



21 – 22 January 2020, Leipzig, Germany

Helmholtz Centre for Environmental Research - UFZ Permoserstraße 15 04318 Leipzig

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Persistent, Mobile and Toxic (PMT) Substances:
A Challenge for analytical chemistry and water quality control



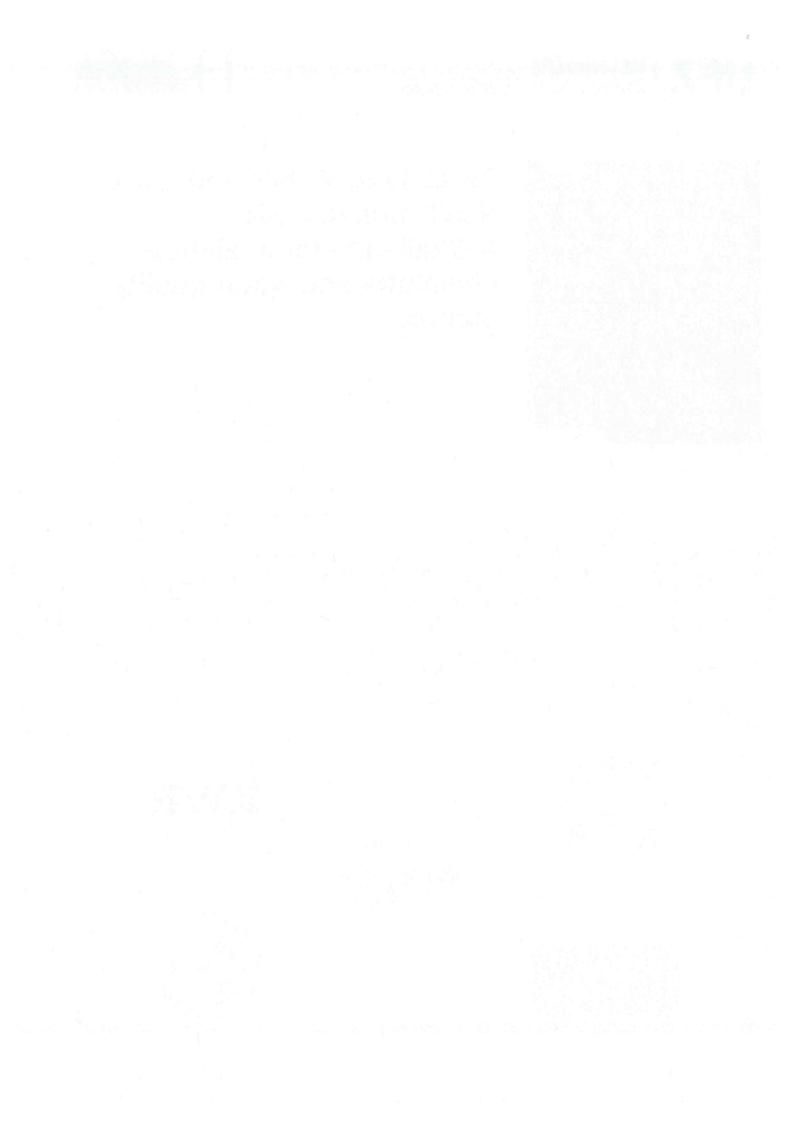




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Welcome

Dear Guests, dear Colleagues,

Welcome to the workshop "Persistent and Mobile Organic Chemicals - A challenge for Analytical Chemistry and Water Quality Control" taking place at the Helmholtz Centre for Environmental Research in Leipzig.

Persistent, mobile and toxic (PMT) substances are an issue of increasing awareness in the water community. While the conceptual importance appears obvious, profound knowledge is still limited, so that the importance of PMT substances for ecological and human health remains a matter of debate.

For this reason the NORMAN network and the Helmholtz Centre for Environmental Research jointly set up this workshop with the following aims:

- Highlighting the present state of analytical methods to determine PM chemicals
- Collect knowledge on the occurrence of PM(T) chemicals, from wastewater to drinking water
- Elaborating the obstacles and shortcomings in the different fields of research on PM chemicals
- Proposing strategies to improve knowledge on PM chemicals

We, the organizers, are convinced that the program of these two days, with oral presentations, poster presentations, and with your active participation in breakout groups and in a final plenum discussion will bring forward knowledge and ideas that help to achieve these aims. And we are more than grateful to our speakers and poster presenters for their willingness to share their expertise and thoughts on PMT compounds with all of us.

The NORMAN network, the German Water Chemical Society, the German Federal Ministry of Education and Research and the Helmholtz Centre for Environmental Research financially support this workshop. The organizers are grateful for this funding.

It is our hope that you will experience two interesting and stimulating days with a lot of novel insights and information on PMT chemicals and that we will manage to identify next steps to make knowledge on PMT compounds more profound!

Urs Berger, Thomas ter Laak, Michael Neumann, Peter von der Ohe and Thorsten Reemtsma







Workshop Programme



Persistent, Mobile and Toxic (PMT) Substances:



A challenge for analytical chemistry and water quality control

21 - 22 January 2020, Leipzig, Germany

Tuesday, 21 Jan	nuary 2020
08:30	Registration
09:15-09:30	Introduction – Thorsten Reemtsma
09:30 – 10:45	 Session 1: Thomas Knepper Hans Peter Arp (NGI, NO) Establishing criteria for Persistence and Mobility: State-of-the-art and research needs. Urs Berger (UFZ, DE) Recent advances in analysis and monitoring of PM substances. Pim de Voogt (Univ. Amsterdam/KWR, NL) Persistent and mobile compounds in drinking water treatment.
10:45 - 11:15	Coffee Break
11:15 – 12:15	 Session 2: Urs Berger Daniel Zahn (HSF, DE) Matrix effects in the analysis of polar organic water contaminants with HILIC-ESI-MS. Isabelle Neuwald (HSF, DE) Are (fluorinated) ionic liquids relevant environmental contaminants? Eric M.J. Verbruggen (RIVM, NL) Screening and prioritising PMT substances: the development of a score for mobility and toxicity.
12:15 – 13:45	Lunch (with posters on display)
13:45 – 15:05	 Session 3: Thomas ter Laak Thomas ter Laak (KWR, NL) Are PMOCs less toxic; how to further close the gap? Erik Verhofstad (MinEnv, NL) From science to practical regulations to protect drinking water sources. Sascha Pawlowski (BASF, DE) Persistent chemicals and water resources protection: Conclusions from an ECETOC Task Force. Anna Lennquist (ChemSec, SE) Inclusion of PMTs to the SIN List promotes substitution in the global supply chain.
15:05 – 15:45	Coffee Breakincl. registration for Working Groups (day 2)
15:45 - 17:00	Posters (with poster spotlights)
	Guided tour Department Analytical Chemistry (optional)
19:00	Dinner at "Ratskeller" (City Centre)

