cycle of a product as has been summarized in Figure 6.

From in-depth analysis of regulatory frameworks SOLUTIONS identified regulatory gaps and derived a number of recommendations to improve the situation (D7.1). In brief, we suggest (a) to harmonize objectives in a way that regulations consider both human health and environment and (b) to closer link emission and receiving-media oriented regulations such as REACH and WFD. REACH could clearly benefit from considering monitoring data collected under WFD. (c) The regulation of only selected and different stages in life cycles may introduce the risk of inefficient implementation and control. Systematic gaps are observed in trade and product use stages. (d) A key requirement for a better harmonized regulation is cooperation and exchange of information. Many chemicals are listed in different regulations. Common objectives, exchange of information and the use of harmonized terminology would substantially improve regulation. Information on use and emissions, physicochemical and toxicological properties, monitoring data and information on efficiencies, costs and applicability of abatement options should be made transparent and shared in common platforms. (e) Additional substances as well as mixtures need to be considered and (f) the international perspective should be strengthened. Despite the regulations on European market authorization of chemicals many other chemicals enter the EU via imported products.

Figure 6: Life cycle stages covered by the regulatory frameworks

2. SP2: Tools

In SP2 novel approaches and tools for chemical and biological monitoring have been developed and integrated to consistent workflows accompanied by user-friendly guidance for practitioners supposed to use the methods.

2.1 WP9: Integration of chemical, effect-based and ecological tools

The development of chemical, effect-based and ecological tools for a solutions-oriented monitoring and assessment of the presence and effects of complex mixtures of contaminants including the many non-regulated CECs was one of the major tasks of SOLUTIONS. It has been defined in detail in an early stage of the project [5] focusing on the development and adaptation of tools to deal with mixtures of pollutants in water resources management. This included, in addition to innovative research and development of tools, the integration in a comprehensive toolbox including a user-friendly guidance document and decision tree for the use of these tools in the identification of River Basin Specific Pollutants (RBSPs), impact assessment, and establishment of cause-effect relationships. The results of these efforts are provided in deliverable D9.1 that has been also submitted as a scientific publication. In addition, the information has been included in a condensed and structured way into RiBaTox (WP4). The toolbox developed in SOLUTIONS included several water sampling technologies, multi-residue target analysis and non-target screening, bioanalytical methods for complementary use in an effect-based water monitoring, effect-directed analysis as a tool to identify drivers of risks and to establish cause-effect relationships and finally ecology-directed

analysis as a lines-of-evidence approach combining the afore-mentioned approaches with in situ-tests and field-based monitoring studies as it is schematically presented in Figure 7.

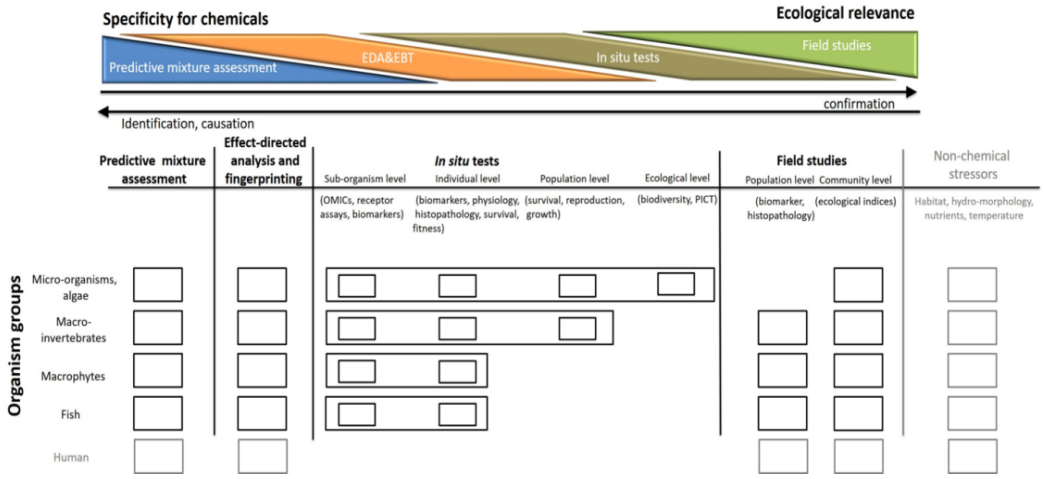

Figure 7: Aggregating information of different lines of evidence in a weight-of-evidence matrix

2.2 WP10: Chemical analytical tools

Major challenges of chemical monitoring of organic micro-pollutants are (a) the detection and quantification of target analytes at very low concentrations including particularly those that have very low predicted non-effect concentrations (PNECs), (b) the screening for the whole mixture including unexpected and unknown chemicals using non-target screening (NTS) and (c) the identification of the chemicals detected with NTS.

A major achievement of SOLUTIONS was the development, advancement and testing of tools for time-integrated sampling and enrichment of water samples for chemical analysis and the application of effect-based methods in order to achieve very low limits of detection and to collect sufficient material for more volume consuming methods such as some of the effect-based tools. In SOLUTIONS, two powerful approaches have been advanced and evaluated for this purpose, namely passive sampling and large volume solid phase extraction (LVSPE). Several partition- and adsorption-based passive samplers have been applied and a detailed guidance for their application has been provided in D10.1. They are powerful screening tools particularly for hydrophobic chemicals with low costs involved. LVSPE has been developed as a mobile tool to extract large volumes of water (50 to 1000L) in the field in order to strongly facilitate logistics related with handling, transportation and storage of large water volumes [6]. Well-reflecting the original mixture in the water sample and excellent recoveries of analytes with a broad range of physico-chemical properties as well as of measured effects [7] suggest LVSPE particularly as a tool for lowly to moderately hydrophobic water contaminant mixtures, while very hydrophilic and very hydrophobic chemicals are outside the domain of this tool. Guidance is given in D10.1. In addition, the feasibility of using high-performance counter-current chromatography has been demonstrated as an alternative to SPE. For cases, where trace contaminants need to be quantified in water samples without the need of biotesting on-line solid phase extraction coupled to liquid chromatography mass spectrometry (SPE-LC-MS) has been explored and recommended (D10.1).

Sensitive and innovative tools in target analysis of emerging pollutants have been reviewed [8] and successfully demonstrated for the analysis of difficult trace components in the context of evaluation

of treatment technologies including pharmaceuticals and iodinated contrast media in hospital wastewater [9], drugs of abuse [10, 11] and cytostatic drugs [12].

A large set of standard operational procedures for target analysis of emerging contaminants has been provided in D10.1.

Since target analysis is necessarily restricted to an (increasing) number of selected analytes, while SOLUTIONS has the ambition to address chemical contamination as a whole, suspect and non-target screening (NTS) got a strong focus in SOLUTIONS. A powerful NTS workflow has been established with a particular emphasis on its application in SOLUTIONS case studies (D10.1). This included methodological developments [13] as well as a collaborative trial [14]. A complete evaluation and the identification of all underlying chemicals are not feasible. Thus, approaches to extract valuable information out of these huge datasets have been developed. These include three complementary approaches: (a) Prioritization of individual peaks or groups of peaks for in-depth analysis according to the specific objectives. This may include the selection of high intensity, high frequency, site-specific peaks, peaks with increasing trends or peak occurrence in time series, peaks occurring after specific sources etc. A powerful example is the application of NTS for monitoring of the River Rhine and the identification of peak emissions including unknown chemicals [15]. (b) Suspect screening by searching NTS data for a large number of exact masses representing suspect chemicals lacking available standards. A typical example is the prediction of and screening for transformation products of known environmental pollutants [16, 17]. (c) The evaluation of whole NTS patterns using multivariate analysis. Several publications are in progress.

