An update of the lists with compounds that are relevant for the production of drinking water from the river Meuse - 2018

Title:	An update of the lists with compounds that are relevant for the production of drinking water from the river Meuse - 2018
Client:	RIWA-Meuse
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Summary

RIWA-Meuse is an international organisation that represents the interests of the drinking water companies in Belgium and the Netherlands that use the River Meuse as a source for their drinking water production. RIWA aims for clean water in the river Meuse to guarantee the sustainable supply of impeccable drinking water. For this reason, RIWA-Meuse closely monitors the quality of the Meuse water and, where necessary, advocates improvement of the water quality. In order to control trends and developments with regard to compounds (of emerging concern) in the Meuse, RIWA makes a compilation of lists of compounds that are considered (potentially) relevant for the drinking water production, namely:

List 1 - Drinking water relevant compounds
List 2 - Candidate drinking water relevant compounds
List 3 - No longer drinking water relevant compounds

For compounds to be considered as drinking water relevant they have to fulfill a fixed set of criteria concerning i.e. their detection frequency, occurrence in concentrations above the ERM target value, (potential) removal by water treatment, toxicity, odor/taste threshold and public perception.

The goal of this study is to update the lists of (candidate) relevant compounds. Therefore, the current list 1 and 2 are re-evaluated based on measurement data from the monitoring stations and intake points along the Meuse in the period 2013-2017, and new candidate drinking water relevant compounds are identified based on a literature study and screening data. For the selected compounds background information is given regarding their toxicological evaluation and possible sources.

Based on the evaluation the following compounds are identified to include in the new joint monitoring program of the drinking water companies along the river Meuse:

List 1: Drinking water relevant compounds		
Industrial compounds	**Pharmaceutical residues**	**X-ray contrast agents**
1,4-dioxane	Gabapentin +	Amidotrizoic acid
Benzo(a)pyrene	Gabapentin lactam	Iohexol
Bisphenol A	Hydrochlorothiazide	Iomeprol
Bis(2-ethylhexyl)phthalate (DEHP)	Lamotrigin	Iopamidol
Diethylenetriaminepentaacetic acid (DTPA)	Metformin +	Iopromide
Diisopropylether (DIPE)	Guanylurea	Ioxitalamic acid
Ethylenediaminetetraacetic acid (EDTA)	Metoprolol	**Pesticides**
Fluoride	Paroxetine	Desphenylchloridazon
Melamine +	Sotalol	Diethyltoluamide (DEET)
Melem	Tramadol	Glyphosate +
Nitriloacetic acid (NTA)	Valsartan +	Aminomethylphosphonic acid AMPA
Pyrazole	Valsartanic acid	N,N-dimethylsulfamid (DMS)
		Terbuthylazine

List 2: Candidate drinking water relevant compounds		
Industrial compounds	**Pharmaceutical residues**	**Pesticides**
Ethylsulphate	Cetirizine	3,5,6-Trichloro-2-pyridinol
Hexa(methoxymethyl)melamine	Citalopram	Sebuthylazine
2,3,3,3-Tetrafluoro-2-(heptafluorpropoxy) propanoate (HFPO-DA; GenX compound)*	Fluconazole	**Hormone disrupting compounds**
Methoxymethyltriphenylphosphonium	Oxipurinol	Anti-AR-Calux
	Telmisartan	
	Venlafaxine +	
	O-Desmethylvenlafaxine	
	Vigabatrin	

*Only at the relevant monitoring stations (Dunea/Evides)

All associated drinking water companies are recommended to monitor the selected compounds on list 1 and 2 in order to have a detailed insight in the water quality of the river Meuse. This is the scientific basis upon which RIWA develops its lobby and advocacy. The recommended monitoring frequencies for list 1 are 13 times a year for 5 years and 13 times a year for 1 year for list 2.

The major sources of the compounds, included in list 1 and 2, are the emissions via municipal and industrial WWTP effluent. These include pharmaceutical residues, X-ray contrast agents and pesticides, as well as industrial compounds, like DIPE, fluoride, melamine, pyrazole and HFPO-DA (GenX), that can be related to specific industrial point sources.
Since toxicity is an important criterion for the selection of drinking water relevant compounds, not all of the compounds that are present in relatively high concentrations (>1 µg/L) end up on the list of drinking water relevant compounds. This is the case for sucralose and methenamine, which are included in List 3. For these compounds, human health effects are expected to be negligible at the detected concentrations.

A recommendation for the future is for the drinking water companies to develop an aligned strategy for the evaluation of screening data for the Meuse. The screening process is qualitative rather than quantitative: substances can be detected, but the exact concentrations cannot be directly known. This makes the list of potential relevant compounds very long and it is difficult to prioritize and select compounds from the screening.

In addition it is recommended to initiate the development of suitable analytical techniques for the monitoring of more polar compounds in water in order to bridge the existing analytical data gap that makes it difficult to monitor and prioritize PMT (polar/mobile/toxic) compounds from the REACH database.

Contents

Abbreviations

4-AAA	4-acetylaminoantipyrine
4-FAA	4-formylaminopyrine
ALZ	Aqualab Zuid
AMPA	Aminomethylphosphonic acid
AR	Androgenic receptor
BAP	Benzo(a)pyrene
BQ	Benchmark Quotient
BRA	Brakel
BTO	Bedrijfstakonderzoek
CALUX	Chemical Activated Luciferase gene eXpression
Ctgb	College voor de toelating van gewasbeschermingsmiddelen en biociden
DDD	Daily Defined Dose
DEET	Diethyltoluamide
DEHP	Bis(2-ethylhexyl)phthalate
DIPE	Diisopropylether
DMS	N,N-Dimethylsulfamid
DMSA	N,N-dimethyl-N'-phenylsulphamide
DTPA	Diethylenetriaminepentaacetic acid
ECB	European Chemicals Bureau
ECHA	European Chemicals Agency
EDTA	Ethylenediaminetetraacetic acid
EFSA	European Food Saftey Authorization
ER	Estrogenic receptor
ERM	European River Memorandum
EYS	Eijsden
F3-MSA	Trifluoromethanesulfonic acid
FRD-902	ammonium, 2,3,3,3,-tetrafluoro-2-(heptafluorpropoxy)-propanoate
FRD-903	2,3,3,3,-tetrafluoro-2-(heptafluorpropoxy)propanoic acid
GR	Glucocorticoid receptor
HAV	Haringvliet
HEE	Heel
HEU	Heusden
HFPO-DA	2,3,3,3-tetrafluoro-2-(heptafluorpropoxy)propanoate
HMMM	Hexa(methoxymethyl)melamine
HWL	Het Waterlaboratorium
KEI	Keizersveer
K_{ow}	Octanol/water partition coefficient
KWR	KWR Watercycle Research Institute
LOD	Limit of detection
LOQ	Limit of quantification
LUI	Liège/Luik
Max	Maximum concentration in the Meuse
MTBE	Methyl-tertiair-butylether
NAM	Namêche
NDMA	N-Nitrosodimethylamine
NGI	Norwegian geotechnical institute
NOAEL	No observable adverse effect level
NTA	Nitrilotriacetic acid
pGLV	Provisional drinking water guideline value
PMT	Persistent, mobile and toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RIVM	Rijksinstituut voor Volksgezondheid en Milieu (Dutch Institute for Health and Environment)
RIWA	Association of River Waterworks

STE	Stellendam
SVHC	Substances of Very High Concern
TAI	Tailfer
TCP	3,5,6-Trichloro-2-pyridinol
TCPP	Tris(1-chloro-2-propyl)phosphate
TFA	Trifluoroacetic acid
TPPO	Triphenylphosphine oxide
TTC	Threshold of toxicological concern
VP	Vapor pressure
UBA	Umweltbundesamt (German environment agency)
vPvM	Very persistent, very mobile
WHO	World Health Organization
WWTP	Wastewater treatment plant
ZZS	Zeer Zorgwekkende Stoffen (Substances of Very High Concern)

1. Background

RIWA-Meuse is an international association of drinking water companies in Belgium and the Netherlands that use the River Meuse as a source for their drinking water production. RIWA-Meuse represents the joint interest of these companies: clean water in the river Meuse for sustainable supply of impeccable drinking water. For this reason, RIWA-Meuse closely monitors the quality of the Meuse water and, where necessary, advocates an improvement of the water quality.

One of the issues for the production of drinking water is the presence of anthropogenic compounds (e.g. pharmaceutical residues, personal care products, industrial compounds, pesticides and the metabolites of these compounds) in the river water. These chemicals can enter the river via various sources like water treatment plants, diffuse emissions by agriculture, but also industrial plants located near the river (**Figure 1**). New chemical compounds are continuously discovered in river water. On the one side, the development and improvement of analytical techniques broadens the spectra of compounds that can be analyzed and, on the other hand, new compounds are introduced into the market.

The countries in the Meuse catchment area are developing an approach for these new, emerging compounds. Several initiatives in this area such as the project DIADeM[1] (Développement d'une approche intégrée pour le diagnostic de la qualité des eaux de la Meuse) and Schone Maaswaterketen[2] are mentioned in the annual report of the RIWA Meuse (RIWA Meuse 2018).