Wednesday, 22 January 2020				
09:00	Introduction to Day 2			
09:15 - 10:40	Morning: Discussion in break-out groups			
	 Detection of PM compounds (monitoring and screening level) 			
	PM findings and knowledge on occurrence			
	Persistency: data quality and test methods			
	Mobility: suitable parameters and options for verification			
	Toxicity and ecotoxicity of PM substances			
	Removal options for PM substances from water			
10:40 - 11:10	Coffee (Posters on display)			
11:10 - 12:00	Reporting Back and Final Conclusions			
	How big is the problem of PMT substances?			
	Which steps to take next?			
12:15	Closure – Thorsten Reemtsma			

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Abstracts (Oral presentations)
(according the programme)

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Oral Abstracts

Establishing Criteria for Persistence and Mobility: State-of-the-Art and Research Needs Hans Peter H. Arp1,2

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The mobility of an organic substance in the subsurface and its likelihood to reach water resources is dependant largely on two processess: its environmental persistence and its sorption to soils from porewater. The greater the persistence and weaker the sorption to soils, the longer the substance will exist in the subsurface and the quicker and further it will be transported. Depending on use and emission patters, PM substances are a concern for their potential accummulation in wastewater reuse cycles within cities, in drinking water as well as in all water resources globally.

An early model to describe mobility is the Groundwater Ubiquity Score that combined soil half-lives as a measure of persistency and the organic carbon-water partition coefficient, Koc, to describe sorption (Gustafson, 1989). To this day, this general framework remains a robust way to describe mobility in the subsurface and through sorbtive barriers (e.g. bankfiltration, conventional water treatment plants); however, there are three complexities for putting this into practice for all organic substances: 1) lack of high-quality persistency and mobility data, 2) environmental heterogeneity of persistence and sorption processes, and 3) where to place "cut-off values" for persistence and sorption data to ensure the best protection from the hazards of persistent and mobile (PM) substances. Recently, a strategy to deal with all three of these complexities in a way that gives a practical definition of a PM substance was put forward (Arp and Hale, 2019). This approach provides guidance on how to use the definiton of persistence in the EU REACH regulation, or alternaltively screening and QSAR data, to assess P. The approach also demonstrates how the mobility cut off of log Koc of 4.0 or less describes most of the substances detected in drinking water, and suggests alternatives for this cut-off when Koc is not available. This strategy was based on modelling data, existing frameworks for chemical hazard assessment, and an analysis of false positive and negatives in relation to how accurately the criteria predicted PM substances in water resources. The development of these recommendations will be presented, as well as a list of substances produced from these recommendations, and suggestions for future research needs regarding generating better P data and understanding sorption processes for complex molecules in complex enviornments.

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Recent advances in analysis and monitoring of PM substances

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The latest decade has seen a steep increase of the number of scientific papers published on the occurrence of polar contaminants in groundwater and drinking water. This may partly be due to the continuously increasing sensitivity of LC-MS instrumentation, but it may also be attributed to the growing awareness of the presence of PM substances in source and drinking water and the development of analytical methods for highly polar (mobile) substances that came along with this awareness.

There are three major challenges in quantitative analysis of PM substances in environmental water samples. 1) To achieve the required analytical sensitivity in order to quantify PM substances at trace levels (down to low ng/L concentrations), an enrichment step is necessary; 2) chromatographic separation in the final instrumental method requires retention of PM substances on a stationary phase; 3) accurate quantification is hampered by strong matrix effects and the lack of isotope-labelled internal standards. Both 1) and 2) are very demanding to achieve for a broad number of PM substances due to their mobility, i. e. the inherent property not to sorb to any surfaces. Suggested solutions for 1) are mixedmode solid phase extraction, direct freeze-drying or (azeotropic) evaporation of water samples. In any case, efficient separation of PM substances from water matrix (e. g. DOM) will not be possible, hampering a simple quantification approach based on external, solventbased calibration (challenge 3). Regarding 2), ion chromatography, mixed-mode LC, hydrophilic interaction LC (HILIC) or supercritical fluid chromatography (SFC) have successfully been developed and employed for retention and separation of PM substances. To correct for matrix effects in quantification (challenge 3), various procedures based on standard addition (to samples or to extracts) or based on matrix-matched calibrations have been suggested. These recent developments made it possible to monitor for more and more PM substances in remote environmental waters.

The presentation will review recent progress in analysis and results from monitoring of PM substances in water samples. Studies published in literature as well as own results from the projects PROMOTE (Protecting Water Resources from Mobile Trace Chemicals) and PROTECT (Persistent and Mobile Organic Chemicals in the Aquatic Environment: Sources, Occurrence and Techniques for Removal in Drinking Water Production) will be shown.

Persistent and mobile compounds in drinking water treatment

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Riverbank filtration (RBF) is a common drinking water pretreatment with potential to remove dissolved micropollutants mainly by sorption and biodegradation. When surface water infiltrates through the hyporheic zone many classes of hydrophilic organics enter RBF systems. Polar substances can easily cross both natural and technological barriers typically used in drinking water production, such as river banks, disinfection and active carbon filtration. They can be highly mobile in RBF systems with long travel times at stable biogeochemical conditions. Common removal processes used in drinking water production appear to remove these polar compounds at most partially and therefore additional treatment might still be necessary.

We investigated a natural drinking water source consisting of a RBF site using non target screening mass spectrometry to study presence and time trends of polar pollutants (Albergamo et al, 2019a). The efficiency of reverse osmosis (RO) for removal of neutral polar, cationic and anionic compounds was studied in pilot-scale drinking water treatment (Albergamo et al, 2019b). In a sampling campaign the persistence and mobility of two perfluorinated compounds was demonstrated by their presence in samples of river bank filtrate and their incomplete removal during drinking water processing (Vughs et al, 2019). The concentrations detected in drinking water give no immediate reason for concern for adverse health effects from drinking tap water produced by the water suppliers. However, concentrations may increase if discharges continue to be permitted.