Compound identification and structure elucidation are typical follow-up steps on NTS. A highly efficient workflow based on the software MetFrag has been developed (10.1) involving novel computational approaches to use exact masses for the derivation of molecular formula and to identify structures. Candidate structures are retrieved by searching compound databases such as PubChem and ChemSpider or by predicting possible structures with MOLGEN. Subsequently, scoring and filtering criteria are used to select most probably structures. These criteria are based on mass spectrometric information including fragmentation and ionization, chromatographic retention time predictions, hydrogen/deuterium exchangeability but also other criteria such as the number of references in the database assuming that a frequently mentioned chemical is more likely to be found than a compound mentioned only few times. Several publications have summarized the new developments [18-21]. Diagnostic derivatization has been developed as a tool to detect specific groups of chemicals such as aromatic amines [22].

2.3 WP11: Effect-directed analysis

Effect-directed analysis (EDA) is designed to identify drivers of toxic effects in complex mixtures such as water, sediment and biota extracts. A consistent conceptual framework for EDA (Figure 8) has been developed in SOLUTIONS and supported by a comprehensive compilation and critical evaluation of available tools [23], (D11.1). Driver identification is considered as a stepwise approach most efficiently exploiting existing information and large scale chemical and effect-based monitoring linked by mass balance approaches and multivariate analysis. Higher tier EDA as a combination of biotesting, fractionation and in-depth chemical analysis is used as a site-specific approach for those cases where neither mass balances nor statistics are able to unravel cause-effect relationships.

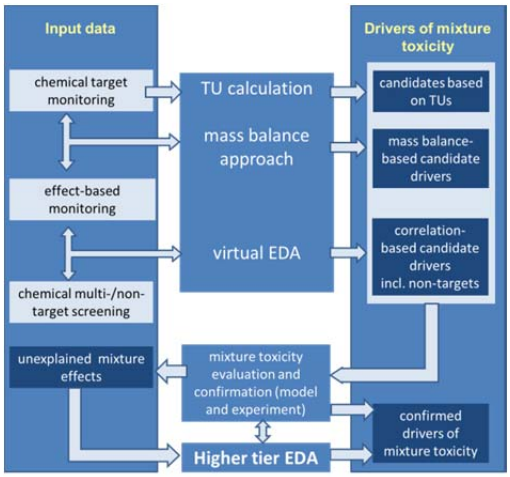

Figure 8: Conceptual framework for EDA as a stepwise approach

Novel method applications and several successful field studies have been performed to demonstrate the power of EDA approaches. This includes mass balance approaches identifying drivers of endocrine disruption and other effects in water of the River Danube impacted by untreated wastewater from the city of Novi Sad [24] but also in small streams in the Rhine catchment [25]. Virtual EDA has been demonstrated as a powerful tool in the identification of diaminophenazines as drivers of mutagenicity in industrial wastewater on the basis of a time series of samples [26, 27]. Several successful higher tier EDA studies have been performed in order to unravel site-specific toxic contamination. In a small German stream strong anti-androgenic effects have been detected and could be linked to coumarin 47, a frequently used fluorescent dye that has never been detected in monitoring so far and that was, thus, unknown as an environmental contaminant [28]. Endocrine disruptors could be identified and quantitatively confirmed in the River Danube [29]. EDA has been also demonstrated as a powerful tool to get insight into mutagenicity in the River Rhine. The effects have been shown to be mixture effects rather than driven by individual chemicals [30]. Mixtures of industrial aromatic amines and natural carboline alkaloids detectable in the river water have been demonstrated to exhibit strong synergistic effects.

2.4 WP12: Effect-based tools

SOLUTIONS strongly recommends effect-based tools and methods (EBM) to complement chemical monitoring in order to determine the likelihood that “surface water bodies will fail to meet environmental quality objectives” (WFD) and to reduce the risk to overlook toxic chemicals not necessarily covered with chemical monitoring. Intensive research has been performed in order to develop improved bioassay solutions (D12.1) and to assess the feasibility of these solutions integrating for environmental monitoring (D12.2). A first important step has been the evaluation of frequently found surface water contaminants for their mode of action (MoA) in order to design a diagnostic test battery that covers all relevant MoAs [31]. Since only for few MoAs specific in vitro assays are available SOLUTIONS suggests the use of a combination of apical tests involving fish embryos, daphnids and algae, also representing WFD BQEs, relevant for the Ecological Status, with MoA-specific in vitro assays on endocrine disruption, mutagenicity and dioxin-like effects. For specific purposes a set of additional tests on adaptive stress responses and changes in metabolism is available and covers links in relevant adverse outcome pathways (AOP) (Figure 9) [32].

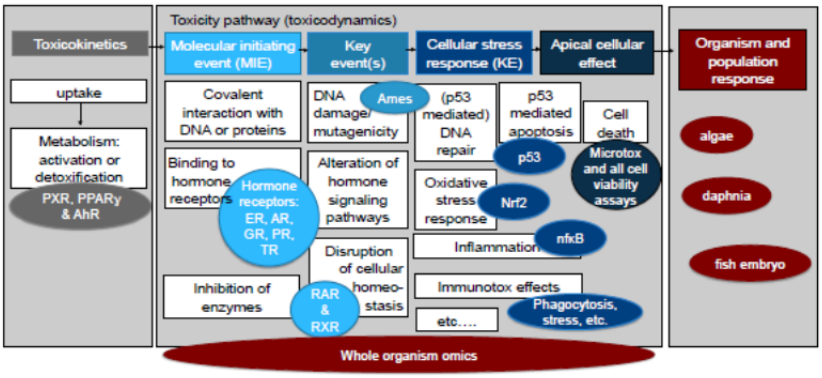

Figure 9: AOP conceptual framework and the bioassays used within SOLUTIONS.

The effects of 34 water pollutants with different MoAs were fingerprinted in a test battery of 20 bioassays. We could demonstrate that the tested battery was able to detect these specific effects individually and in mixtures.

Interlaboratory investigations further enhanced the degree of confidence into the application of EBMs in monitoring of complex mixtures [33, 34]. A specific focus was given on the detectability of mixture responses of active compounds against a background of other inactive compounds. The majority of in vitro and in vivo tests produced mixture responses in agreement with additivity expectation of concentration addition [34]. Our findings support the application and further development of effect-based methods for water quality assessment, safeguarding specific water uses and diagnosis of complex contamination. This was also recommended in a policy brief released by SOLUTIONS and suggesting the test battery shown in Figure 10.