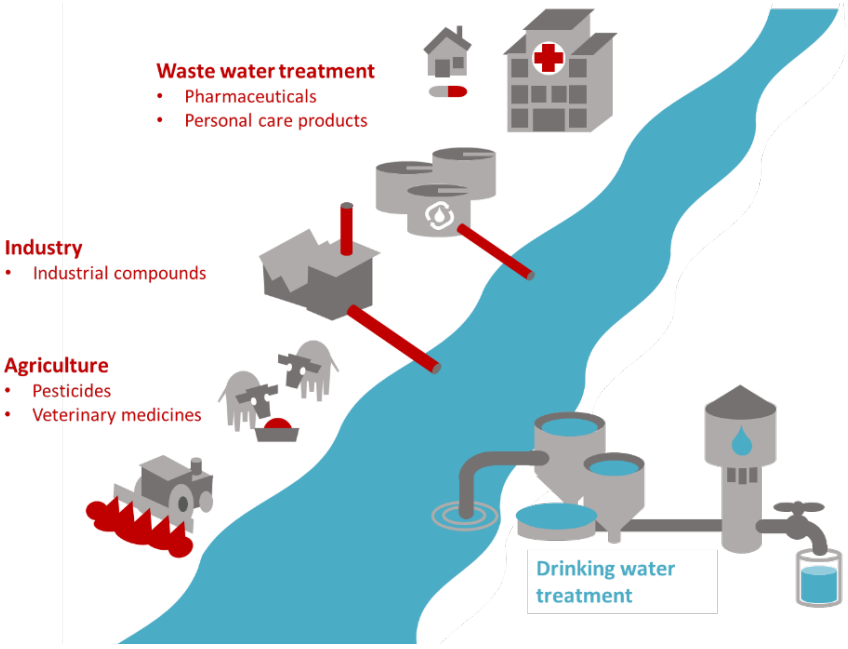


Figure 1. *A schematic representation of possible sources of anthropogenic compounds in the river Meuse*

[1] http://www.interregdiadem.eu/

[2] http://www.samenwerkenaanwater.nl/inspiratie/kansenkaart-drinkwater/schone-maaswaterketen/

To be able to follow the developments with regard to (emerging) compounds in the Meuse, in 2007 RIWA-Meuse started with the compilation of lists of compounds that are considered (potentially) relevant for drinking water production (van den Berg et al. 2007). The selected compounds are monitored by all associated drinking water companies and used to advocate a good water quality of the river Meuse.

The lists of relevant compounds were revised in 2011 and 2015 (Fischer et al. 2011, Van der Hoek et al., 2015). During the previous revision in 2015 a number of changes were made to the methodology on the basis of new insights. RIWA-Meuse now works with three separate lists:

List 1 - Drinking water relevant compounds
List 2 - Candidate drinking water relevant compounds
List 3 - No longer drinking water relevant compounds

For compounds to be considered as drinking water relevant compounds for the Meuse and to be included in list 1, they have to fulfill a fixed set of criteria. These criteria comprise, amongst others, the exceedance of the ERM target value, and the detection frequency and the distribution of the occurrence in the Meuse catchment area. It is only possible to check if compounds fulfill these criteria in case monitoring data for the Meuse is sufficiently available.
This is the reason that list 2 was introduced: on this list all compounds are placed that, based on various sources (literature, screening data, monitoring data from other parties, data on usage), are expected to be a drinking water relevant compound for the Meuse. When enough monitoring data is collected, it can be evaluated if the compounds should be placed on list 1.
List 3 contains all compounds that were placed on list 1 or 2, and which are completely evaluated, but do not or no longer fulfill the criteria. This list is kept in order to secure the information with regard to the evaluation of these compounds and to avoid duplication of efforts during a following evaluation. It is not intended as a list of compounds that drinking water companies should stop monitoring, as there can be several valid reasons to continue measuring, like a legal obligation. Each drinking water company can decide individually to keep these compounds in their monitoring program or remove them or follow them via screening methods.

In order to keep the lists up to date and significant, a new evaluation is carried out in this project. The specific goal of this project is to compile new lists of (candidate) relevant compounds for the joint monitoring program of the drinking water companies along the river Meuse.
Therefore the following activities are carried out:

- The current list 1 and 2 are evaluated based on recent monitoring data from the period 2013-2017
- New candidate drinking water relevant compounds are identified based on a literature study

Additionally, a source study is carried out for the compounds that meet the criteria for list 1 and 2. Knowledge of the source of compounds can help the lobby for a better water quality because a first step can be to reduce the emission of a compound, for example in consultation with the industry.

In the following chapters firstly the methodology for compiling the relevant compound lists is explained (Chapter **2**), followed by an overview of the newly proposed lists of drinking water relevant compounds (Chapter **3.1**). Subsequently, background information is provided regarding their toxicological evaluation and possible sources (Chapter **3.2**). Also, the preparation of the list of candidate drinking water relevant compounds is discussed in more detail (Chapter **3.3**). Finally, in Chapter **4** and **5** the conclusions and recommendations are described.

2. Methodology

2.1 Ranking methodology

To define a compound as a relevant compound for the drinking water production using the Meuse as a source, it had to fulfil certain criteria which are related to the following characteristics:

- The measured concentrations
- The frequency of detection
- The distribution of the compound in the Meuse catchment area
- Recent occurrence
- The toxicological properties of the compound
- The (potential) degree of removal of the compound during the water treatment process
- The public perception of the compound

} these last three characteristics are used to calculate an individual compound score (see Appendix 1)

Figure 2 shows a schematic representation of the flow scheme that was followed for the evaluation of the compounds. The specific criteria for each list are given in the boxes below.

Criteria for List 1: Drinking water relevant compounds

1. The compound was detected at two or more RIWA Meuse monitoring stations or intake points in the last 5 years (for a minimum of two years), with a frequency of at least 7% of the measurements[1] ***and***
2. The compound was found to exceed ERM target values or the Drinking Water Standards from the Dutch Drinking Water Regulation on at least two different RIWA Meuse monitoring stations or intake points in the past 5 years (taking into account possible removal by conventional treatment), with a frequency of at least 1% of the measurements ***and***
3. The compound was found to exceed the drinking water standard or the ERM target value used by the drinking water companies, at least once in the past 3 years ***and***
4. The total score of the compound has to be 10 or higher, of which at least 4 points are awarded by compound removal (sum of polarity, volatility, and biodegradability points) (the exact calculation of the score is explained in Appendix 1)

If the benchmark quotient of the compound is 1 or higher, the compound is considered drinking water relevant and criteria 2, 3, and 4 can be neglected.

[1] If the compound is monitored more than 13 times per year, it has to be detected at two or more RIWA Meuse monitoring stations with a frequency of at least 7% of the measurements per year. This criterion is equivalent to the criterion requiring that the compound with a monitoring frequency of 13 times a year, is detected at least once a year.

Criteria for List 2: Candidate compounds

1. The compound is present in the river Meuse at concentrations well above the ERM target value ***or***
2. The concentration of the compound is expected to increase due to increased use in the catchment area in the near future (e.g. due to a change in usage of pesticides) (based on expert judgement) ***or***
3. The compound has undesirable properties for the production of drinking water and is expected to be present in the river Meuse (based on research) ***and***
4. The compound can be monitored with an affordable measuring technique with a reasonable limit of detection

For the list the following monitoring frequencies are maintained:
List 1: **13 times a year** for **5 years**
List 2: **13 times a year** for **1 year**
List 3: need for monitoring decided by drinking water companies individually

It can happen that as well the parent compound as (one of) its metabolite(s) are placed on List 1 and/or 2. As a rule the parent compound and the metabolite will be coupled together and placed on one list. Having both the monitoring data of the parent compound and its relevant metabolite available helps to demonstrate that the use of a certain parent compound causes problems when it degrades in a persistent metabolite (Van der Hoek et al., 2015).

Criteria for List 3: No longer drinking water relevant compounds

Former list 1 and 2 compounds which have not been found to fulfill the criteria of list 1 in the past 5 years.

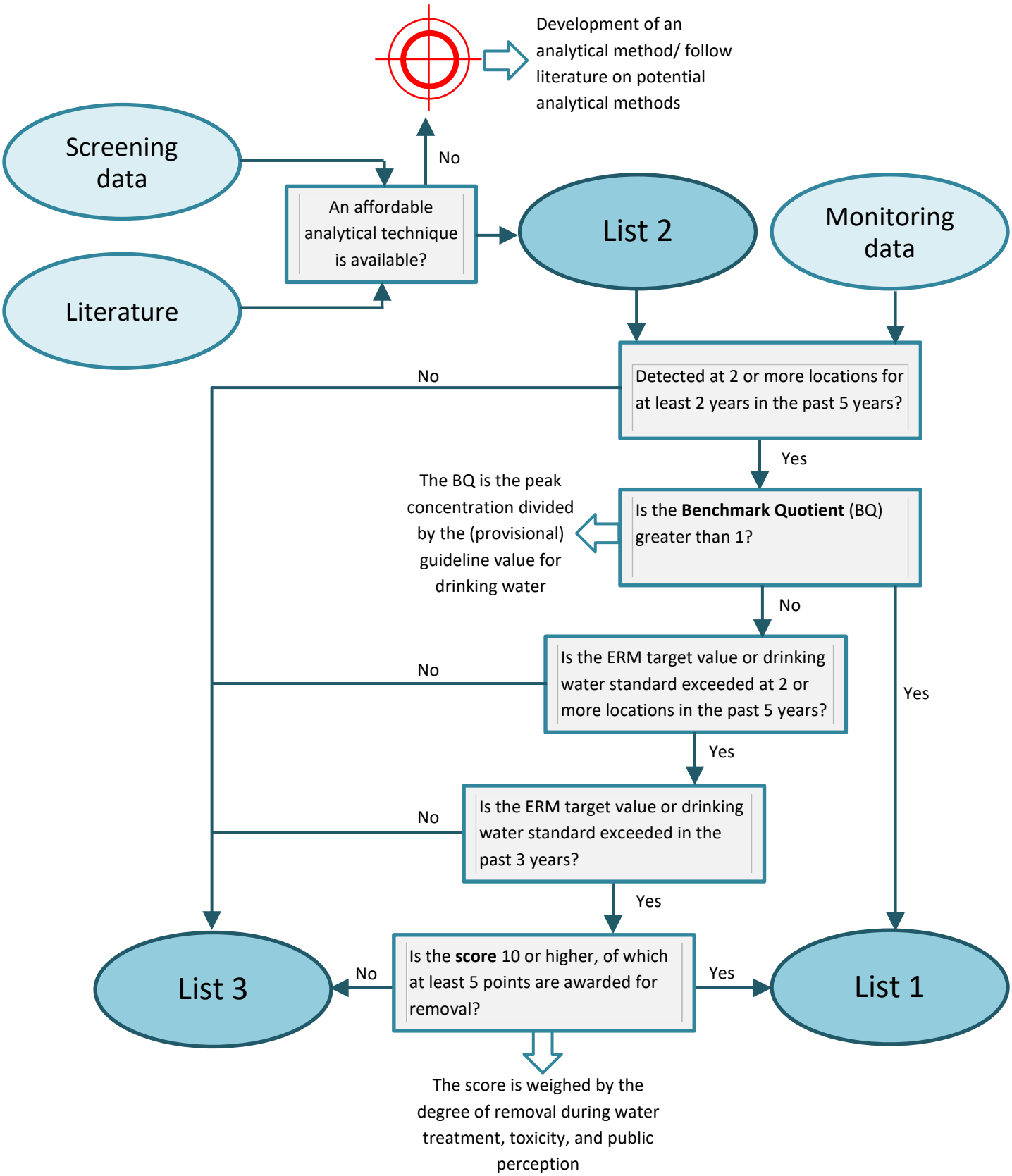


Figure 2. *A schematic overview of the ranking scheme used to establish the list of drinking water relevant compounds*