Reverse osmosis (RO) proved to be a robust barrier against most polar MPs. Overall, the passage figures observed for the investigated set of compounds ranged from less than 1%—25% in standard conditions. Statistical analysis showed significant influence of physicochemical properties on compound passage. Compound size and passage were highly correlated for neutral MPs, and charge for anionic MPs.

To avoid contamination with many legacy pollutants from the 1990s the use of young groundwater to produce potable water is recommended, whereas advanced treatment should be applied to the old groundwater.

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Matrix effects in the analysis of polar organic water contaminants with HILIC-ESI-MS

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Persistent and mobile organic chemicals (PMOC) are able to penetrate natural and artificial barriers, and thus spread quickly in the water cycle [1]. It is currently considered to integrate these chemicals into REACH regulation as persistent mobile and toxic (PMT) or very persistent and very mobile (vPvM) substances [2]. Consequently, the accurate trace analysis of these chemicals is of ever-increasing importance. Besides difficulties in their chromatographic separation and enrichment from aqueous matrices, several studies observed pronounced partially highly variable matrix effects for some very polar water contaminants [3, 4]. While matrix effects in reversed phase chromatography – electrospray ionization (ESI) have been investigated for years, matrix effects in hydrophilic interaction liquid chromatography (HILIC) are still only scarcely studied [4].

To address this issue, we investigated the matrix effects when analysing drinking water (DW) and wastewater treatment plant (WWTP) effluent. We enriched these samples with two sample preparation methods suitable for very polar analytes, namely the evaporation of the aqueous matrix and a multi-layer solid phase extraction (mISPE) method [5] and utilized post-column infusion of 26 polar model analytes to investigate their matrix effects throughout the chromatographic run [6]. These experiments showed that there is general ion suppression that coincides with a high total ion count and can thus be attributed to limitations in the generated excess charge and therefore the total amount of free gas-phase ions. Additionally, defined retention time ranges with pronounced highly structure-specific matrix effects were observed. Matrix effects in these areas ranged from almost total ion suppression to 500% ion enhancement with significant differences even for structurally closely related analytes like mono- and dihalogenated methanesulfonic acids. Structural elucidation of substances whose retention time, profile, and peak shape coincided with the observed structure-specific matrix effects revealed clusters of inorganic ions as potential cause for these matrix effects. This hypothesis was confirmed when solutions of inorganic ions were used as test matrices. Knowledge about the cause and extent of these matrix effects can proove valuable during method development, especially during analysis of critical substances that are strongly influenced by the presence of specific inorganic ions and for which no isotope-labelled internal standards are available.

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Are (fluorinated) ionic liquids relevant environmental contaminants?

A high-resolution mass spectrometric screening approach for per- and polyfluoroalkyl substances in various matrices led to the detection of a novel fluorinated ionic liquid

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Due to the toxicity of some legacy per- and polyfluoroalkyl substances (PFASs), industry tends to use and produce shorter chain alternatives or fluorinated replacement chemicals that are less harmful but still exhibit the typical PFAS properties. Their widespread and versatile use causes inevitable release into the environment and potentially leads to an increasing number of hitherto unknown fluorinated environmental contaminants.

In this work we present a rather scarcely used HRMS approach called fragmentation flagging (FF) for the assessment of fluorinated compounds in environmental water samples, as well as building materials, fabrics and foils. This method is able to indicate the retention time of fluorinated chemicals through the formation of their diagnostic in-source fragments, such as C2F5- and C3F7-. This approach has led to the detection of various well-known legacy PFASs (perfluorooctanoic and perfluorooctanesulfonic acid), their shorter chain alternatives perfluorohexanoic and perfluorobutanoic acid, and some only rarely analyzed ultra-short chain PFASs like trifluoromethanesulfonic acid.

In addition, an unknown fluorinated compound was detected and identified as tris(perfluoroalkyl)trifluorophosphate (FAP), an ionic liquid anion that is used, among others, in electrochemistry (e.g. supercapacitors) and as lubrication or extraction agent (Blanco et al., 2011; Pandey and Hashmi, 2013). Quantification of FAP in 21 surface waters showed concentrations up to 3.4 μ g/L. The contamination of FAP was limited to one area affecting only three connected rivers (Neuwald et al., submitted). This finding raises the question whether ionic liquids might be of environmental concern.

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To further assess the potential of ILs being possible environmental contaminants, a thorough literature research was performed. It revealed that multiple laboratory scale tests have been conducted so far in order to examine the toxicity of various IL an- and cations and concerns have been raised, especially regarding the fluorinated ILs (Pham *et al.*, 2010). Environmental monitoring data that proves their presence in the environment is, to the best of our knowledge, so far not available. Particularly fluorinated ionic liquids and ionic liquid anions may be prime candidates for persistent, mobile and toxic (PMT) or very persistent and very mobile (vPvM) substances or act as precursors thereof. Thus, they might be able to overcome natural and artificial barriers in the water cycle, finally reach drinking water and in some cases may even pose a risk to human health.

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Screening and prioritising PMT substances: the development of a score for mobility and toxicity

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In 2011 a PB-score (Persistence and Bioaccumulation score) was developed at RIVM to screen and prioritise chemicals that are potentially PBT and/or vPvB (Rorije et al, 2011). A continuous scoring system was developed as this was thought superior to binning as used by other methodologies. The scores (0-1) were centered around the vP and vB criteria in such a way that the dicriminating power was highest around these criteria. The P- and B-score are based on QSAR-generated physico-chemical properties (US EPA, 2019), used for estimates of overall persistence and higher trophic level bioaccumulation.

Recent concern for persistent mobile, and toxic substances has led to a further development of our scoring tools to implement these properties in the hazard assessment. For PMT screening the P-score, derived from BIOWIN3 estimates (US EPA 2019), focusses on the aquatic environment rather than overall persistence, because this is the primary compartment of concern for PMT substances. Secondly, a score for Mobility, which is best characterised by log Koc (Neumann, 2019), was added. Volatility was also taken into account as a mitigating factor in the PMT scoring.

The absence of a Toxicity-score was a potential drawback of the original PB-score. Here we present the first results of the development of a score using endpoint specific profilers from the OECD QSAR toolbox (OECD, 2019) as well as similarity to CMR and ED substances (Wassenaar, 2019). The challenges for transforming these data into T-scores arises from i) the lack of potency information from the profilers and ii) the weighing of the relative importance of the different endpoints (i.e. C, M, R, and ED).

Next steps involve extending these scoring functions with monitoring data, especially non-target screening as well as emission data. This work is done in collaboration with water authorities and drinking water companies.

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Are PMOCs less toxic; how to further close the gap?