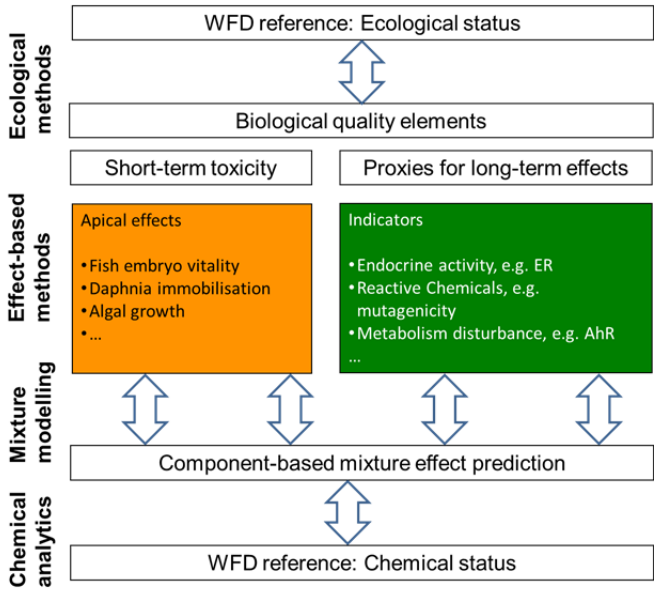

Figure 10: Recommended test battery bridging Chemical and Ecological Status

2.5 WP13: Ecological assessment tools

SOLUTIONS developed weight-of-evidence (WoE) approach that may be used for impact description, identification and quantification and for stressor identification and the establishment of cause-effect relationships. Four line of evidence (LoE) are considered including (a) chemical monitoring profiles

and predictive mixture modelling, (b) effect-based monitoring and fingerprinting, (c) in situ approaches for the identification of chemical exposure or effects (e.g. biomarkers), (d) community indices based on field surveys of community composition. Available tools as well as the integrated concept are described in depth in D13.1.

This approach has been fully or in relevant parts applied and demonstrated in the large SOLUTIONS case studies Danube and Rhine as well as in an additional field study in the River Holtemme in Germany.

The WoE study in the case study Danube has been performed as a joint activity of WPs 13 and 19 and is based on data collected during Joint Danube Survey (JDS) 3 by ICPDR and SOLUTIONS. This demonstration study involved all four LoEs suggested above including chemical analysis and toxicity modelling based on toxic units (TU), in vitro bioassays, a battery of in situ biomarkers in sentinel fish and taxonomy- and trait-based analysis of fish and macroinvertebrate community. LoE1 based on chemical analysis indicated a considerable risk for macroinvertebrates. LoE2 representing effect-based fingerprinting used large-volume solid phase extracts for testing fish embryo toxicity, effects on algal growth and photosynthesis inhibition as well as nine receptor-based in vitro assays, including endocrine disruption, mutagenicity, neurotoxicity and adaptive stress responses. Along the River Danube significant effects at many sites have been detected for different endpoints without strong differentiation. Some tributaries inhibited stronger effects. LoE3 involved a substantial battery of biomarkers in wild fish including DNA damage, enzyme activities indicating changes in phase I and II biotransformation, oxidative stress and neurotoxicity, gene expression analysis in liver samples as well as histopathology. As for LoE3 similar biomarker responses have been detected along the Danube however with some significant peaks of neurotoxicity and genotoxicity [35]. Taxonomy- and trait-based assessment of aquatic communities focused on macroinvertebrate and fish community structure using indices based on species richness, heterogeneity of the community, and other taxonomic and functional indicators for fish and three characteristic indices for macroinvertebrates including the Average Score Per Taxon (ASPT), the well-known saprobic index and the trait-based indicator $SPEAR_{pesticide}$ reflecting the effect of toxic pollution. Most sites exhibited a moderate status with some significant exceptions with poor to bad status downstream of big cities such as Belgrade. The LoEs were integrated using quality classes for each of them: no effect, moderate effect, clear effect. In agreement with expectations for a large river with high dilution potential on the one hand but a lot of significant input of pollution from many sources, the WoE evaluation indicated clear anthropogenic impact and toxic pressure as a potential cause of degradation but also a ‘flat’ profile with not very pronounced differences and no real reference sites.

The WoE in the case study Rhine was performed as a joint activity with WP20 and focused on two LoEs, namely chemical analysis and TU distributions and in situ experiments with complex algal communities based on structure and pollution-induced community tolerance (PICT) [36]. The study focused on the impact of wastewater treatment plants (WWTP) on river ecosystems and was designed as an upstream-downstream gradient study but as well as a Before-and-After-Impact study integrating the evaluation of the upgrade of one of the WWTPs. The study clearly indicated the strong impact of the WWTPs on the TU distributions with clear increase downstream based on pesticides and antibiotics. After WWTP upgrade with a fourth treatment step using powder-activated carbon filtration there was no more significant difference between upstream and downstream. This result was confirmed by the investigation of bacterial and algal structure. Principal component analysis (PCA) indicated clearly different communities upstream and downstream for non-upgraded

WWTPs while the communities were very similar in structure after upgrade. PICT, indicating increased tolerance by the disappearance of sensitive species provided a further LoE confirming the occurrence of tolerant communities downstream the WWTPs without upgrade, while the upgraded WWTP had no impact on tolerance (Figure 11).

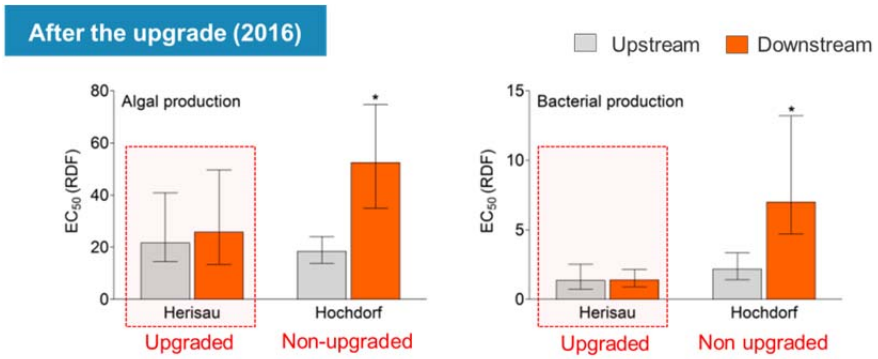

Figure 11: Tolerance of algal and bacterial production upstream and downstream of an upgraded and a non-upgraded WWTP

The WoE in the Holtemme River combined the analysis of toxic unit distribution for algae, daphnids and fish [37] with in situ biomarker responses in fish and genetic structure and body burdens of *Gammarus pulex* [38]. All LoEs indicated significant risks and the strong and different impact of the two WWTPs along the river. The TU evaluation indicated significant risks to invertebrates, algae and fish with seasonal and random peaks of pesticides predominating acute toxicity while chronic and sublethal effects to fish were driven by constantly emitted pharmaceuticals [37]. Water contamination was well reflected by internal concentrations in *Gammarus pulex* [39] as well as in genetic diversity in *Gammarus* populations [38]. Detectable mutagenicity downstream of one of the WWTPs was reflected in Gammarus as the occurrence of private alleles.