2.2 Data collection

2.1.1 Monitoring data

The monitoring data of compounds was obtained from the RIWA Meuse database. This database is assembled using data provided by drinking water companies and water management agencies located near the Meuse (**Figure 3**). The monitoring stations are shown in **Table 1.**

Figure 3. *The Meuse catchment area with the RIWA monitoring stations and intake points.*

Table 1. RIWA monitoring stations located near the Meuse, in order of downstream appearance.

Monitoring station / intake point		Abbreviation	Drinking water company / water management agency
1	Tailfer	TAI	Vivaqua
2	Namêche	NAM	Water-link
3	Liège/Luik	LUI	Water-link
4	Eijsden	EYS	Rijkswaterstaat Water, Verkeer en Leefomgeving
5	Heel	HEE	NV Waterleiding Maatschappij Limburg
6	Brakel	BRA	Dunea
7	Heusden	HEU	Dunea
8	Keizersveer	KEI	Evides NV/WBB
9	Haringvliet/Stellendam (combined)	HAV/STE	Evides NV

2.1.2 Compound information

To rank compounds in order of increasing relevance for the drinking water function of the river Meuse, the compounds were scored based on following properties:

- Toxicity (benchmark quotient)
- Removal by water treatment (polarity, volatility, biodegradability).
- Odor/taste threshold.
- Public perception.

The scoring system is described in **Appendix 1**, and explained in detail in the 2011 RIWA Meuse report (Fischer et al., 2011).

For the calculation of a benchmark quotient the maximum concentration in the surface water is compared to a (provisional) drinking water guideline value (pGLV) that is based on toxicity data. Most pGLVs were taken or calculated from the following sources:

- Recommendations given by the Dutch "Rijksinstituut voor Volksgezondheid en Milieu" (RIVM) (Smit and Wuijts 2012; van Leerdam et al. 2018; Versteegh et al. 2007, and pGLV's related to the exemptions for compounds that exceed the signaling parameter of 1 µg/L for anthropogenic substances in the Dutch Drinking Water Regulation (2011)).
- Guidelines for Drinking-water Quality, Fourth Edition (World Health Organization (WHO), 2011).
- Pharmaceutical residues in drinking water and drinking water sources. Results from the monitoring program 2005/2006 (Versteegh et al., 2007).
- Toxicological relevance of emerging contaminants for drinking water quality (Schriks et al., 2010).

For compounds that did not have a pGLV yet, toxicity data was collected from risk assessment reports, the REACH registration dossiers (https://www.echa.europa.eu/nl), information from the site of the Dutch Board for the Authorization of Plant Protection Products and Biocides (https://toelatingen.ctgb.nl) or literature. For

pharmaceutical residues the defined daily dose (DDD) was used to calculate a pGLV in case an ADI was not available. Based on these toxicity data, a pGLV was calculated as described in **Appendix 1**.
If no toxicity data or a DDD was available, the threshold of toxicological concern (TTC) was used (Kroes et al. 2004). De TTC-value is a threshold value for the exposure level of all chemicals below which an adverse effect to human health is not expected. For most compounds the TTC-value is 0,1 µg/L.

Information needed to estimate the removal by water treatment was either collected from the REACH registration dossiers; the TOXNET database (https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm); or from the program EPI Suite™, v4.11 (https://www.epa.gov/tsca-screening-tools). It concerned the following parameters:

- **The octanol / water partition coefficient** (Log K_{ow}) as an indicator of polarity. The log K_{ow} was obtained as an experimental value or estimated using "KOWWIN v1.68 Log K_{ow} estimate" in EPI Suite™.
- **The vapor pressure** of the compound as an estimate of volatility. The vapor pressure was obtained as an experimental value or estimated using the "mean vapor pressure of Antoine & Grain methods" in EPI Suite™.
- **The biodegradability** was derived from estimations using the "BioWIN3 Ultimate Survey Model" in the EPI Suite™

2.3 Literature study

To select candidate drinking water relevant compounds (List 2) various sources of information were used, namely: scientific literature studies, reports published by KWR Watercycle Research Institute (KWR), that performs joint research studies for the Dutch drinking water companies (bedrijfstakonderzoek - BTO), RIVM reports, measurement data from RIWA and Rijkswaterstaat, and screening data from Aqualab Zuid (ALZ), Het Waterlaboratorium (HWL) and Water-link. For scientific literature, the websites https://www.sciencedirect.com and https://scholar.google.nl have been used. BTO reports have been requested via www.btonet.nl.
In 2017, Het Waterlaboratorium performed a literature study to compile a list of relevant compounds with regard to the new monitoring strategy of anthropogenic compounds for the drinking water companies Dunea, PWN, and Waternet (Van der Velden-Slootweg 2018). This study also included extensive BTO studies concerning the presence and prioritization of relevant compounds in the sources for drinking water production (Sjerps et al. 2015a,b;2016; Ter Laak et al., 2016; Van Leerdam et al., 2017). Besides, in 2018, a report describing the broad screening of pesticides and emerging compounds in the Meuse was published (Verhagen et al. 2018). These studies were used as the basis for the selection of candidate drinking water compounds.
New information was only collected from the years 2017 and 2018. Hereby the following search terms were used (in various combinations):

1. compound / pollutant
2. emerging
3. water (drinking, surface, waste)
4. screening (non-target, suspect, target)

3. Results

3.1 Proposal for the new monitoring program for the Meuse

The lists of drinking water relevant compounds (List 1) is re-evaluated based on new monitoring data from the period 2013-2017. The list of candidate drinking water relevant compounds (List 2) is proposed based on a literature study and measurement data. The new list of no longer drinking water relevant compounds (List 3) consists of all compounds that are tested on the criteria of list 1 or 2, but did not meet them. Below, an overview is given of the new lists of 2018, including the compounds which are recommended for monitoring in 2019. More details about the compounds and background information on how the lists are established are given in Chapter **3.2** and **3.3**.

3.1.1 Drinking water relevant compounds

The evaluation of the monitoring data resulted in the proposal of a new list of drinking water relevant compounds (**Table 2**). Compared to the former List 1, 12 compounds are newly included and four compounds have been removed. The new compounds contain five substances with an industrial application (1,4-dioxane; bisphenol A; melamine, melem and pyrazole), six pharmaceutical residues (gabapentin; hydrochlorothiazide; lamotrigin; tramadol; valsartan and valsartanic acid) and one x-ray contrast agent (ioxitalamic acid).

Most new compounds were placed on List 2 in 2015 and based on the collected monitoring data they do fulfill the criteria for List 1. 1,4-Dioxane was not on a RIWA-list before, but was included recently in the monitoring programs. Ioxitalamic acid was already included in the monitoring programs before 2015, but did not meet the criteria before. For valsartanic acid, a metabolite of the antihypertensive drug valsartan, there is not enough monitoring data available to evaluate if the compound fulfills the criteria for List 1. It was however decided that if a parent compound and a metabolite are both on List 1 and/or 2, it is recommended to couple them. The same applies for melem, a metabolite of melamine.

Table 2. Proposed list of drinking water relevant compounds for the river Meuse (List 1).

#	Compound	CAS #	Category	Score[1]	Previous list
1a	1,3,5-Triazine-2,4,6-triamine (melamine)	108-78-1	Industrial compound	**20**	2
1b	Melem (triazine)	1502-47-2	Industrial compound	**27**	New
2	1,4-Dioxane	123-91-1	Industrial compound	**18**	New
3	Amidotrizoic acid	117-96-4	X-ray contrast agent	**11**	1
4	Benzo(a)pyrene (BAP)	50-32-8	Industrial compound	**18**	1
5	Bisphenol A	80-05-7	Industrial compound	**18**	2
6	Desphenylchloridazon	6339-19-1	Pesticide (metabolite)	**20**	1
7	Bis(2-ethylhexyl)phthalate (DEHP)	117-81-7	Industrial compound	**17**	1
8	Diethylenetriaminepentaacetic acid (DTPA)	67-43-6	Industrial compound	**13**	1
9	Diethyltoluamide (DEET)	134-62-3	Pesticide	**10**	1
10	Diisopropylether (DIPE)[2]	108-20-3	Industrial compound	**13**	1
11	Ethylenediaminetetraacetic acid (EDTA)	60-00-4	Industrial compound	**12**	1
12	Fluoride[3]	16984-48-8	Industrial compound	**0**	1
13	Gabapentin	60142-96-3	Pharmaceutical	**11**	2
14a	Glyphosate	1071-83-6	Pesticide	**11**	1
14b	Aminomethylphosphonic acid (AMPA)	1066-51-9	Pesticide (metabolite)	**11**	1
15	Hydrochlorothiazide	58-93-5	Pharmaceutical	**12**	New
16	Iohexol	66108-95-0	X-ray contrast agent	**12**	1
17	Iomeprol	78649-41-9	X-ray contrast agent	**12**	1
18	Iopamidol	60166-93-0	X-ray contrast agent	**12**	1
19	Iopromide	73334-07-3	X-ray contrast agent	**12**	1
20	Ioxitalamic acid	28179-44-4	X-ray contrast agent	**11**	New
21	Lamotrigine	84057-84-1	Pharmaceutical	**23**	2
22a	Metformin	657-24-9	Pharmaceutical	**17**	1
22b	Guanylurea	141-83-3	Pharmaceutical (metabolite)	**23**	1
23	Metoprolol	37350-58-6	Pharmaceutical	**16**	1
24	N,N-Dimethylsulfamid (DMS)	3984-14-3	Pesticide	**11**	1
25	Nitrilotriacetic acid (NTA)	139-13-9	Industrial compound	**13**	1
26	Paroxetine	61869-08-7	Pharmaceutical	**22**	1
27	Pyrazole	288-13-1	Industrial compound	**26**	2
28	Sotalol	3930-20-9	Pharmaceutical	**10**	1
29	Terbuthylazine	5915-41-3	Pesticide	**16**	1
30	Tramadol	27203-92-5	Pharmaceutical	**17**	2
31a	Valsartan	137862-53-4	Pharmaceutical	**28**	2
31b	Valsartanic acid	164265-78-5	Pharmaceutical (metabolite)	**28**	New

[1] The score of compounds was calculated using the scoring system described in **Appendix 1**. See **Appendix 2 f**or details.