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Reemtsma et al. (2016) illustrated that persistent and mobile organic chemicals (PMOC) were long ignored in environmental studies including those dedicated to the quality of drinking water and its sources (Reemtsma, Berger et al. 2016). Recent studies show their presence in concentrations above the Threshold of Toxicological Concern (Baken and Sjerps 2016) or signaling levels for anthropogenic chemicals in surface water and groundwater, including drinking water sources (Kolkman, Vughs et al. 2018, Vughs, Kolkman et al. 2019).

With the emergence of this class of anthropogenic organic contaminants, the 'so what' question rises. We realize that these chemicals are present in the environment, that they can pass natural as well as technological barriers applied in watewater treatment and drinking water production (exposure) but we still have limited knowledge on distribution within the aqueous environment. On top of that there is insufficient information about human and environmental toxicity (hazard) of these emerging contaminants. Therefore, proper risk assessment (exposure x hazard = risk) is precluded.

Here we propose an approach to elucidate to what extent PMOC properties can be related to toxicity and toxic modes of action. It is hypothized that chemicals that have a low tendency to leave the aqueous phase to sorb to / complexate with solid phases or dissolve in hydrophobic liquid phases, and do not react easily under environmental conditions, possibly hold a low toxicity potential, which is the result of accumulation and interaction (or reaction) with biological systems.

This hypothesis whilrls up many questions on behavior of chemicals in biological systems in relation to the physicochmemical properties of the chemicals and the modes of action in organisms. The evaluation of the hypothesis needs various studies and probably won't leave single or simple answer. We therefore want to discuss the essential aspects with experts in this field to obtain the needed research questions and define reserach approaches to allow substantial human and the environment risk assessment. This knowledge can support future resrearch and eventually decision-making related to the design of monitoring activities as well as water quality assessment and risk assessment of emerging PMOC substances in the water cycle.

ABSTRACTS (ORAL PRESENTATIONS)

This inventory for research is supported by the Dutch and Flemish drinking water sector (BTO).

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From science to practical regulations to protect drinking water sources

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In the Netherlands, the ministry of Infrastructure and Water management, together with RIVM, Rijkswaterstaat, Industry and water supply companies, are working together to develop a complete framework to prevent that the most harmful of the PMT/vPvM substances pollute surface waters that are also used as sources for drinking water. The basic idea is to identify the most harmful PMT/vPvM substances for drinking water, and to use practical existing tools and regulatory frameworks to prevent that discharges of these substances will lead to unacceptable risks for the drinking water supply. We expect to come up with a draft in the summer of 2020 and regulations in 2021.

References

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Persistent chemicals and water resources protection: Conclusions from an ECETOC Task Force

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Chemicals from various sources may be released into the environment and potentially reach ground- and drinking water resources. The PMT/vPvM-concept was developed by the German Environmental Protection Agency (UBA) with the aim to better protect these resources from such substances regulated under REACh (UBA 2019). However, the exercise indicated that hazard-based data evaluation resulted in a serious number of false positive and a certain number of false negative candidates which indicates an urgent need for further adjustment of the concept. Furthermore, available monitoring data illustrated a broader range of substances, which are not REACh-related, that are present in ground- and drinking water and these substances will not be addressed by the REACH PMT/vPvM-concept.

An ECETOC Task Force was established to elaborate relevant topics central to such an approach. These included a review of existing legislations, elaboration of the applicability of an alternative risk-based approach, review of existing monitoring data and the level of relevant metabolite concentrations, possibility of NER-formation, appropriateness of the chosen Persistence (P) Mobility (M)- and Toxicity (T) criteria. Results: A risk-based approach using available phys.-chem. and e-fate parameters is applicable. A survey of monitoring data revealed no correlation with logKoc. Employing a 0.1% as relevant metabolite threshold is not practically applicable due to expected low concentrations (≤1ng/L). In EU plant protection product (PPP) regulation, metabolite thresholds are 10% and 5%. NERs are not relevant for water-soluble substances. M cannot be a stand-alone criterion to identify substances with leaching potential to ground and drinking water resources. Including the additional T-criteria will not significantly contribute to an enhanced safety of drinking water. Discussion and conclusion: A risk-based approach is a suitable alternative, compared to the initial hazard based PMT/vPvM-concept, as it allows for the exclusion of both false positive and false negative candidates. For this purpose, additional higher tier data may be required on a case by case basis. The results from the monitoring survey suggests that PMT may not be predictive of actual exposures. A 10% and 5% threshold level for metabolites similar to PPP is recommended. The criteria for 'T' as set out in Annex XIII of REACH already fulfils the protection goal of ensuring human and environmental safety in a conservative manner.

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Inclusion of PMTs to the SIN List promotes substitution in the global supplychain

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The SIN (Substitute It Now) List¹ was first introduced in 2008 by the non-profit organisation ChemSec. Its aim since then has been to predict and influence the development of the REACH Candidate List, by listing chemicals fulfilling REACH criteria for being Substances of Very High Concern, SVHCs. This initative has been much appreciated by companies, financial investors, public procurers and by other organisations wanting to be prepared for upcoming regulation. The last year the SIN List had 21 000 users from all over the world. It is also included in the Dow Jones sustainability index as a measure of progressive chemicals managent.

The PMT concept and the proposed criteria captured the interest of ChemSec as an obvious next development of the SIN List. During 2019 ChemSec had discussions with representatives from UBA, and professor Hans Peter Arp. A list of in total 344 chemicals that had been screened by UBA for PMT properties^{1,2,3} was compiled, and the most promising candidates further evaluated. This evaluation was lead by professor Martin Scheringer, ETH Zurich. Professor Scheringer and coworkers perfomed a litterature review using scientific databases, they used of a number of databases and estimation methods to investigate the PMT properties, and they screened information provided in ECHA databases⁵.

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The decision on wether or not to include a chemcial on the SIN List was based on i) fulfillment of UBA PMT criteria ii) structural similarity to substances included on REACH Candidate List or the Stockholm convention on POPs as P, vP or T iii) degradation into a substance fulfulling PMT criteria. In total 16 PMT chemicals were included in the SIN List on November 14 2019.

With this inclusion ChemSec hopes and excpect that these PMT chemicals get attention for substitution in the global supply chain, over time limiting the use and release of these chemicals.

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Poster abstracts

Quantification of persistent and mobile organic substances in water using supercritical fluid chromatography coupled to high-resolution mass spectrometry

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To reduce the analytical gap of persistent and mobile organic compounds (PM substances), we propose a quantitative method for trace analysis based on supercritical fluid chromatography (SFC) coupled to high-resolution mass spectrometry (HRMS).