3. SP3: Models

3.1 WP14: Integrated Models

SOLUTIONS provided the approaches and tools for a more holistic and solutions-oriented monitoring that covers a large set of chemicals, measurable effects in laboratory test systems and in situ, and community alterations. However, there will be always gaps in compounds covered, in time, in space and in matrix under consideration. Thus, SOLUTIONS developed an integrated system of models called the SOLUTIONS model train that helps identify gaps of specific concern and thus provide indications on monitoring needs with high priority and tentatively fill these gaps, and identify chemicals, regions and times with low or no risk that do not require major monitoring efforts. The SOLUTIONS model train comprises four highly integrated modules including emission modelling (WP15), transport and fate modelling (WP16), substance metabolism and properties modelling (WP17) and human and ecological risk modelling of pollutant mixtures (WP18). A scheme of the integrated model train and external data used is compiled in Figure 12. The model train operates on the scale of Europe as a whole or for one or more individual river basins. The spatial schematization as well as hydrology, soil type, land use and crop cover are derived from the Europe-wide hydrology model E-hype developed by SMHI. The SOLUTIONS model train is designed to provide temporarily and spatially explicit predictions of exposure and risks. The whole modelling framework is described in more detail in D14.1.

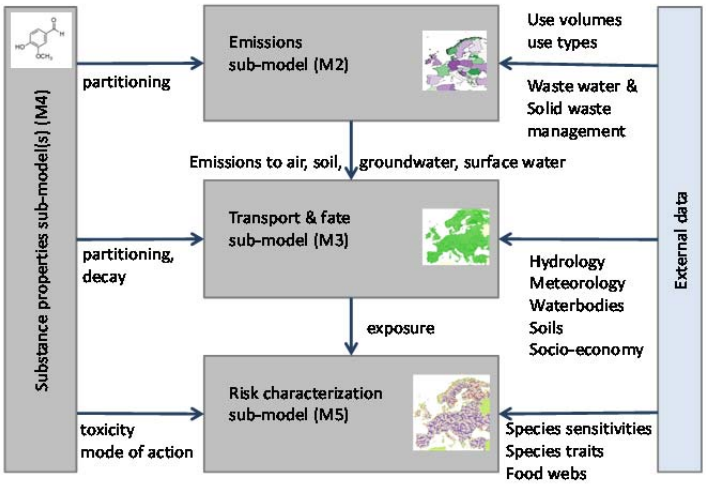

Figure 12: Scheme of the SOLUTIONS modelling system and its modules

3.2 WP15: Emission modelling

Emission modelling has been derived from the Dutch Pollutant Release and Transfer Register (PRTR) as a basis of the European Pollutant Release and Transfer Register (E-PRTR, http://prtr.ec.europa.eu/#/home). The emission modelling separates three groups of substances (pesticides, pharmaceuticals and chemicals registered under REACH) and provides temporally and spatially resolved emissions to surface waters and soils (D14.1).

The losses of pharmaceuticals are estimated based on per-capita sales in different countries. Human excretion is assumed to be 12% of the amount sold on average and all losses are assumed to reach the wastewater. The losses of pesticides to air, surface water and soil have been estimated using the harvested-area approach combining crop- and substance-specific application rates with known agricultural land uses. The losses of REACH registered organic chemicals have been estimated based on registered amounts produced, imported and exported submitted to the European Chemicals Agency as a part of REACH registration dossiers. This information is confidential, but SOLUTIONS was allowed to use the numbers for the purpose of EU wide analysis of impacts. Emissions are assumed to reach air (8.5%), water (12%) and soil (3.0%), calculated from loss factors for various use categories. Due to a lack of compound-specific information the general assumptions given above had to be done, however being well aware that this is a source of uncertainty that can be reduced only with more transparency in compound related data.

The losses to the environment are spatially distributed on the basis of so-called locator values. For REACH-registered chemicals and pharmaceuticals SOLUTIONS assumed that a higher standard of living implies (gross domestic product based on purchasing-power-parity, GDP-PPP taken from the World Bank) a higher use of chemicals. At the same time, increased standard of living is also related to higher environmental awareness quantifiable as the share of wastewater collected and treated (Figure 13).

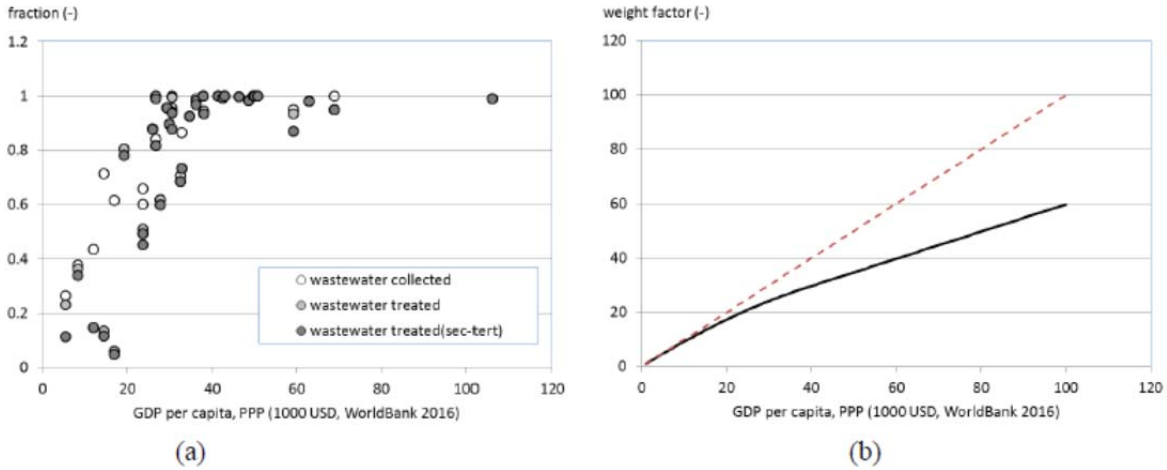

Figure 13: Country-by-country indicators for wastewater management (a) and GDP dependent population weight factor used in spatial distribution of emissions

Based on simulations with the model Simple Treat developed at RIVM, the fate of individual chemicals in wastewater treatment is calculated.

For pesticides, the losses to water, soil and air are spatially distributed according to the agricultural land use considering distribution in time by taking into account spring crops, autumn and perennial crops.

In total emissions have been modeled for 621 pharmaceuticals, 408 plant protection products and 4159 REACH registered chemicals for the entire European Union plus few other countries spanning a period of 5 years (2009 to 2013). As an example, spatial distribution of emissions of the pharmaceutical flukonazol to surface water is given in Figure 14.