[2] DIPE has a clear emitting source (Société de Prayon, Ruisbroek) and it is proposed to monitor the compound only at the monitoring stations downstream from this source.

[3] For fluoride it is not possible to calculate a score based on the EPI Suite™ models because these are not suitable for this compound. Based on the criteria the compound does not get any points. However, fluoride remains on the list based on political reasons.

3.1.2 Candidates for the list of drinking water relevant compound

A literature study on emerging compounds was carried out and the screening data from the drinking water companies were evaluated to check for potentially relevant compounds to the drinking water function of the river Meuse (see also Chapter **3.3**). This results in the proposal of 15 new compounds for the candidate list. For 6 compounds it is not known if analytical methods are available (**Table 4**). For these compounds it is recommended to develop an analytical method.

For the other compounds it is proposed to add them to the joint monitoring program of the Meuse in 2019. It concerns the pharmaceutical residues cetirizine, citalopram, oxipurinol, and vigabatrin and the industrial compounds ethylsulphate, hexa(methoxymethyl)melamine (HMMM), 2,3,3,3-tetrafluoro-2-(heptafluorpropoxy)-propanoate (HFPO-DA) and methoxymethyltriphenylphosphonium (**Table 3**). Since HFPO-DA has a known emitting source, it is recommended to monitor this compound only at the drinking water intake points where the compound can be expected based on hydrology and dispersion.

Table 3. Proposed candidate drinking water relevant compounds for the river Meuse (List 2). Compounds are scored based on removal by water treatment, toxicity, odor/taste threshold and public perception.

#	Compound	CAS #	Category	Score[1]	Previous list
Compounds proposed for the monitoring program in 2019					
1	3,5,6-Trichloro-2-pyridinol (TCP)	6515-38-4	Pesticide (metabolite)	**≥10**	2
2	Anti-AR-Calux	not applicable	Hormone activity	**N.A.**	2
3	Cetirizine	83881-51-0	Pharmaceutical	**29**	New
4	Citalopram	59729-33-8	Pharmaceutical	**≥10**	New
5	Ethylsulphate	540-82-9	Industrial compound	**26**	New
6	Fluconazole	86386-73-4	Pharmaceutical	**≥11**	2
7	Hexa(methoxymethyl)melamine	68002-20-0	Industrial compound	**27**	New
8	HFPO-DA (GenX)[2]	62037-80-3	Industrial compound	**19**	New
9	Methoxymethyltriphenylphosphonium	4009-98-7	Industrial compound	**26**	New
10	Oxipurinol	2465-59-0	Pharmaceutical	**20**	New
11	Sebuthylazine	7286-69-3	Pesticide	**≥11**	New
12	Telmisartan	144701-48-4	Pharmaceutical	**≥9**	2
13a	Venlafaxine	93413-69-5	Pharmaceutical	**≥10**	2
13b	O-desmethylvenlafaxine	93413-62-8	Pharmaceutical (metabolite)	**≥11**	2
14	Vigabatrin	60643-86-9	Pharmaceutical	**10**	New

[1] The score of compounds was calculated using the scoring system described in **Appendix 1**. See **Appendix 3** for details; [2] HFPO-DA has a clear emitting source (DuPont, Dordrecht) and it is proposed to monitor the compound only at the monitoring stations downstream from this source.

Table 4. Proposed candidate drinking water relevant compounds for the river Meuse (List 2) with an unknown concentration. Monitoring is proposed in a later stage (when analytical techniques are available)

#	Compound	CAS #	Category	Score[1]	Previous list
Compounds to keep in sight[3]					
15	1,2,4-Triazole	288-88-0	Industrial compound	**≥8**	New
16	2,2,6,6-Tetramethyl-4-oxopiperidinonoxy	2896-70-0	Industrial compound	**≥7**	New
17	4-Aminophenol	123-30-8	Industrial compound	**≥8**	New
18	4-Mesyl-2-nitrotoluene	1671-49-4	Industrial compound	**≥7**	New
19	Fexofenadine	83799-24-0	Pharmaceutical	**≥11**	New
20	Ritalinic acid	19395-41-6	Pharmaceutical (metabolite)	**≥11**	New

[3] The complete list of candidate compounds for which an analytical technique is not available is shown in **Appendix 5**.

From the former list 2 not all compounds have been monitored (sufficiently) yet, and it is recommended to add also these compounds to the monitoring program of 2019. This concerns the pesticide (metabolite) 3,5,6-trichloro-2-pyridinol (TCP), the bioassay for anti-androgenic activity (the Anti-AR-Calux), and the pharmaceutical residues fluconazole, telmisartan and venlafaxine and its metabolite o-desmethylvenlafaxine[3] (Table 3).

After one year the compounds that have been monitored can be evaluated according to the methodology in Chapter **2.1** and it can be decided to either add the compounds to List 1 or List 3.

Table 5. List of compounds that are currently on list 2 and for which monitoring data is (partly) available.

#	Compound	CAS #	Category	Remark
Compounds currently monitored along the Meuse (evaluation possible at the end of 2018)				
21	4-FAA (metabolite metamizol)	1672-58-8	Pharmaceutical (metabolite)	Evaluation at the end of 2018: possibly included as list 1 compounds in joint monitoring program in 2020
22	4-AAA (metabolite metamizol)	83-15-8	Pharmaceutical (metabolite)	
23	Irbesartan	138402-11-6	Pharmaceutical	
24	Metazachlor ethane sulfonic acid	172960-62-2	Pesticide (metabolite)	
25	Metazachlor oxalic acid	1231244-60-2	Pesticide (metabolite)	
26	Metolachlor ethane sulfonic acid	171118-09-5	Pesticide (metabolite)	
Compounds for which monitoring data is available for some locations along the Meuse				
27	Aniline	62-53-3	Industrial compound	Measured at several monitoring stations, concentrations < 0,1 µg/L[1]
28	Benzylalcohol	100-51-6	Industrial compound	Below LOQ in Heel (ALZ)
29	Tert-butyl alcohol (metabolite MTBE)	75-65-0	Industrial compound	Below LOQ (measured by Vivaqua)

[1] RIWA Meuse (2017)

[3] O-Desmethylvenlafaxine has the same molecular formula and retention time as the compound tramadol ($C_{16}H_{25}NO_2$), which is placed on List 1. It is therefore impossible to chromatographically separate these compounds (personal communication P. Joos, Water-link)

Table 5 lists the compounds that were included on List 2 in 2015 (Van der Hoek et al. 2015) and that are either currently monitored (number 21 till 26) or for which some monitoring data is available indicating that the compounds are not present in concentrations above the LOQ (number 27 till 29). For the compounds that are being monitored in 2018 it is recommended to evaluate the monitoring data at the end of 2018 and then decide if the monitoring should be continued or not. For the compounds that are not found above the LOQ, the urgency to monitor them at all locations is not high and it is proposed not to include these compounds in the joint monitoring programme of the RIWA Meuse in 2019.

In appendix 7 is indicated for the compounds on List 2 which drinking water laboratories have an analytical technique available.

3.1.3 No longer drinking water relevant compounds

Compounds that were previously on List 1 or 2 and have the necessary parameters available to calculate the score, but were not found to exceed the ERM target values often enough or were not detected often enough (see Chapter **2.1**) were moved to the list of evaluated no longer drinking water relevant compounds (List 3). The compounds are shown in **Table 6**. The reason that the compounds will not be placed on List 1 or 2 is given in the field “Remark”.
For the compounds that were on List 1, the main reasons are a decrease in the maximum concentration or the detection frequency. For ibuprofen the pGLV that was determined by Houtman et al. (2014) was used instead of the TTC value, resulting in a lower BQ.
For the compounds that were on List 2 the main reason for removal is the low concentrations in the Meuse. Methenamine has been detected in concentrations above the 1 µg/L, but based on the relative low toxicity of the compound (RIVM has determined a GLV of 500 µg/L) and corresponding low BQ, the total score of methenamine is lower than 10.

The candidate compounds that were selected from literature or screening were evaluated according to the methodology. Several compounds did not meet the criteria, because they had a relatively low toxicity which resulted in scores below 10 (**Table 7**). Since these compounds were evaluated, they were placed on List 3.
The complete list of no longer drinking water relevant compounds is shown in **Appendix 6**.

Table 6. Compounds that are considered to be no longer drinking water relevant (List 3).