Reversed-phase liquid chromatography (RPLC) coupled to MS is the method of choice for screening or quantitative analysis of trace levels of polar environmental pollutants in water. However, RPLC is not suited for separation of persistent and highly mobile (i. e. very polar) substances, due to low or no retention on the non-polar stationary phase (Reemtsma et al., 2016). Recently, methods based on hydrophilic interaction (HILIC, Zahn et al., 2016) or mixed-mode liquid chromatography (Montes et al., 2019) with better retention for PM substances have been developed. SFC-HRMS is an alternative approach offering the possibility of using normal-phase chromatographic columns.

The proposed SFC-HRMS method is based on a quick and simple enrichment step by azeotropic evaporation of the water sample using acetonitrile to form a minimum azeotrope. After filtration, the concentrated sample is directly injected into the SFC and PM substances are separated on a BEH column (for analyses in positive ion mode) or Torus Diol column (for analyses in negative ion mode) (both columns from Waters) using a carbon dioxide-methanol/water gradient containing 0.2% ammonium hydroxide in the methanol/water co-solvent. A methanol/water make-up flow containing 0.1% formic acid is used to transfer the column effluent into the quadrupole time-of-flight HRMS, operating alternatively in electrospray positive or negative ion mode.

Full method validation was performed and showed method detection limits for 17 tested PM substances in the range of 2 – 50 ng/L (partly influenced by procedural blank contamination). Recoveries were typically between 55 and 95%, while apparent recoveries were additionally influenced by (usually suppressive) matrix effects and ranged between 30 and 100%. Apparent recoveries were comparable between different types of surface water and tap water, thus, the apparent recovery factors, determined from one type of water/matrix, can be used for quantification of PM substances in a variety of water samples. Precision, expressed as relative standard deviation of four replicate quantifications of a spiked surface water sample, ranged between 4 and 14% (mean 7%), while trueness (percentage deviation from spiked concentration) ranged between -25 and +28% (mean +15%) (with the exception of +64% for one analyte).

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The potential of carbon-based material for the extraction and analysis of 1,2,4-triazole and other triazol-fungicide metabolites in groundwater

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1,2,4-triazole is a frequently detectet pollutant in the upper groundwater. To date, 1,2,4-triazole is analysed only directly by HPLC-MS/MS, with detection limits just below the thresholds value for pesticides of $0.1 \,\mu\text{g/L}$ (European Parliament and Council 2000).

Based on an intenstive method development, a solid phase extraction method for 1,2,4-triazole in groundwater was developed. As known LC-methods for analysis of 1,2,4-triazole are based on ThermoFisher Hypercarb columns (Blondel et al. 2018), empahsis was put on testing carbon-based materials like ThermoFisher's HyperSep Hypercarb and Supelco's EnviCarb cartridges.

A final SPE-UPLC-MS/MS method was validated using an EnviCarb sorbent for the extraction. With extraction recovery of 98% and a detection limit of 0.003 μ g/L, the developed method is feasible for extraction of 1,2,4-triazole. Likewise it has been tested for other triazole-metabolites and is very promissing to be used for other small, polar polutants.

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Occurrence of 1,4-Dioxane and volatile organochlorinated compounds in groundwater at the metropolitan area of Barcelona.

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Several studies of groundwater have evidenced the presence of antropogenic compounds due to their use in industrial processes. The realease and disposal of these contaminants to the environment has occurred during years, especially when there was no regulation at that

time. Today, some of these compounds still remain into the aquifers where populated areas use its groundwater as a supply for drinking water treatment plants. Historically, chlorinated solvents such as trichloroetylene, perchloroethylene, dichloromethane and carbon tetrachloride, have been used in a huge range of industrial applications because of their low boiling point, stability, solvent power efficency, availability and low cost. As well, solvent stabilizers have also been detected in groundwater sources. Stabilizers solvents have been used in order to ensure the stability of some chlorinated solvents. Among them, 1,4-Dioxane has been used a stabilizer solvent of 1,1,1-Tricholoroethane for many years, however, it has been discontinued. Nowadays 1,4-Dioxane is still being used as a industrial solvent and can be a by-product in many manufacturation processes and industrial applications.

A groundwater sampling campaing was performed in 2019 in Besos and Llobregat aquifer in order to monitor 1,4-Dioxane by SPE-GC-MS/MS and 19 different organochlorinated volatile compounds by purge and trap-GC-MS (Method EPA 524.2). Evaluation of 1,4-Dioxane has become a matter of concerrn because it has been classified a Class IIB probable human carcinogen that easily migrates to groundwater due to its physico-chemical properties. Additionally, diffusion processes provoques its mobility into the aquifer and recent studies has proved that removal of 1,4-Dioxane in drinking water treatment plants with conventional and advanced treatments are not efficient enough.

In Besos's aquifer 1,4-Dioxane's results showed significant higher values than in Llobregat's aquifer with mean concentrations of 1890 μ g/L (n=22) and 6100 μ g/L(n=6)

respectively. When considering organochlorinated compounds, in most of the collected samples taken in the Llobregat's Aquifer, tetrachlorethylene, tricloroethylene and 1,1,2-Trichloroethane were detected above their repective limit of quantification, whereas in Besos' Aquifer samples, only tetrachloroethylene exceeded it. In the Llobregat's aquifer, mean calculated concentrations of trichloroethylene, tetrachlorethylene and 1,1,2-trichloroethane were about 3,0 μ g/L (n=217), 5,1 μ g/L (n=208) and 22 μ g/L(n=162) respectively. In Besos' Aquifer, a resulting mean concentration of tetrachloroethyle of 3,5 μ g/L (n=8) was quantified. As well, other organochlorinated volatile compounds were detected above their limit of quantification but in less extend such as 1,2-dichloroethane (0,76 μ g/L n=62) and 1,1-Dichloroethylene (1,8 μ g/L n=50).