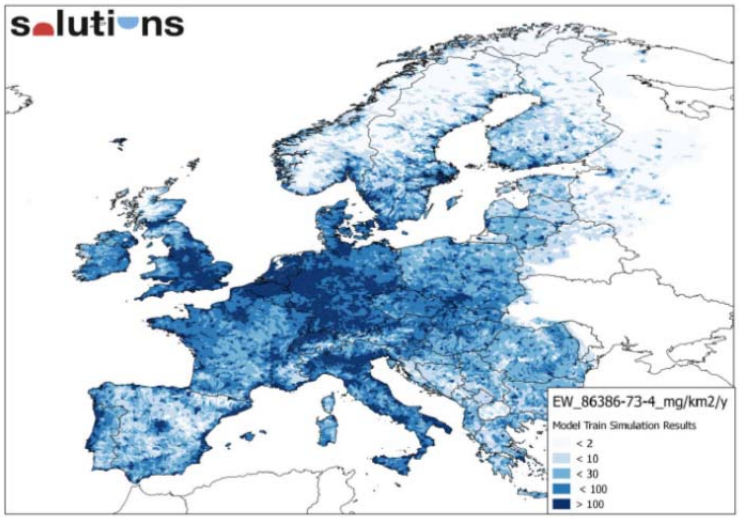

Figure 14: Simulated spatial distribution of emissions of fukonazole to surface water

3.3 WP16: Fate and transport modelling

For fate and transport modelling, a dynamic mass balance model called STREAM-EU has been developed. Its description and several relevant applications with a specific focus on the perfluorinated surfactants PFOS and PFOA in the SOLUTIONS case studies have been published [40-42]. STREAM-EU was implemented in the Delft3D-WAQ open source modelling framework was used to calculate contaminant concentrations in a spatially and temporally resolved way in all relevant environmental compartments including surface water, groundwater, snow, soil and sediment. The compartments are considered as well mixed and contain different phases. Partitioning between the phases is modelled using the fugacity concept. Precipitation, dissolution and ionization as well as biodegradation have been implemented in the model. Within the compartment with an atmosphere interface volatilization is included. In order to properly cover particle-bound contamination, the fate and transport model needs information about erosion and sedimentation fluxes which is derived from a separate dynamic mass balance simulation driven by E-Hype schematization and hydrology.

With a focus on the fish consumption pathway for human health risk assessment the fate and transport model was expanded with a module to quantify expected bioaccumulation in fish combining the estimation of rate constants with food-web modelling. Bioaccumulation was modelled for several fish species at different trophic levels. Internal equilibrium concentrations modeling involved also the uptake and elimination rates for ionogenic organic chemicals using the innovative BIONIC model [43].

In addition to the European scale, mean concentrations of pesticides, pharmaceuticals and REACH chemicals were modeled for the big SOLUTIONS case study Rivers Danube and Rhine, Spanish rivers and Vegea River in Sweden in order to evaluate modeling data with monitoring data that were provided by SOLUTIONS in WPs 19 to 21 or available from external sources. To summarize the results for pesticides, although correlations between predicted and observed concentrations of different compounds were quite dependent on the investigated basin, the overall bias was less than one order of magnitude in 72% of cases and less than two orders of magnitude in 94% of cases (Figure 15).

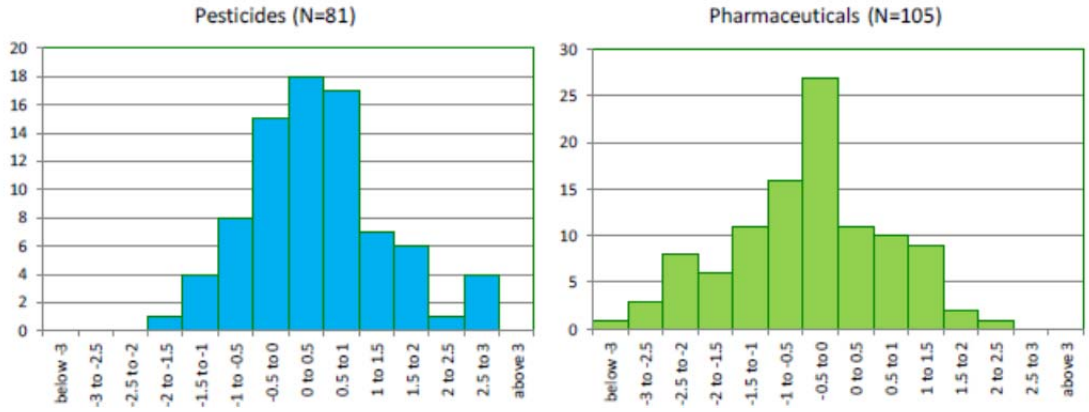

Figure 15: Histogram of bias for individual pesticides (left) and pharmaceuticals (right) for all investigated cases

For data sets with good temporal coverage a very good fit could be achieved as exemplified for the River Vegea in Figure 16.

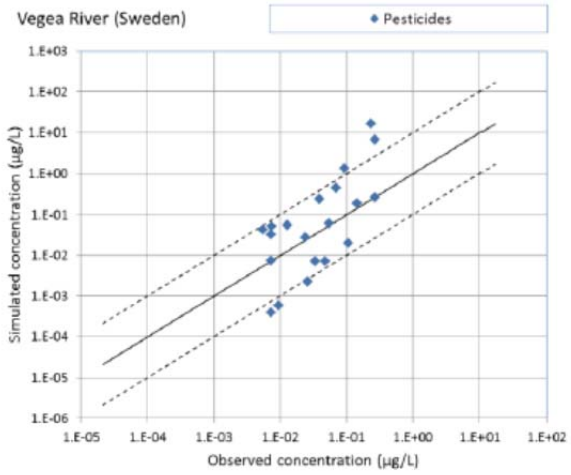

Figure 16: Simulated vs. observed concentrations of pesticides for River Vegea

The deviations between simulated and measured concentrations for pharmaceuticals were low for Spanish rivers and River Rhine but higher for the Danube (no data for River Vegea were available). Altogether the bias is less than one order of magnitude in 61% of all cases and less than two orders of magnitude in 88% (Figure 15). All simulations were based on available pharmaceutical sales in Sweden and Great Britain, which obviously only poorly reflected pharmaceutical consumption in the Danube countries. Better data availability will probably improve predictions.

For REACH registered chemicals again the bias is dependent on the river basin under consideration. Deviations occurred particularly for volatile chemicals despite the fact that volatilization from soils and surface waters in included in the model.

3.4 WP17: Substance metabolism and properties modelling

Data gaps with respect to chemical fate and effects of emerging compounds are one of the major obstacles for the evaluation of monitoring data as well as for simulating emissions and fate and transport with models. Thus, SOLUTIONS put major efforts on closing these data gaps using QSAR models (D17.2). For prediction of sorption and bioaccumulation of emerging contaminants novel experimentally-based LSER models were developed (D17.1).

For the large set of chemicals used in modelling as well as for the chemicals detected in the aquatic environment in SOLUTIONS case studies physico-chemical properties including water solubility, partition coefficients and other pure compound molecular properties have been calculated using the model suite developed for and compiled in ChemProp at UFZ have been estimated. Where needed this approach was complemented with the commercial software package ACD/Percepta and EPI Suite models.

The CATALOGIC software suite, developed by LMC, is a platform for models and databases to predict the environmental fate of chemicals including abiotic and biotic degradation, bioaccumulation but also acute ecotoxicity to algae, daphnid and fish for narcotic chemicals. These models were complemented by a set of TIMES models developed by LMC for the prediction of an extensive set of sublethal endpoints relevant for human health as well as partially for effects on aquatic organisms including genotoxicity such as Ames mutagenicity, chromosomal aberrations (both including S) activation), in vivo Comet genotoxicity, in vivo liver clastogenicity, in vivo liver transgenic rodent

mutagenicity, in vivo bone marrow micronucleus test, other types of reactive toxicity such as skin and eye irritation and skin sensitization, phototoxicity, aromatase inhibition and three nuclear receptor based endpoints involving AhR, AR and ER. In total 11 large sets of chemicals for different purposes have been modelled feeding the results into many different SOLUTIONS work packages.