Compound	CAS #	Category	Remark
From list 1			
Acetone	67-64-1	Industrial compound	A lower maximal concentration results in a lower BQ: new score below 10
ER-CALUX	not applicable	Hormone activity	Concentrations below the ERM target value in the last 3 years
Ibuprofen	15687-27-1	Pharmaceutical	New pGLV available resulting in a lower BQ: new score below 10
Isoproturon	34123-59-6	Pesticide	Compound no longer authorised in the EU; few exceedances of the
Nicosulfuron	111991-09-4	Pesticide	<1% of the measurements above the ERM target value
From list 2			
Amoxicillin	26787-78-0	Pharmaceutical	Concentrations < 0,02 µg/L in Meuse
Ciprofloxacin	85721-33-1	Pharmaceutical	Concentrations < 0,02 µg/L in Meuse
Clarithromycin	81103-11-9	Pharmaceutical	Concentrations < 0,01 µg/L in Meuse
Clindamycin	18323-44-9	Pharmaceutical	Concentrations < 0,02 µg/L in Meuse
Erythromycin	114-07-8	Pharmaceutical	Concentrations < 0,01 µg/L in Meuse
Propyphenazone	479-92-5	Pharmaceutical	Concentrations < 0,01 µg/L in Meuse
GR-CALUX	not applicable	Hormone activity	Concentrations < ERM target value in the last 2 yrs
Methenamine	100-97-0	Industrial compound	Low toxicity, resulting in a low BQ and a score below 10
Oxadiazon	19666-30-9	Pesticide	Concentrations < 0,05 µg/L in Meuse

Table 7. Compounds that were considered as candidate compounds on List 2, but had a score below 10 (see **appendix 4** for details)

Compound	CAS #	Category
1,2-Benzisothiazol-3(2H)-one	2634-33-5	Industrial compound
1,3-Diethyldiphenylurea	85-98-3	Industrial compound
1,3-Diphenylguanidine	102-06-7	Industrial compound
Azelaic acid	123-99-9	Pharmaceutical
Trichloroacetic acid (TCA)	76-03-9	Industrial compound
Trifluoroacetic acid (TFA)	76-05-1	Industrial compound
Trifluoromethanesulfonic acid (F3-MSA)	1493-13-6	Industrial compound
Tris(1-chloro-2-propyl)phosphate (TCPP)	13674-84-5	Industrial compound
Triphenylphosphine oxide (TPPO)	791-28-6	Industrial compound

3.2 Sources of relevant and candidate compounds

3.2.1 Pharmaceutical residues

Pharmaceutical residues can be found as a result of the use of prescription and over the counter medicines, therapeutic drugs and veterinary drugs. Human pharmaceuticals are primarily introduced into the environment via human excretion which ends up in sewage water that is cleaned in wastewater treatment plants (WWTP). Traces of pharmaceutical residues or their metabolites can end up in WWTP effluent if the compounds are not fully removed or transformed during the water treatment. Veterinary pharmaceuticals can enter the environment via agricultural runoff, and livestock and veterinary waste (WHO 2012).

List 1 and 2 both contain 11 (metabolites) of pharmaceutical residues. **Metformin**, a drug that is used for the treatment of diabetes type 2 and to a lesser extent reduced fertility, and its major metabolite **guanylurea** are the pharmaceutical residues that are found in the highest concentrations in the surface water of the Meuse. Guanylurea is also a metabolite of the industrial compound melamine. Based on a number of daily defined doses (DDD) of >155 million in 2017, metformin is on the 12th place of most used pharmaceuticals in the Netherlands (www.gipdatabank.nl). In Belgium it is by far the most commonly consumed peroral antidiabetic. Nearly 500.000 patients were prescribed this medication in 2014 (www.fagg.be). Metformin and guanylurea are detected in concentrations above 1 µg/L in the Meuse. WML, Evides and Dunea have exemptions for metformin and/or guanylurea.

The anticonvulsants **gabapentin** and **lamotrigin** were placed as candidate drinking water relevant compounds on List 2 in 2015. Based on the new monitoring data they are now moved to List 1. Lamotrigin is one of the few drinking water relevant compounds with a pGLV below 1 µg/L. **Vigabatrin** is another anticonvulsant that was detected in the surface water of the Meuse in concentrations above the ERM target value at Haringvliet and was therefore placed on List 2. For vigabatrin there was no ADI available and a pGLV was determined on the basis of the lowest therapeutic dose for children.
The antihypertensive drugs **metoprolol** and **sotalol** (both beta-blockers that are used to treat abnormal heart rhythms) remain on List 1. Metoprolol and sotalol only exceed the ERM target value in less than 5% of the samples. Metoprolol on the 6^{tµh} place of most used pharmaceuticals in the Netherlands with 171 million DDD in 2017 (gipdatabank).

Valsartan (**Figure 4**) and **telmisartan** are angiotensin II-receptor blockers used for the treatment of high blood pressure and heart failure. Valsartan remains on List 1 and telmisartan remains on List 2 because for this compound monitoring data is not available for the Meuse. Telmisartan was placed on List 2 because it was detected in European surface waters with screening methods (Van der Hoek et al. 2015). Valsartan and telmisartan are in the top 100 of most used pharmaceuticals in the Netherlands with 92 and 18 million DDD, respectively

(gipdatabank). New in the category of antihypertensives is the metabolite of valsartan, **valsartanic acid** (**Figure 4**). Valsartanic acid is measured since 2018 at Brakel, where it was detected in concentrations above the ERM target value. Valsartanic acid is coupled to valsartan and therefore directly placed on List 1. Since toxicity data could not be found for valsartanic acid, the pGLV is based on the TTC value of 0,1 µg/L. Valsartan has a low pGLV of 0,2 µg/L based on an ADI determined by Khan and Nicell (2015). The maximum concentrations for valsartan and its metabolite are above the pGLV resulting in high BQ scores (**Appendix 2**). With total scores of 28 they are at the top of the ranking of the drinking water relevant compounds.

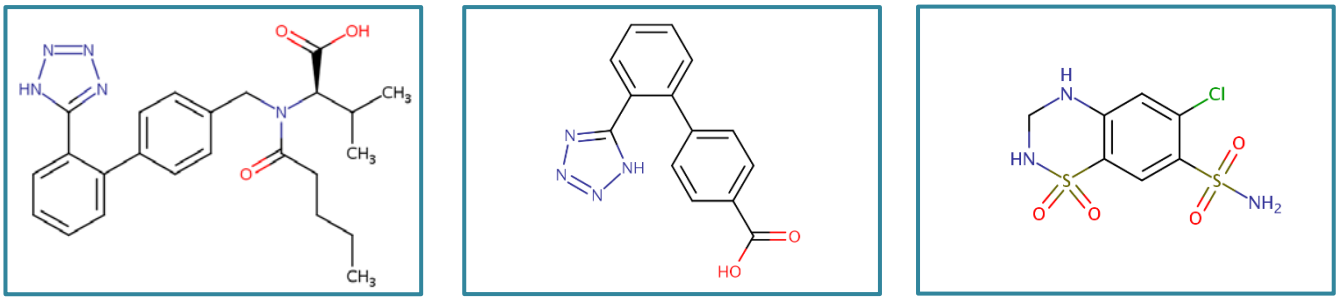


Figure 4. *Molecular structures of valsartan (left), valsartanic acid (middle) and hydrochlorothiazide (right)*

Antihypertensives are often prescribed in combination with diuretics like **hydrochlorothiazide** (**Figure 4**) (www.farmacotherapeutischkompas.nl). For hydrochlorothiazide monitoring data is available for the surface water of the Meuse. The compound was detected with a maximum concentration of 0,3 µg/L. Based on the score of 12 is was placed directly on List 1. Hydrochlorothiazide is an often used pharmaceutical with almost 127 million DDD in the Netherlands in 2017 (gipdatabank).

The opioid painkiller **tramadol** is also a widely used medicine. It is not in the top 100 based on DDD in the Netherlands, but the medicines tramagetic® and zaldiar® are both in the top of 100 of used medicines based on the number of users (600.000 for the two medicines together) (gipdatabank). Based on the new monitoring data tramadol moved from the candidate list 2 to List 1.

The antidepressant **paroxetine** remains on List 1. The number of DDD is decreasing the last years in the Netherlands, but with 51 million DDD in 2017, it is still a widely used pharmaceutical (gipdatabank). List 2 contains the antidepressants **citalopram** and **venlafaxine** (and its metabolite **O-desmethylvenlafaxine**). All three compounds were already placed on List 2 in 2015. Citalopram and venlafaxine are also in the top 100 of most used pharmaceuticals in the Netherlands with 48 and 39 million DDD, respectively.

Cetirizine and **fexofenadine** are antihistamine drugs used in the treatment of allergy symptoms, such as hay fever and urticaria. Cetirizine is monitored only in Namêche and Luik where it was detected in concentrations above the ERM target value (RIWA Maas 2018). The maximum measured concentration of 0,24 µg/L is almost equal to the pGLV of 0,25 µg/L that was based on an ADI determined by Khan and Nicell (2015). Fexofenadine was detected with LC-screening in more than 75% of the samples taken at Brakel in 2016 and was therefore selected as a candidate compound. It is not known if an analytical technique is available for this compound and it is proposed to monitor the compound in a later stage.

Fluconazole is an antifungal pharmaceutical used for a number of fungal infections. It was placed on List 2 in 2015 because it was detected in European surface waters in concentrations above 0,1 µg/L (Van der Hoek et al. 2015). No monitoring data for the Meuse is available for fluconazole and the compound remains on List 2.
The last two new compounds on List 2 are metabolites of pharmaceuticals. **Oxipurinol** is the metabolite of allopurinol, a medicine used to decrease high blood uric acid levels. Allopurinol is often prescribed with almost 20 million DDD in the Netherlands in 2017 (gipdatabank). Oxipurinol was detected in the river Rhine in concentrations above the ERM target value, since its mother compound has a widespread use it is also selected as a candidate compound for the river Meuse. **Ritalinic acid** is the inactive metabolite of the psychostimulant drugs methylphenidate (brand name concerta®). Methylphenidate improves the attention and mood and is used for people suffering from ADHD (attention deficit hyperactivity disorder) and narcolepsy (sleeping disease. Methyphenidate is also a widely used medicine with almost 52 million DDD in the Netherlands in 2017 (gipdatabank). Ritalinic acid was detected with LC-screening in more than 75% of the samples taken at Brakel in 2016 and was therefore selected as a candidate compound.