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Monitoring of PFAS in an agricultural area impacted by a fluorochemical plant

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In 2013, large-scale contamination with PFAAs was discovered in Veneto region, northern Italy, as a consequence of the emissions from a fluorochemical plant (Miteni company) in the province of Vicenza (WHO, 2017). PFAS emitted by the plant for decades diffused into the groudwater used as potable water resource because of teir mobility and persistence characteristics. Nowadays the total catchment area cover more than 540 km2 and 350,000 inhabitants, Veneto region matched the results of the biomonitoring study to those of chemical analyses in order to define 3 areas with different health impacts (Red, Yellow and Green). Even though elevated serum PFAAs concentrations were detected in the residents of the contaminated areas in Veneto, connected with contaminated drinking water consumption (Ingelido et al., 2018), comprehensive health risk assessment and research considering the food consumption are still lacking. For that reason, the LIFE project envisages an extensive monitoring program to assess the distribution of PFAS in different environmental matrices (water, soil, plants) in agriculture areas in the three areas, with a specific focus on more mobile but shorther chain PFAS. These sites are all characterized by the presence of a water body and enough soil to characterise the area of plants growth, moreover the selected stations are all featured by the presence of one ubiquitous aquatic vegetal species (Phragmites australis) and edible vegetables (Zea mais, Lactuca sativa, Cichorium intybus, Allium cepa). Water, soil and biological samples have been collected in 10 areas, including uncompromised site. The monitoring activity started in May 2018 and will last in March 2020. On the selected sampling sites surface and ground-waters, vegetables (3 different periods of the irrigation season for 24 months), soil and animals (3 periods every 12 months) will be analysed. Preliminary data show that PFAS concentrations in irrigation water do not exactly match with the exposure levels of the population, because both surface and groundwaters are used for irrigation in these areas. Nevertheless soil contamination more reflects the exposure areas, but in soil long chain PFAS prevail. Plants, both aquatic and edible plants are not significantly impacted by the PFAS contamination, even if plants from red area present a larger number of positive results, especially for the aquatic species phragmites, which are directly exposed to the contaminated waters. Positive findings in edible vegetables are very few and connected risks for population are very limited.

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LIFE PHOENIX project: a new project for the management of water pollution from short chain perfluoroalkyl acids in Veneto region (Italy)

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In 2013 a significant episode of PFAS pollution of surface, ground- and drinking water has been discovered in a large area of the Veneto region, in Northern Italy. The most important source of pollution was identified in a fluorochemical plant, sited in an area of groundwater recharge who impacted for decades groundwater, used as potable water source, in a large area (about 540 km2), because of the persitence and mobility characteristics of PFAS. The Veneto Region immediately put in place mitigation actions that were more effective for long chain PFAS than for short chain ones. Within the framework of the Community Life Program, a project on the management of short-chain perfluorinated compounds (PFAS), coordinated by the Department of Health Protection, Food and Veterinary Safety of the Veneto Region, in association with CNR IRSA, ARPAV, Azienda Zero and University of Padua, has been funded. The LIFE-PHOENIX project, acronym for "Perfluorinated compounds Holistic Environmental Institutional experience", started in September 2017 and will end in March 2021. The approach requires the involvement of regional authorities, developing tools, such as shared common datawarehouse, transferable to other geographical contexts characterised by episodes of similar environmental contamination but also proposes mitigation strategies based on innovative technologies. The activities are focused on a real scale case constituted by the PFAS pollution episode. The project includes the field monitoring of PFAS in abiotic (water, soil) and biotic (vegetables and animals) in agricultural field. Meanwhile, some innovative technological tools for mitigation of PFAS concentration in water are being validated and compared for irrigation and drinking water purification, using full-scale plant (wetland system) and physico-chemical plans breakdown system (filters). Finally, a typical local crop (red chicory) was cultivated in a greenhouse as model crop, under varying concentrations of pre-contaminated soil and irrigation water. The obtained results are a valuable empirical base for the validation of the existing plant uptake models and can support a mechanicistic understanding of contaminants transport from soil

to crop. All project activities offer well-timed and innovative environmental tools for the estimation of PFAS distribution and risks based on multidisciplinary datasets aimed to implement policy measures to prevent or limit problems related to the diffusion of persistent mobile organic contaminants.

Assessing occurrence of organic contaminants of emerging concerns in Groundwater: may the Gustafson's force be with us!

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In 1989, Gustafson demonstrated that if other physical properties than soil organic carbon and water (Koc) and half-life in soil ($t_{1/2}$), such as water solubility, octanol/water partition coefficient, and volatility from soil, have often been involved as indicators of leachability, they are found to have no useful power in discriminating between "leachers" and "non-leachers" organic active pesticides. Author developed and validated the GUS index (Gustafson, D. I., 1989) for assessing the leachability of pesticides, for which Koc and $t_{1/2\text{-soil}}$ properties were widely available. Nowadays, with the improvement of knowledge on physic-chemical properties of organic Contaminants of Emerging Concerns (CECs), it becomes possible to calculate and to test the GUS index for other micro-organic contaminants than pesticides.

To test the potential for the GUS index to predict the leachability of organic compounds others than pesticides, it is proposed to plot CECs whose occurrence in groundwater is known in a diagram $log(t_{1/2-soil}) = f(log(Koc))$. We choose the worst-case scenario plotting the minimum Koc versus the maximum $t_{1/2 \ soil}$. Occurrence data of CECs in groundwater have been obtained from a national screening of French groundwater for more than 400 regulated and emerging contaminants carried out in 2011 for almost 500 sites (Lopez, B. et al., 2015). The diagram reveals that substances for which half-life in soil is less than 1 year (log[Half-Life]=2.56) mainly occur in groundwater only if GUS index value is above 1.4. Moreover, the diagram shows that CECs with half-life in soil above 1 year can reach groundwater whatever their sorption abilities (expressed with Log (Koc) value).

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As a first assessment of organic CECs groundwater leachability, GUS index seems to be usable only if half-life in soil is less than 1 year. A $t_{1/2\text{-soil}}$ of 1 year represents a cutt-off value above which organic CECs are estimated to have a groundwater leaching potential.

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Filling the knowledge gap: Suspect Screening for over 1400 PM(T)-substances in German surface waters

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Persistent and mobile chemicals (PM-substances) are particularly difficult to remove in partially closed water cycles and thus can even reach drinking water [1]. However, for screening routinely applied reversed phase liquid chromatography (RPLC) coupled to high resolution mass spectrometry (HRMS) does not fully cover this class of substances (« analytical gap »). Hence, only very limited knowledge is available on the extent to which PM-substances occur in the water cycle. This is of special concern for PM-substances that are also toxic (PMT-substances).

The analytical window can be extended to highly polar substances by the use of hydrophilic interaction liquid chromatography (HILIC) [2] and supercritical fluid chromatography (SFC) [3]. In a recent monitoring study for 60 PM-substances three quarters of the chemicals were detected in the aquatic environment [3].