3.5 WP18: Human and ecological risk modelling of pollutant mixtures

Estimating ecosystem and human health risks from predicted and measured exposure is an important building block for an integrated modelling framework, which can be used for the prioritization of emerging pollutants and for the assessment of abatement options. In SOLUTIONS we developed a common tiered framework for human and ecological mixture risk assessment (MRA), which has been further extended with the specific aim of increasing the predictive modelling capacity with respect to the ecological effects of emerging compounds, both described in detail in D18.1.

The common and advanced framework for human and ecological mixture risk assessment uses a component-based tiered approach based on the model of concentration addition (CA) as a lower tier approach, complemented with the model of independent action (IA) in higher tier. In Tier 1, regulatory values such as ADI, TDI and EQS (or their equivalents such as PNECs) are used together with modelled or measured data on exposures in order to calculate a Hazard Index (HI), a Point of departure Index (PODI) or related quotients. These indices are conservative approaches that consider and mix all toxicological endpoints and use assessment factors (from 10 to 10,000) to consider uncertainty. In Tier 2 the influence of assessment factors of differing magnitude is removed and taxa-specific PODs are used coming up with risk quotients (RQ). In Tier 3, subgroups of mixture components that affect a common endpoint through a similar mode of action are compiled and hybrid approach using CA for similarly acting compounds within a group and IA as tool for aggregation of the groups. A detailed guidance is given providing the assessment rules main and sub-tiers. All tiers are detailed with workflow schemes based on the same principle for human health and ecosystems.

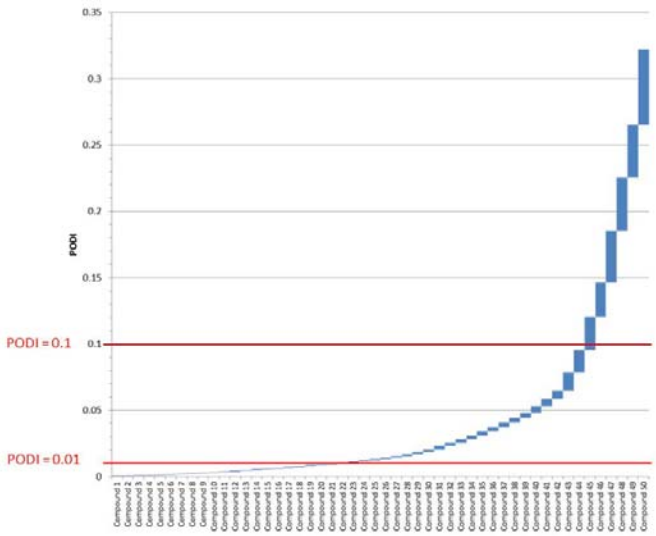

Figure 17: The principle of driver identification based on their contribution to mixture effects compared to PODIs as thresholds of acceptable exposures.

For driver identification in mixtures existing approaches have been discussed in D18.1 and complemented by an approach sorting the chemicals under consideration in ascending order according to the size of their RQ. PODIs of concern need to be established as the limit of acceptable exposures (typically 0.01 or 0.1). The components of the mixture with cumulative HQs exceeding the PODI are considered as drivers of toxicity (Figure 17).

Human health risk assessment was based on the exposure pathways drinking water and consumption of freshwater fish. In order to answer the question "Is the fish caught from a given freshwater site safe for human consumption water concentrations were converted into expectable concentrations in fish tissues using bioaccumulation modelling based on trophic levels and lipid contents. The approach was demonstrated for the assessment of chronic mixture risks to fish and humans in the River Danube on the basis of JDS3 data. In total four chemicals have been identified as drivers of mixture risks for human fish consumption including three pharmaceuticals and one insecticide.

On the basis of modelled concentrations of 1800 compounds MRA was performed for all case studies (Rivers Danube, Rhine and the Iberian river basins) and the endpoints algal reproduction, immobilization of Daphnia and toxicity to fish deriving endpoint-specific lists of toxicity drivers including 40, 19 and 7 compounds, respectively. Statistical and trait-based approaches together with the alignment of modeled risks with the ecological status have been performed. It was shown that mixture exposure is a significant factor that limits reaching or maintaining good or high ecological status with higher mixture toxic pressure (msPAF) implying higher limitations (Figure 18).

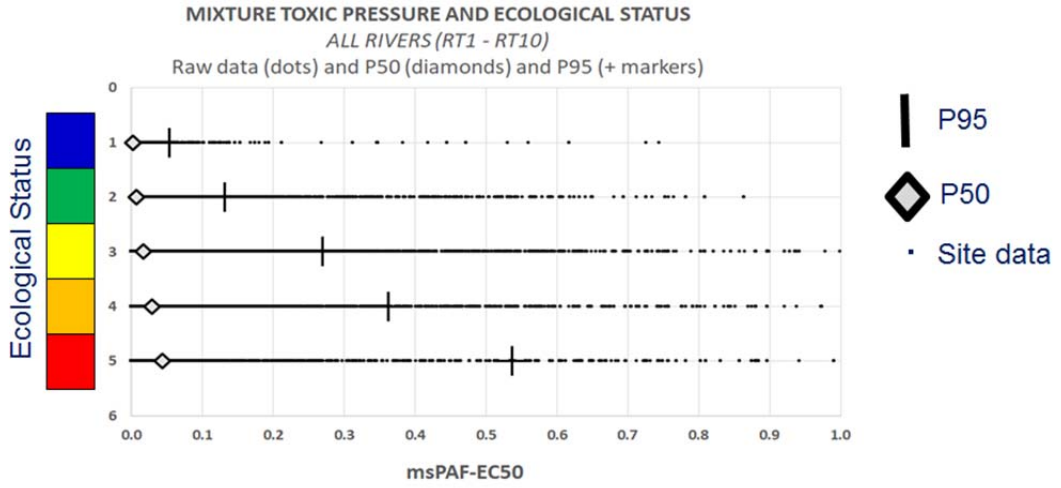

Figure 18: Empirical relationship between mixture toxic pressure (msPAF) and Ecological Status

4. SP4: Cases

SP Cases has been designed to evaluate, demonstrate and mutually validate monitoring tools and models in the large case studies on the Rivers Danube and Rhine as well as on several Spanish rivers. In addition, smaller cases for specific purposes such as the Rivers Holtemme (Germany) and Vegea (Sweden) have been involved. Many of these tasks have been already reported above in SPs 2 and 3 in order to demonstrate the power of the tools and models developed in these sub-projects. Thus, the major focus of the reporting in WP19 to 21 will be on activities that have not been reported elsewhere.

4.1 WP19: Danube river basin case study

A major basis and anchoring point of the Danube river basin case study was the Joint Danube Survey 3 (JDS3) two months before the official start of SOLUTIONS. Several members of the SOLUTIONS consortium participated in JDS3 safeguarding that samples were collected in a way that they could be analyzed and evaluated by SOLUTIONS to support the specific objectives of this project.