The **anti-AR-CALUX®** is a bioassay that is used to detect the presence of compounds with an anti-androgenic mode of action. In several researches performed by drinking water companies in the Netherlands, a potent response was found in the anti-AR-CALUX in surface water (e.g. Schriks et al. 2016; monitoring data Dunea). Since it is not known which compounds are the cause of the response, it is not possible to tell if the responses indicate a risk or not. For bioassays, trigger values that are developed specifically for the bioassay are often used as a first indication for risk. For the anti-AR-CALUX, this trigger value is currently being developed in BTO and a comparison with the responses found in the Meuse is not possible yet. However, since an anti-androgenic response is found in the surface water of the Meuse, it is recommended to keep monitoring the anti-AR-CALUX and evaluate the results as soon as the trigger value is available.

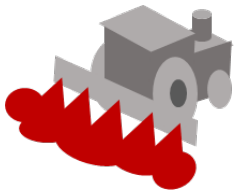
At the moment there are no veterinary pharmaceuticals included in the Lists of (candidate) drinking water relevant compounds. Ter Laak and Kools (2016) performed a quick scan in which the monitoring data of veterinary compounds was compiled. Only for a small percentage of the known pharmaceuticals monitoring data was available, and the measured concentrations in surface water were in the ng/L range for most compounds. In the near future a project on veterinary pharmaceuticals will be performed within the "knowledge impulse" (kennisimpuls) of the Delta-approach water quality and freshwater initiated by the Dutch government. Within this project a large number of participating institutions, e.g. KWR, one of the goals is to identify the knowledge gaps concerning veterinary pharmaceuticals in aquatic systems and gain insight in the risks. The outcome of the project can be used as input for the selection of new candidate compounds during the following evaluation of drinking water relevant compounds for the Meuse.

3.2.2 X-ray contrast agents

List 1 contains six X-ray contrast agents: **amidotrizoic acid**; **iohexol**; **iomeprol**; **iopamidol**; **iopromide** and **ioxitalamic acid**. The compounds are used to enhance the visibility of vascular structures and organs during radiographic procedures. Although these compounds are found in relatively high concentrations in the surface water, they all have a very low toxicity with pGLV's varying between 0,25 and 1 gram (which is a 10^7 difference compared to the lowest pGLV of 0,2 µg/L of valsartan!)

Contrast agents are broadly used in the whole Meuse catchment area. Emissions mainly come from households, and not from hospitals, because patients return home after a radiological examination where they excrete the contrast agents. The contrast agents therefore mainly enter the surface water of the Meuse via the wastewater effluent of WWTP (Rijkswaterstaat 2018).

3.2.3 Pesticides



The lists of (candidate) drinking water relevant compounds contain five pesticides and three metabolites of pesticides.

One pesticide, **sebuthylazine**, is newly added to List 2. Sebuthylazine is a herbicide that was used in combination with other compounds for weed control. It has no authorized use as a pesticide in Europe. Still it was found with a screening method in the surface water of the Meuse. The metabolite **3,5,6-trichloro-2-pyridinol** (3,5,6-TCP) can be formed by hydrolysis of either the organophosphate insecticide chlorpyrifos or the pyridine herbicide triclopyr. TCP was found to be a relevant metabolite in groundwater in Germany and was added to List 2 in 2015 (Reemtsma et al. 2013). Since it is not yet monitored in the Meuse, it remains on List 2.

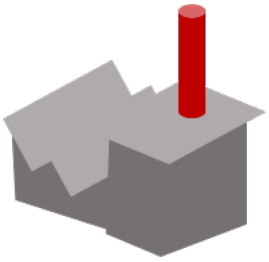
The other pesticides were already on List 1. **DEET** is the most common active ingredient in insect repellents. It is often detected in the surface water of the Meuse, but exceeds the ERM target value only in 1% of the samples. DEET mainly enters the surface water via the effluent of WWTP (Verhagen et al. 2018).

Glyphosate is also known as its brand name Roundup. It is a broad-spectrum herbicide which is used to kill weeds. In Belgium the use of glyphosate is prohibited for private individuals since July 2017. In the Netherlands, the professional use of chemical weed killers is forbidden in public spaces since November 2017 (with a few exceptions). Glyphosate is degraded into its metabolite **AMPA**. AMPA is also a degradation product of various phosphonates used in cooling water. AMPA was detected in the surface water of the Meuse in concentrations up to 8 µg/L. Glyphosate and AMPA mainly enter the surface water via WWTP effluent. The direct emission from agriculture is a factor 50 smaller. AMPA also has an emission pathway via the use of cooling water. The increase in the load of AMPA between Eijsden and Keizersveer can be attributed for more or less 1/3 to the lateral canal Ur, where AMPA ends up in the water as a result of the use of phosphonates in cooling water from chemical industries (RIWA Meuse 2018). In the Netherlands, the drinking water companies along the Meuse have received an exemption to take in AMPA and glyphosate. The exemption concentrations for glyphosate and AMPA are 0,3

and 3 µg/L, respectively. These concentrations are much lower than the health-based pGLV of 1500 µg/L that was determined by RIVM.

Effluent of WWTP also form a significant emission pathway for **terbuthylazine** and **desphenylchloridazon** (the metabolite of chloridazon) (Verhagen et al. 2018). Chloridazon is an authorized pesticide in Belgium and the Netherlands with an application as herbicide in the cultivation of e.g. beets, flower bulbs and onions. Desphenylchloridazon is defined as a not toxicologically relevant metabolite and therefore has a drinking water standard of 1 µg/L as well in Belgium as in the Netherlands (RIWA Meuse 2018).
Terbuthylazine is used as herbicide in agriculture and horticulture. In Belgium and the Netherlands terbuthylazine has an authorization as herbicide in the cultivation of maize (www.fytoweb.be; www.ctgb.nl). Besides the emission via WWTP, terbuthylazine can also enter the surface water directly via run-off, drainage and drift (RIWA Meuse 2018). The compound is frequently detected, but the ERM target value is exceeded in only 1% of the samples.
DMS is a degradation product of tolylfluanide, the active ingredient in fungicides used for the conservation of wood. Tolylfluanide does not have an authorized use in Belgium and the Netherlands anymore. DMS can also be formed from DMSA, the major degradation product of dichlofluanide which was used in antifouling on ships. Dichlofluanide does not have an authorized use in Belgium[4], and in the Netherlands it has only an authorization as film preservative (www.ctgb.nl; RIWA Meuse 2018). DMS itself is not very toxic with a pGLV of 700 µg/L, but during ozonation it can be converted to the genotoxic compound NDMA.

3.2.4 Industrial compounds



The highest share of the exceedances (38,7%) of the ERM target value in the Meuse can be attributed to industrial compounds (RIWA Meuse 2018). These compounds can enter the surface water via the industrial effluents. For a part of the industrial compounds industries have discharge permits. At the moment it is not easy to gain insight in these permits to find out which compounds are exactly discharged by industries in the Meuse catchment area. Furthermore there are many unknown compounds and transformation products present in the effluent. To get a better grip on the compounds in industrial effluent, at least two studies will be performed in 2018/2019. In the first project, performed by Rijkswaterstaat, some 70 discharge permits that are granted in the Netherlands will be fully screened. KWR will perform a project for Evides named “Grip op stoffen” (grip on substances) in which they will evaluate both the PMT substances and the list with 327 potential Substances of Very High Concern (SVHC) (Lijst met potentiële Zeer Zorgwekkende Stoffen (ZZS)) that was prepared by RIVM[5]. One goal is to investigate possible sources of these compounds for the river Meuse.
In this project emission data and information in the discharge permits is not included. Only industrial compounds that are found in screenings and literature are considered as potential candidate compounds. Compared to the

[4] https://www.health.belgium.be/nl/lijst-van-toegelaten-biociden-en-jaarverslag#1

[5] https://rvs.rivm.nl/stoffenlijsten/Zeer-Zorgwekkende-Stoffen/Potentiele-ZZS

last evaluation, ten industrial compounds are newly added to the lists of (candidate) drinking water relevant compounds. Ten compounds remain on the list, giving a total of 20 industrial compounds.

The complexing agents **EDTA**, **DTPA** and **NTA** are already known as relevant drinking water compounds for a long time. For EDTA the highest concentrations are measured with a maximum of 48 µg/L, but DTPA and NTA are also detected in concentrations far above the ERM target value of 1 µg/L. For EDTA and DTPA most drinking water companies in the Netherlands have an exemption with an exemption values of 50 µg/L and 10 µg/L, respectively. DTPA is on the SVHC list that was compiled by RIVM.
The main sources of EDTA, DTPA and NTA emissions to the environment are via wastewater effluent (because of their use in detergents, as a food additive and a variety of consumer products) and industrial effluents (because of their use as a complexing agent in industrial applications, e.g. inactivation of metal ions in the pulp and paper industry) (US EPA 2004). NTA is used increasingly since 1960 as a replacement of EDTA in detergents since it is better biodegradable. NTA is regarded as a potential carcinogenic compound by WHO (IARC class 2B) (RIWA Meuse 2018).

DIPE and **fluoride** have a known emitting source in the Walloon part of the Meuse catchment area. The company Société de Prayon developed and patented an extraction process using the solvents DIPE (85-95%) and tributylphosphate (5-15%) with which technical phosphoric acid can be upgraded to phosphoric acid with food quality. Since 1983, this process has been applied at the Engis plant and currently there is an installation that can treat 120 000 tonnes per year (expressed in P2O5). Fluoride is an impurity in the technical phosphoric acid. In the first step the amount of fluoride is reduced in phosphoric acid and partly recovered and sold in the form of hexafluorosilicic acid (H2SiF6). This process was optimized in 2014 resulting in a higher recovery of fluoride and less discharge. The loads of fluoride are decreasing in the last years (RIWA Meuse 2018). Based on the criteria fluoride is no longer a drinking water relevant compounds, but it is recommended to keep it on List 1 to verify that the trend downwards continues. WML has received an exemption for DIPE with an exemption value of 1400 µg/L. The maximum detected concentration in the Meuse is 28 µg/L. For DIPE a taste/odour threshold value is established at 10 µg/L (Smit and Wuijts 2012). Fluoride has a deviating ERM target value of 1000 µg/L.