In the present study an extensive suspect screening by HILIC- and SFC-HRMS for over 1400 potential PM(T)-substances in German surface waters was carried out, in order to substantially reduce the existing knowledge gap regarding their occurrence in the water cycle. The list of PM(T)-suspects was compiled from previous prioritisation and identification studies [4, 5]. The main focus was on REACH chemicals. In addition, pharmaceuticals, chemicals for plant protection, artificial sweeteners and ionic liquids were considered. More than 100 substances were tentatively detected and partially already confirmed with authentic reference standards

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The results underline that SFC and HILIC are promising techniques for the analysis of PM(T)-substances. A number of analytes eluted in RPLC as broad peaks was separated as sharp peaks in SFC and thus sensitively detected. Thus, both techniques significantly contribute to widen the polarity window that can be analyzed and consequently to fill the existing knowledge gap for these compounds. Therefore, SFC and HILIC are powerful tools to learn more about the occurrence of PM(T)-substances in the aquatic environment and to prioritize these chemicals for future activities aiming at a reduction of their discharge or at the development of novel methods for their removal from the water cycle.

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Fluoropolymer Stability: How Can You Prove a Negative (Absence of Leachable Substances of Concern Over Time)?

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Certain per- and polyfluoroalkyl substances (PFAS) have been detected in environmental compartments and biota. Globally, regulators are struggling how to manage the grouping and regulation of the 4,730 **PFAS** (including polymers) OECD.Polytetrafluoroethylene (PTFE), a fluoropolymer, meets the OECD Polymer of Low Concern (PLC) classification criteria. As such PTFE is not toxic or bioaccumulative. PTFE is stable and does not degrade, breakdown, or form toxic transformation products. The stability of PTFE means that it possesses a long environmental half-life, which translates into a classification of "persistent" under common regulatory and hazard assessment frameworks. Persistence alone cannot, by definition, present a risk to biota or the environment in the absence of inherent hazard, either from the fluoropolymer itself or from leachable substances of concern from the fluoropolymer. How then can the absence of leachable substances of concern from PTFE over time be proven?

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We propose a testing scheme based on our knowledge of PTFE manufacturing processes, their chemical, physical and thermal properties, and existing OECD and OPPTS test guidelines for environmental fate to determine what may leach out over time from PTFE. One objective of the proposed testing framework is to provide consistent evidence that persistence of a substance does not necessarily imply toxicity or bioaccumulation, nor does it imply future degradation, release, or transformation into a continuous source of substances of concern.

Keywords: PTFE, PFAS, environmental fate, OECD test guideline, OPPTS test guideline, biotic and abiotic stability, persistence

Removal of PM substances from drinking water by adsorption onto activated carbon

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Within the broad range of organic micropollutants, compounds with the intrinsic properties of being persis-tent and mobile in the environment are of growing concern due to their tendency to enrich in the water cycle as well as the risk of reaching drinking water sources (Neumann and Schliebner, 2017; Reemtsma et al., 2016). In recent years, numerous compounds meeting PM criteria have been newly identified (Schulze et al., 2019; Zahn et al., 2019). Hence, little is known about their behaviours in natural and technical water treatment processes (Reemtsma et al., 2016). Adsorption onto activated carbon is an established process for the removal of organic micropollutants in water treatment that is expected to achieve low removals of PM substances, which has been indicated by previous studies (Ridder et al., 2010). The affinity of an ad-sorbate towards activated carbon depends on a variety of compound characteristics such as polarity, mo-lecular weight, aromaticity and electric charge.

A total amount of 20 compounds with varying properties (log D between -3.06 and 2.25 at pH 7.5, anionic, neutral and cationic at pH 7.5, aromatic and aliphatic) were analysed regarding their adsorption potential in equilibrium. For this purpose, batch experiments were conducted with pulverized (CryoMill, Retsch; 30 s, 30 Hz) granular activated carbon (Hydraffin CC, Donaucarbon, Germany). Doses of 2, 10 and 50 mg/L activated carbon were added to 50 mL of Berlin tap water (DOC \approx 4.5 mg/L, pH \approx 7.5) spiked with 10 µg/L of each PM substance. After 48 h contact time on a horizontal shaker all samples were filtered (0.45 µm). Prior to PM substance measurements by supercritical fluid chromatography with high-resolution mass spec-trometry (SFC-HRMS) (Waters Acquity UPC2 BEH 3.0 x 100 mm, 1.7 µm; Waters Acquity UPC2 system) all samples were pre-treated by azeotropic evaporation (XcelVap, Biotage). PM substance removal was calculated using peak area ratios assuming a linear relation between analyte concentration and peak area.

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The investigated PM substances exhibited very different adsorbability onto activated carbon in equilibrium. At a feasible/realistic carbon dose of 10 mg/L, half of the PM substances only adsorbed poorly or not at all (removal < 60 %). The lowest removals were achieved for trifluoromethanesulfonic acid (log D = -1.23), 2-methyl-2-propene-1-sulfonic acid (log D = -2.21) and 4-hydroxy-1-(2-hydroxyehtyl)-2,2,6,6,-tetramethylpi-peridine (log D = -2.19), all relatively small (150-201 g/mol) aliphatic compounds with low log D values. However, five PM substances revealed good to very good adsorbability by activated carbon (80-100 % removal with 10 mg/L activated carbon). Contrary to expectations based on their low log D and N-(3-(dimethylamino)respectively) oxipurinol values (-2.86)and -1.37, propyl)methacrylamide demonstrated a high adsorbability. The high affinity of oxipurinol towards activated carbon was indicated by Sperlich et al. (2017) in a fixed-bed granular activated carbon filter in a similar matrix. In conclusion, no clear correlation between log D and the removal by activated carbon from tap water was found for the PM substances analysed. Consequently, log D is not a good descriptor and other substance characteristics as well as interactions with background organic matter play an important role defining the adsorbability of the PM substances investigated.

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Break-out Groups

The work in break-out groups is the major point on the workshop schedule of day 2. This should give us the opportunity to dive deeper into specific aspects of PMT substances you are interested in.

On the basis of reports and discussion on day 1, these break-out groups offer the opportunity for all participants to share their experience and view with the other workshop participants.

A chairperson has been nominated for each group to moderate the discussion and for reporting back to the plenum. This will be the last point on the workshop agenda. The organizers will document the reports of all break-out groups and make them available to all participants of the workshop.

To foster the discussion in the break-out groups the organizers together with the chairs have collected a number of questions for each discussion topic (see below). These questions may but do not have to be discussed.