In addition to large scale method testing, demonstration and evaluation, the identification of River Basin Specific Pollutants (RBSP) for the Danube was a key objective of the case study. This included the development of a methodology together with the guidance for application as well as the RBSP list itself for introduction into Danube River Basin Management Plans by ICPDR as a stakeholder directly involved into the SOLUTIONS consortium. The methodology and guidance is based on the NORMAN prioritization framework (Figure 19) involving the approaches and tools developed in the SPs on tools and models. Chemical monitoring data measured by SOLUTIONS and additional laboratories in JDS3 samples are the basis of the prioritization complemented by the screening and evaluation of a 12 WWTPs in the Danube river basin as a source related dataset. The prioritization framework is explained in detail in D19.4.

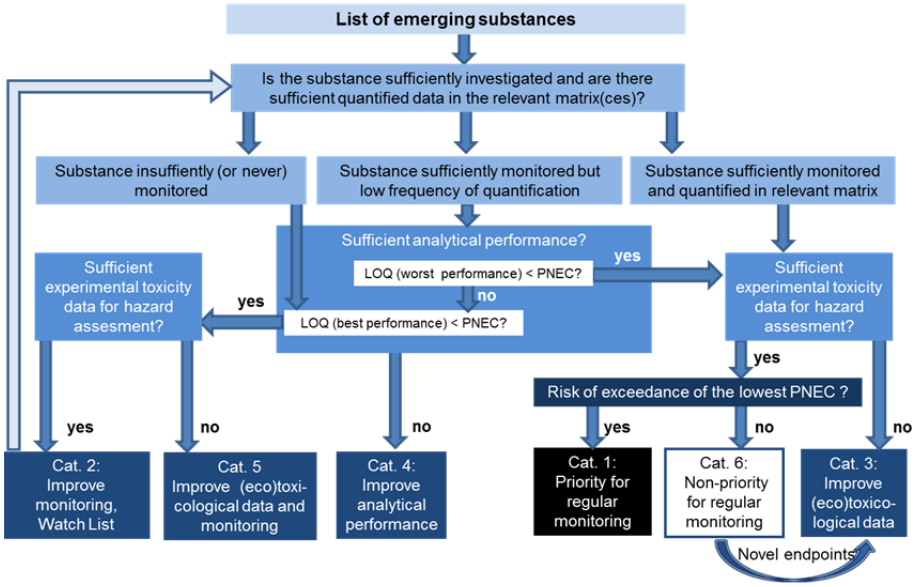

Figure 19: Decision tree for the categorization and prioritization of chemicals

The categorization of measured chemicals according to the decision tree in Figure 19 and a prioritization of those chemicals that have been sufficiently monitored using the extent of exceedance of the lowest PNEC and the spatial frequency of exceedance of the lowest PNEC as criteria to calculate the final ranking scores, SOLUTIONS came up with an interims list of 20 substances that have been presented in the 2015 update of the Danube River Basin Management Plan. Extensive curation of monitoring data has been carried out to exclude outliers. This resulted for example in an exclusion of PAHs from the RBSP list. An updated version of a list of 20 RBSP may be found in D19.4 and has been submitted to ICPDR. This list includes PFOS, isoproturon and some metals as WFD Priority Substances together several pesticides, pharmaceuticals and some industrial chemicals such as bisphenol A.

SOLUTIONS came to the conclusion that there is a need to involve modelling, effect-based monitoring and ecological monitoring into a multiple LoE approach on prioritization (see WP2). Thus, these methods were tested in the case study Danube investigating them for their potential to provide additional candidates for RBSPs that may be considered in upcoming JDS4 and other monitoring activities in the River Danube. This included an in-depth study of the River Danube downstream of the city of Novi Sad as a potential pollution source due to the emission of untreated wastewater into the Danube as well as an emission-based modelling exercise for the whole River Danube using the SOLUTIONS model train as detailed in the report on SP3.

Integrated effect-based and chemical monitoring in the River Danube downstream of Novi Sad with a focus on endocrine disruption and other specific in vitro assays together with a mass balance approach involving default mixture toxicity modelling and an EDA study revealed a list of 14 chemicals driving ER- and AR-mediated effects [24, 29]. These chemicals include natural steroids, phytoestrogens and synthetic steroids used for medication. Due to their very low PNECs the limits of detection of chemical screening are too high to detect them in river water. Thus, using the chemical monitoring-based approach alone, they are overlooked and ignored in RBSP lists. This finding highlights the importance of involving effect-based methods into monitoring, assessment and prioritization.

A prioritization exercise modelling exposure and risks for 1835 chemicals known to be emitted in the Danube basin together with the extent of exceedance/frequency of exceedance scoring revealed a top hundred list of potential candidates (D19.4). This list may be seen as complementary and will be considered when designing the list of compounds for monitoring in JDS4.

4.2 WP20: Assessment of abatement options in the River Rhine catchment

The case study in the River Rhine catchment was designed as a test field for abatement options, the application of new effect-based and chemical methods for evaluation of abatement efficiency and the derivation of emission limit values (ELVs) and provisional drinking water guideline values.

Building on the toolbox provided in WP9, a targeted toolbox for abatement assessment has been established (D20.1). This includes sampling strategies that allow for the calculation of elimination efficiencies and the impact of wastewater to river water quality. Grab sampling typically used in monitoring is compared to time-integrated sampling techniques. Enrichment and sample preparation techniques have been investigated suggesting SPE with multi-layer cartridges as a tool to enrich a broad spectrum of compounds with in situ LVSPE as a major advancement. Care needs to be taken to avoid toxic blanks. To observe the performance of certain abatements chemical analysis and effect-based methods are recommended. Guidance is given on the selection of marker compounds for specific purposes. Polar and ionic chemicals are suggested to be targeted for testing breakthrough in activated carbon filtration, chemicals with low reactivity should be in the focus of efficiency of reactive abatement processes such as ozonation, while bank filtration needs to be tested with persistent and mobile organic compounds (PMOC) with poor removal. Also different sources can be addressed with marker compounds for agricultural runoff and urban wastewater. Effect-based methods representing endpoints with human health concern such as genotoxicity and endocrine disruption as a part of the modular test battery suggested in WP11 should be in the focus of drinking-water-quality related assessments. In upstream-downstream studies at WWTPs in Switzerland integrated effect-based and chemical monitoring has been demonstrated to assess the impact of

wastewaters on river water quality [25, 44]. Ecological assessment tools (discussed in WP13) further supported the development of cause-effect relationships using PICT of microbial communities and the SPEcies At Risk ($SPEAR_{pesticide}$) index for the assessment of macroinvertebrate communities. A significant correlation between $SPEAR_{pesticides}$ and toxic contamination characterized by msPAF has been detected.

Since WWTPs emitting complex mixtures of chemicals are one of the major sources of deterioration of surface water qualities Emission Limit Values (ELVs) are required and have been provided by SOLUTIONS for a large number of chemicals based on EQS for Priority Substances and RBSPs considering the dilution of the discharged water in the receiving river during dry weather flow conditions.

While ELVs target the regulation of emissions, provisional drinking water guideline values (pGLVs) are required to protect drinking water and thus human health as a major receptor from contamination and adverse effects. While the concept of the Threshold of Toxicological Concern (TTC) is a pragmatic approach using information on chemical structure to sort chemicals in three so-called Cramer classes with a uniform threshold value, SOLUTIONS derived compound-specific pGLVs based on available toxicological information for 142 chemicals [45]. The latter were derived from a set of 686 chemicals detected in water resources in general by selecting those 76 that have been detected in produced drinking water together with 87 substances in raw drinking water or direct sources. For most chemicals SOLUTIONS did not find appreciable human health risk, while for several compounds including vinylchloride, trichlorothene, bromosichloromethane, aniline, phenol, 2-chlorobenzamine, mevinphos, 1,4-dioxane and nitrilotriacetic acid human health risks could not be excluded.