Besides the five compounds mentioned above, two other compounds remain on List 1: benzo(a)pyrene (BAP) and Bis(2-ethylhexyl)phthalate (DEHP). **BAP** is a polycyclic aromatic hydrocarbon and is formed during the incomplete combustion of fossil fuels. BAP is a carcinogenic compound and listed as a priority compound in the European Water policy (Directive 2013/39/EU). BAP has a drinking water standard of 0,01 µg/L. BAP enters the surface water of the Meuse via indirect atmospheric deposition (62%) and direct emission mainly from traffic (37%) (Klein et al. 2013).
DEHP belongs to the group of phthalates and was one of the most widely used plasticizers worldwide (Van Walleghem 2011). Phthalates are mainly used in polyvinyl chloride (PVC) which consist for up to 95% of plasticizers. The overall production of DEHP was estimated to be several million tonnes per year in 1994. After it became known that children could get exposed to phthalates through soft PVC toys, the EU limited the use of

DEHP and other phthalates in toys and childcare articles (Moleveld 2006). In Europe, the use of DEHP is also prohibited in personal care products. Because there is no covalent bond between the phthalates and the plastics in which they are mixed, phthalates can easily leak out of the material and end up in the environment (Heise and Lintz 2004). Phthalates mainly enter the environment through direct emissions into the air and waste water, and through sewage sludge and solid waste (ECB 2008). DEHP is listed as a priority compound in the European Water policy (Directive 2013/39/EU).

Three industrial compounds that were placed on List 2 in 2015 are now included in List 1 based on monitoring data. These concerns the compounds bisphenol A (BPA), melamine and pyrazole.

BPA is used as starting material for the synthesis of plastics, primarily polycarbonates and epoxy resins. These plastics are for example used as protective coating on the inside of food packaging material, in medical devices and bottles for drinking water. In the EU the use of BPA has been banned in baby bottles (Smit and Wuijts 2012). BPA is a hormone disrupting compound that can mimic the mode of action of oestrogen. Its use has become controversial and the cause of debate in the last years. Concentrations of BPA in the Meuse exceed the ERM target value in only 2% of the samples. Emission occurs mainly through the leakage from plastic materials and the compound can enter the surface water via effluent from WWTP or industries.

Melamine is a synthetic substance that is used in the production of plastics, resins, fire-resistant foam and coatings (ECHA registration dossier). The compound has been in production since the 1930s. Melamine plastics are strong, hard, light and resistant to acids and bases. That is why melamine is used for example to make plastic plates and cutlery. Melamine has a flame retardant property and is therefore also used as an additive in flame retardants (HSDB). The user volume of melamine in Europe is between 100 000 and 1 000 000 tonnes per year (ECHA registration dossier). Due to the high production volume and the use of melamine in all kinds of materials, the compound can end up in the environment via different waste streams. In the Meuse melamine concentrations are often above 1 µg/L. The drinking water companies along the Meuse have an exemption to take in melamine in concentrations up to 5 µg/L. Rijkswaterstaat is performing a study in cooperation with partners in Belgium and the water boards to track down the sources of melamine in the Meuse. One source for the Meuse is the melamine factory from OCI Nitrogen which is located at the Chemelot industrial park (RIWA Meuse 2018). Melamine is on the Dutch list of potential substances of very high concern under REACH (RIVM). **Melem** is a practical insoluble transformation product of melamine. Still it was found in concentrations above the 0,1 µg/L and therefore melem is selected as a candidate compound (Sjerps et al. 2018). ALZ is developing an analytical method to monitor the most relevant transformation products of melamine in the Meuse in the near future.

Pyrazole is an industrial compound that is used as an intermediate in the production of various chemicals, including acrylonitrile, pesticides and various pharmaceutical agents (Emke and Beacon 2015). In the summer of 2015 an incident took place with pyrazole in the Maas near Heel. Large quantities of pyrazole were emitted in the Meuse via the industrial effluent coming the WWTP of Sitech Services located at the Chemelot industrial park which also treats the wastewater of AnQore, a company that produces acrylonitrile. Normally pyrazole is largely

removed through microbial degradation in the WWTP of Sitech, but this temporarily did not function well. In 2016 and 2017 the ERM target value was not exceeded in the Meuse at most locations. Exceedances of the ERM target value at Haringvliet are caused by the presence of pyrazole in the river Rhine where it is emitted by the acrylonitrile factory INEOS in Dormagen at Cologne (RIWA Meuse 2018). Since July 2017, pyrazole is included in the Dutch drinking water directive with a drinking water standard of 3 µg/L.

1,4-Dioxane is a new drinking water relevant compound that was not listed before. It was detected in the surface water of the Meuse in concentrations up to 1,1 µg/L. It is an industrial compound with a wide range of applications. It is used as solvent in the paper-, cotton- and textile, in coolants, as a starting material for the synthesis of other substances, as a foaming agent in the polymer industry and in the production of cosmetics and shampoos (RIWA Meuse 2018). Due to its toxicological properties, the industry was obligated to limit the 1,4-dioxane content in shampoos to 10 mg/kg (ARW 2017). The direct use of 1,4-dioxane in personal care products is not permitted because the compound is regarded as a potential carcinogenic compound by WHO (IARC class 2B). The REACH registration dossier shows that there is at least one ethylene oxide factory along the Meuse and that there are also at least two producers located along the Albert Canal (RIWA Meuse 2018). RIVM has determined a health-based GLV of 3 µg/L for 1,4-dioxane.

New candidate compounds which are proposed to be included in the monitoring program of 2019 are ethylsulphate, HMMM, HFPO-DA and methoxymethyltriphenylphosphonium. **Ethylsulphate** is a conjugation product of ethanol and sulphate which is formed by humans after the consumption of alcohol. The compound is also used as an intermediate in the production of ethanol from ethylene. A REACH registration dossier is not yet available for ethyl sulphate. Ethyl sulphate is measured in surface water in concentrations up to 0,53 µg/L (Sjerps et al. 2018). A pGLV could not be established for ethylsulphate and the TTC-value of 0,1 µg/L was used to determine the BQ. As a transformation product of ethanol it could enter the surface water via domestic WWTP effluent, but it is also possible that the compound has some industrial emissions.
HMMM is used as cross-linker in coatings and paints. Related substances (such as hexakis (hydroxymethyl) melamine) are permitted as additives in food packaging products (Van Genderen and Stoks 2004). The compound is moderately toxic when it is orally ingested, but since no information could be found on the chronic toxicity, the TTC value of 0,1 µg/L was used to determine the BQ. HMMM is often detected with screening methods. It has been detected in the surface water of the Rhine and Meuse in concentrations above the ERM target value. It is not known if there is a specific source for this compound causing the presence of this compound in the Meuse.
Methoxymethyltriphenylphosphonium only has a registered use as an intermediate compound. Triphenyl phosphonium compounds are used worldwide by the chemical industry to synthesize alkenes. It is primarily discharged by the chemical industry (Schlüsener et al. 2015). Methoxymethyltriphenylphosphonium has been detected in the river Rhine in concentrations above the ERM target value (Schlüsener et al. 2015).

GenX is a technology for the production coatings, which are used for example as non-stick coating in pans. In the GenX technology the compounds FRD-902, FRD-903 and E1 are used. In water FRD-902 and FRD-903 dissociate

into **HFPO-DA** (RIVM 2016). HFPO-DA was detected in the surface water of the Meuse and in drinking water in South Holland. Because of the harmful properties of the compound (similar to PFOA it is potentially carcinogenic) the presence in drinking water received a lot of media attention in the Netherlands. HFPO-DA has a clear emitting source, namely the company Chemours in Dordrecht in the Netherlands. Chemours has recently reduced the discharge of HFPO-DA by 85% due to a new filter installation with carbon beds that has been used since July 2017[6]. The concentrations in the Meuse are in the low ng/L range, but since the pGLV that is advised by RIVM is only 118 ng/L (Ministry Infrastructure and Water Management 2018), the resulting BQ is still 0,1. RIVM has placed HFPO-DA on the SVHC list. It is recommended to monitor HFPO-DA only at the intake point of Brakel and downstream.

The following compounds have been selected as candidate compound on List 2 because they belong to the REACH compounds that were assessed to be persistent in aquatic environments, mobile and toxic (P_{aq}MT): **1,2,4-triazole** is used as intermediate for the production of other chemicals, e.g. fungicides, but also as additive in fertilizer (Berger et al. 2018). It is one of the REACH compounds that were assessed to be persistent in aquatic environments, mobile and toxic (P_{aq}MT). 1,2,4-Triazole has registrants in Germany and France and has a registered production volume of 1000-10 000 tonnes per year (REACH registration dossier). **2,2,6,6-Tetramethyl-4-oxopiperidinonoxy** is used as intermediate for the production of pharmaceuticals, paper chemicals and petroleum additives (TOXNET). It has a registered production volume of 100-1000 tonnes per year (REACH registration dossier). **4-Aminophenol** is also used as intermediate, for example for the synthesis of paracetamol and in the manufacturing of sulphur- and azo-dyes. The compound acts as a corrosion inhibitor in paints and as an anticorrosion-lubricating agent in engine fuels. 4-Aminophenol has multiple registrants, also in the Netherlands and a registered production volume of 10-100 tonnes per year (REACH registration dossier). The registration dossier also identifies “wide dispersive use”, “industrial use” and “professional use” as intended uses. Therefore, emissions to the environment are expected also for this substance (Berger et al. 2018). **4-Mesyl-2-nitrotoluene** has a registrant in Sweden and is registered with a low production volume of 0-10 tonnes per year and a confidential tonnage data (REACH registration dossier). The compound has an unknown application.
It is not known if analytical techniques are available for these compounds and therefore they have been marked as “compounds to keep in sight”

[6] https://www.rijnmond.nl/nieuws/170664/Koolstofbedden-verminderen-lozing-GenX

3.3 Compiling the candidate list

The surface water of the Meuse can be polluted with anthropogenic compounds via different sources like emissions from wastewater treatment plants, industrial emissions, shipping and agriculture. Via these pathways a broad range of compounds, like pharmaceutical residues, personal care products, pesticides and industrial compounds can reach the surface water (as is also demonstrated in Chapter **3.2**). Because of the amount and the variety of compounds, it is not possible to analyse all compounds that are potentially present in the Meuse. Therefore it is important to select and prioritize the most relevant compounds for the drinking water production. Signalling emerging compounds that form a potential threat to the drinking water production gets a lot of attention in Europe (see e.g. http://www.norman-network.net). Also in the joint research of the Dutch drinking water companies (BTO) projects are performed in which the focus is on the development of strategies for the signalling and prioritization of emerging, relevant compounds (Sjerps et al. 2015a; Ter Laak et al. 2016).