Organisational remark:

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Discussion in groups becomes difficult if a group is too large. Therefore the organizers would prefer an even distribution of participants to the groups, so that no group exceeds the number of 15 participants.

To arrange this process we kindly ask all participants interested in the break-out groups to register on one of the six lists displayed on poster boards during the coffee break on Tuesday afternoon.

You are also invited to add missing aspects you would like to discuss in your group at that board.

Break-out Group Titles	Proposed	Possible questions
4	Chairs	
Analysis of PM compounds (monitoring and screening level)	Pim de Voogt	 Pros and cons of HILIC, SFC, MMLC, IC? Is "polarity extended" RPLC sufficient? Enrichment from water?
2. Findings and knowledge on occurrence of PM compounds	Urs Berger	 Which compounds have been found? Are these critical in terms of "T"? Should we care for "non-T" compounds? What do we expect next? Strategies to locate sources of PM compounds How to avoid (release of) PM substances?

3.	Hans Peter Arp	Do you agree that there is general
Persistence: data quality	Tians reter Arp	insufficient P data for hazard/risk
and test methods		
and test methods	ü	assessment?
	-	Do you think (time-consuming,
		expensive) simulation tests are the
	" " " " " " " " " " " " " " " " " " "	only way to adequately assess P?
	· · · · · · · · · · · · · · · · · · ·	 What alternative types of test could
an .		be used as an alternative (e.g.
		inherent biodegradability tests?)
		 How can we best adapt QSARs/read-
	, , ,	across?
→ ⁸		Identification of "P"-precursors?
4.	Thorsten	Parameters to assess mobility
Mobility: suitable	Reemtsma	Adequate cut-off values?
parameters and options for	(prelim.)	Modeling versus experimental data
verification	e see	for "M"?
	*	Test systems for "M"
٠ ´ ا		 Is true "enrichment" in organisms
* .		possible to occur?
5.	Thomas ter	Do we expect many "T" compounds
Toxicity and ecotoxicity of	Laak	among "PM" compounds?
PM compounds		Do we have sufficient knowledge on
		"T" for the PM compounds already
		reported?
		Which modes of actions appear most
		likely?
6.	Aki Ruhl	To which extent do (advanced)
Removal options for PM	2 mm 11 mm	oxidation and adsorption help?
compounds from water		 Which alternatives are promising?
ozpodilas irom water	2	
	ψ.	 Can we estimate/predict eliminations in treatment processes?
	=	Do we expect additional PM
	e e	substances originating from
	•	disinfection or oxidation or
		biotransformation?

Questions for all groups:

- Urgent questions that science should answer next
- Suitable approaches to tackle these questions

Project Overview



Persistent mobile organic chemicals in the aquatic environment: Sources, occurrence and technical processes for their removal in the drinking water supply (PROTECT)

Water is an essential resource of our planet. However, the discharge of man-made, persistent and mobile organic

chemicals (PM substances) into the environment threats the quality of water and thus not only the aquatic environment, but also human health.

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Persistent and mobile substances are particularly difficult to remove in partially closed water cycles where they can reach drinking water. However, existing monitoring methods do not fully cover this class of substances. Hence, only very limited knowledge is available on the extent to which PM-substances do indeed reach from waste water to raw or even drinking water. While PM-substances therefore pose a risk to the drinking water supply on the one hand, knowledge about their fate in the entire water cycle is very limited on the other.

Based on the results of the previous research project PROMOTE a consortium of six partners will apply novel analytical methods that are dedicated to very polar, mobile compounds to screen for PM-substances in all compartments of the water cycle and to monitor the efficacy of natural and technical barriers (wastewater treatment, subsurface passage, drinking water treatment) in removing PM-substances. PM-substances are most critical, if they are also toxic (PMT-substances). Therefore, prominent PM-substances will be evaluated for their toxicity and ecotoxicity. Simultaneously, technologies for the removal of PM-substances from raw water used for drinking water production will be studied in full-scale for their removal of PM-substances and innovative procedures like membrane separation will be developed in lab scale. The consideration of the whole water cycle and the combination with improved removal technologies will eventually allow recommending a set of mitigation measures to reduce the risk that PM-substances pose to water resources. Highest priority will be given to PMT-substances.

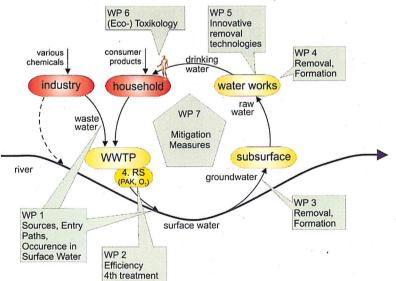


Abb. 1 Seven working packages (WPs) of PROTECT arranged along a partially closed water cycle.

The consortium will achieve its goals through seven working packages which are arranged along a partially closed water cycle (Fig. 1)

Duration of the project: 01/02/2019 - 31/01/2022

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About the UFZ

Our Vision

The UFZ is one of the world's leading research centres in the field of environmental research, enjoying high social recognition. It demonstrates ways in which a sustainable use of our natural resource base is possible for the benefit of both humankind and the environment.

Our Mission

Biodiversity, functioning ecosystems, clean water and intact soils all make up our natural resource base. In the face of global change, employees at the Helmholtz Centre for Environmental Research – UFZ are united by the goal of demonstrating ways to combine societal development with a healthy environment.

The UFZ with its approximately 1100 employees conducts excellent research and takes on a shaping role in the scientific community. As a reliable partner, the UFZ supports the political arena, the economy and the general public to better understand the consequences of human actions on the environment and to develop options for social decision - making processes. For this purpose, the UFZ responds to the stimuli created by society and by producing know - how and technologies that should help to rapidly identify problems comprising conflicting priorities between the environment and society. The UFZ will consequently work on precautionary measures.

In dealing with complex environmental issues, the disciplinary borders between the natural-, engineering- and social sciences need to be overcome. The UFZ has extensive competences in integrated environmental research. It boasts innovative scientific infrastructures and nurtures indispensable national and international cooperation, enabling problem - solving at the highest level.



Organisation

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Dinner Location for January 21th, 7 pm:

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Tel. +49(0)341 123 45 67 www.ratskeller-leipzig.de

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Change at the central station to tram 10 (direction Lößnig via Connewitz Kreuz) to "Wilhelm-Leuschner-Platz" or take a 15 minutes' walk through the city centre to "Neues Rathaus".