Riverbank filtration (RBF) is considered as a cost-efficient approach to produce high-quality drinking water making use of natural processes. SOLUTIONS investigated this process involving filtration, biodegradation and sorption for improvement of water quality at 10 RBF sites along the River Rhine and its tributaries. For one RBF system with detailed long-term hydrological, hydrogeological and chemical observation data a detailed reactive transport modelling study was varied out to assess the long-term/long-distance behavior of organic compounds. A major uncertainty in estimating degradation is the calculation of degradation rate constants. In SOLUTIONS, these rate constants were calculated with QSAR technology using the CATALOGIC platform described in WP17. For a total of 82 substances concentrations in raw drinking water after RBF could be estimated from river water concentrations suggesting that at the in-depth investigation site of Rodenhuis (The Netherlands) 1,4-dioxane, iopamidol and tolyltriazole may exceed 100 ng/L regularly, diclofenac and dyglyme at least occasionally. Investigations at the Lek River (The Netherlands) indicated that there were 10 compounds that were fully persistent during RBF even after 3.6 years of transit time, five others were only partially removed. Reversed osmosis (RO) is considered as a tool for further purification of riverbank filtrates. SOLUTIONS used effect-based methods to test water quality at a Dutch drinking water treatment plant after RO detecting no positive response up to a relative enrichment of 2000.

In the Swiss part of the Rhine catchment five times lower residence times in RBF are legally required (10 days) compared to EU. Based on 526 targeted compounds no health risk of drinking water was indicated under normal conditions. However, the short residence times result in vulnerability to contamination peaks in case of heavy rain events, during pesticide application periods, accidents etc..

4.3 WP21: Iberian river basins

The Iberian case study involved four river basins including Ebro, Llobregat, Júcar and Guadalquivir was performed in collaboration with the Spanish national project SCARCE and had a specific focus on prioritization of chemicals under water scarcity, which is considered as a major bundle of non-chemical stressors, and thus on the relationship between chemical and non-chemical stressors.

On the basis of about 200 compounds detected, prioritization of chemicals was performed based on TUs for the green algae, *Daphnia magna* and fish using a ranking according to the frequency of occurrence (sites) of a chemical in rank classes defined as ranges of log TU (D21.1). Highest risks were concluded for six insecticides (chlorfenvinphos, chlorpyriphos, dichlofenthion, ethion, diazinon and carbofuran), the fungicide prochloraz and the herbicide diuron, as well nonylphenol and octylphenol. Sediment assessment at the same river basins involving the equilibrium partitioning approach to estimate corresponding water concentrations prioritized a similar selection however including the insecticide malathion and the antibiotic ciprofloxacin. In fish tissues 135 compounds were analysed with highest frequency of detection and highest concentration for several perfluorinated compounds, some pesticides and polychlorinated flame retardants.

The study on the relationship between chemical and non-chemical stressors used biofilms and invertebrate communities as representative receptors and used TUs as an indicator for toxic stress. Using an assessment approach published at the beginning of SOLUTIONS [46], dependent of the basis under consideration up top 74 % of the sites were under acute toxic risk driven mainly by pesticides and metals, while for chronic risks pharmaceuticals such as the antidepressant sertraline played an important role. Toxic stress could be confirmed by the correlation of the disappearance of sensitive macroinvertebrate species (SPEAR) with TUs. However, the results were suffering from a limited gradient since reference conditions with low concentrations and well established macro invertebrate communities were lacking in all investigated river basins.

In close interaction with SP3 (WP16), the SOLUTIONS model train was applied to more than 200 organic pollutants monitored in the Iberian river basins. Grouping the chemicals according to pesticides, pharmaceuticals and REACH compounds similar to other basins most substance average concentrations could be predicted within one or two orders of magnitude.

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List of official Deliverables public available via the SOLUTIONS website (from February 2019)

Del. No.	Title
D1.1	Conceptual framework as basis for implementation in RiBaTox and the toxicant knowledge base on the basis of specified stakeholder problems and requirements
D1.2	Integrated publications on novel solutions for risks of mixture of emerging pollutants in water resources
D2.1	Advanced methodological framework for the identification and prioritisation of contaminants and contaminant mixtures
D3.1	Technical and non-technical abatement options implemented in RiBaTox including rules for placement of abatement options, removal efficiencies and prioritisation
D3.2	Example cases for the application of the Chemical Footprint and the (Planetary) Boundaries concept to abatement strategies
D4.1	RiBaTox fully documented on-line 'final' version
D5.1	Integrated Data Portal for SOLUTIONS (IDPS)
D5.2	Web-based knowledge base integrated with IPCheM and RiBaTox
D6.1	Recommendations: Pollution of tomorrow: options to act on future risk and final report
D8.1	Functional interactive SOLUTIONS web-side, stakeholder communication platform and intranet
D8.2	Final products (RiBaTox, models, knowledge base and guidelines) accessible via the SOLUTIONS web-site
D8.3	Final Report on Communication, dissemination and training
D9.1	Guidance document and decision tree for use of chemical, bioanalytical and ecological tools in RBSP identification, impact assessment and establishment of cause-effect relationships
D10.1	Guidelines for target and non-target analysis of emerging contaminants in water and biota
D11.1	SOP for mutually validated virtual and higher tier EDA of surface waters and fish tissue ready for translation into guidelines
D12.1	Improved bioassay solutions for environmental monitoring based on adverse outcome pathways
D12.2	Feasibility assessment of extract-bioassay approaches for environmental monitoring
D13.1	Diagnostic toolbox for ecological effects of pollutant mixtures, including bio-tests, trait-based database and detection tool and WoE studies at hot-spot sites
D14.1	Modelling framework and model-based assessment for substance screening
D14.2	Europe wide modelling and simulations of emerging pollutants risk including think tank scenarios
D15.1	Peer reviewed paper on the entire process of estimating emissions of chemical substances

D16.1	Evaluation of the basin-wide river catchment and soil-to-groundwater-to-surface water transport model including sensitivity and uncertainty analyses
D17.1	Novel experimentally-based LSER models for sorption and bioaccumulation of emerging pollutants
D17.2	Predictions of transformation products, physico-chemical properties, fate and toxicity of candidate compounds from chemical screening, EDA and emission modelling
D18.1	Common assessment framework for HRA and ERA higher tier assessments including fish and drinking water and multi-species ERA via SSD, population-level ERA via IBM and food web vulnerability ERA
D19.4	Guidance for identification of RBSPs and list of Danube RBSP including quantification of their ecological impact and modeling-based exposure and risk predictions validated with case-study data
D20.1	Targeted tool-box for the assessment of abatement options, derivation of ELVs and pGLVs for drinking water and assessment of natural attenuation during river bank filtration
D21.1	Guidance for identification of RBSPs in Mediterranean river basins and list of RBSP including quantification of their ecological impact and modeling-based exposure and risk predictions validated
D23.1	Risk Management Contingency Plan