There are different starting points to select potentially relevant compounds. It is for example possible to try to estimate the presence of compounds based on emission data in combination with data on the compound's properties (behaviour and toxicology). On the other hand, it is possible to use monitoring data that gives information on the actual presence of compounds in the water. Additionally to the target analyses that are performed to detect compounds in a quantitative way, the application of chemical suspect and non-target screenings has increased considerably in the last years. These screenings can provide qualitative information on the presence of a broad range of (unknown) compounds in water samples. In literature several studies are available in which results of suspect or non-target screening analysis are presented for different water matrices in Europe (e.g. Bade et al. 2015; Bletsou et al. 2015; Blum et al. 2017; Gago-Ferrero et al. 2015; Gros et al. 2017; Newton et al. 2017; Vergeynst et al. 2014). The lists of compounds that are found in these screenings are very long, and in case of non-target screening also contain many unknown compounds.

For the selection and prioritization of the new candidate drinking water compounds for the Meuse it was not feasible to consider all available information. Therefore, it was decided to focus firstly on compounds for which quantitative monitoring data in surface waters of European rivers is already available, and secondly on compounds that were already prioritized in other relevant projects like the European projects that focus on the prioritization of industrial compounds that pose a hazard for the drinking water production (NGI 2018) and BTO projects which focuses on datamining in screening data (Sjerps et al. 2015b;2016, Berger et al. 2018).

3.3.1 PMT compounds in the REACH database

Because of the implementation of REACH (Registration, Evaluation and Authorization of Chemicals) in Europe, industrial compounds are now registered and, depending on the production volumes, information on the compounds (behaviour and toxicology) has to be provided by industries. The REACH database gives a basis on which compounds could be selected. However, with the amount of compounds that are registered (>15000 in 2017), this is not an easy task (NGI 2018). The governmental environmental agency of Germany, the

Umweltbundesamt (UBA) and the Norwegian geotechnical institute (NGI) have proposed criteria for ranking compounds that could pose a hazard for the drinking water production. Hereby they focused on compounds that were **p**ersistent and **m**obile in the aquatic environment and **t**oxic (PMT) and compounds that are **v**ery **p**ersistent and **v**ery **m**obile (vPvM). Also they assessed and ranked the compounds with respect to their potential for environmental emissions (Berger et al. 2018; NGI 2018). In a first assessment Berger et al. (2018) ranked 167 pre-selected polar compounds. A larger preliminary assessment was performed on 15469 compounds in REACH based on similar criteria for PMT and vPvM (NGI 2018). Both studies were used as input for the selection of candidate drinking water relevant compounds.

From the 167 pre-selected compounds 9 were determined as being PMT for the aquatic environment. Another 125 were identified as suspected PMT compounds, indicating that there is still a considerable data gap for experimental data to confirm if a compound fulfils the PMT criteria. From the 9 confirmed PMT compounds, 4 compounds are not yet included in the monitoring programs of drinking water companies, namely: 1,2,4-triazole; 2,2,6,6-tetramethyl-4-oxopiperidinonoxy; 4-aminophenol; and 4-mesyl-2-nitrotoluene. These compounds were considered as candidate compounds for List 2 and evaluated according to the ranking methodology (ch. **2.1**).

In the second assessment by NGI, 240 compounds were considered to fulfil the PMT and vPvM criteria with sufficient weight-of-evidence. For these compounds it was also indicated if they were detected in drinking water or groundwater based on monitoring data in literature, and a relative emission rank was given (NGI 2018). For the selection of the RIWA candidate relevant drinking water compounds in this study, only those compounds were considered that a) were not yet included in the monitoring programs along the Meuse; b) were indicated with a known presence in drinking water; and c) had a production volume > 1000 tonnes per year. This concerned only 1,2,4-triazole and 1,3-diphenylguanidine. 1,2,4-Triazole was already included for evaluation in this study based on the assessment by Berger et al. (2018).

For the compounds for which a presence in drinking water is not known yet, it is recommended to investigate if there are possible sources of emission for these compounds along the Meuse. This will be done in the “Grip op stoffen” (grip on substances). The outcome of this project will give important information for the next evaluation of the drinking water relevant compounds of the Meuse.

For the PMT compounds it is known that there is an analytical and monitoring data gap because of the analytical challenges to detect and quantify polar (mobile) compounds in water (Berger et al. 2018). Berger et al. (2018) suggest that it would be good to initiate the development of suitable analytical techniques for the monitoring of polar compounds in water.

3.3.2 Screening data

KWR has performed a broad suspect screening study specifically for the Netherlands, in which the presence of more than 5200 preselected anthropogenic chemicals was evaluated in 151 Dutch water samples (effluent, surface water, groundwater and drinking water) (Sjerps et al. 2015a). This resulted in the indication of 1260 candidate compounds. In a follow-up study, 243 compounds were prioritized. A next step was to try to elucidate the identity of these compounds. For 35 compounds the identity could be confirmed (Sjerps et al. 2016; Van Leerdam et al.

2017). All compounds for which target monitoring data was not available for the Meuse were considered for inclusion as candidate compounds in List 2. This concerned the following compounds:

- 1,2-Benzisothiazol-3(2H)-one
- 1,3-Diethyldiphenylurea
- 1,3-Diphenylguanidine
- 4-acetylaminoantipyrine (4-AAA)
- Azelaic acid
- **Gabapentin lactam**
- Irbesartan
- Propyphenazone
- Tris(1-chloro-2-propyl)phosphate (TCPP)
- Triphenylphosphine oxide (TPPO)

4-AAA; irbesartan and propyphenazone were already included on List 2 since 2015. For 4-AAA and irbesartan monitoring data is being collected in 2018, and it is recommended to perform an evaluation when all data is available for 2018. Propyphenazone is not detected in the Meuse in concentrations above 0,01 µg/L and is therefore considered to be no longer relevant (List 3). The other compounds were all evaluated in Van der Velden-Slootweg (2018). The industrial compounds 1,2-benzisothiazol-3(2H)-one; 1,3-diethyldiphenylurea; 1,3-diphenylguanidine; TCPP and TPPO were all not selected as relevant compounds because they were detected in low concentrations in surface water and have a relative low toxicity. The same applies for the pharmaceutical azelaic acid.
Gabapentin-lactam is included as a candidate compound on List 2.

HWL, ALZ and Water-link also routinely perform GC- and LC-screening studies for the drinking water companies along the river Meuse to detect compounds that cannot be monitored with target analyses. With these screening analyses many known and unknown compounds have been detected in the surface water of the Meuse. In 2017 Van Lieverloo et al. carried out a statistical survey of the GC-screening data of Dunea of the period 2010-2015. This survey gives for example insight in the compounds that have been detected most frequently. Still, to select candidate compounds based on the screening results, it would be necessary to evaluate the data more deeply. In 2018 the evaluation of the screening data will be continued for Dunea in a separate project. It is recommended to await the results of this evaluation for the selection of new candidate compounds based on the GC-screening results.
In the LC suspect screening, a number of compounds are regularly found. Vester (2017) has checked for the intake point of Dunea at Brakel which compounds were found in more than 75% of the samples. This concerns mainly pharmaceutical residues. For some of these compounds monitoring data is available for surface waters in Europe. In case the monitoring data indicated that the compounds were present in concentrations above the 0,1 µg/L, they were selected as candidate drinking water relevant compounds. This concerns **fexofenadine; ritalinic acid; sebuthylazine** and **venlafaxine**.

In the LC-screening performed by ALZ in the surface water of the Meuse near Heel and Roosteren the unknown compound LCAqua-057 was regularly detected. Due to the efforts of ALZ and KWR this compound could be identified as 8-hydroxypenillic acid. Based on the measuring results it became clear that the concentrations in the Meuse were in the range of 10-100 µg/L (communication P. van Diepenbeek, WML). 8-Hydroxypenillic acid is a compound that was added during the wastewater treatment process at the WWTP of Sitech Services located at the Chemelot industrial park. Because of the high concentrations of 8-hydropenillic acid in the Meuse Sitech has stopped the use of the compound and the emission has ended. Therefore, 8-hydropenillic acid is not included as a candidate compound on List 2.

3.3.3 Monitoring data

In 2017, Het Waterlaboratorium performed a literature study to compile a list of relevant compounds with regard to the new monitoring strategy of anthropogenic compounds for the drinking water companies Dunea, PWN, and Waternet (Van der Velden-Slootweg 2018). More than 100 recent papers and reports on emerging compounds in water matrices (target monitoring and screenings) were consulted (see **Appendix 8** for an overview). The following compounds were detected in surface waters in concentrations above the 0,1 µg/L and were evaluated as candidate drinking water relevant compound:

- **Cetirizine** RIWA Meuse database
- **Ethylsulphate** Sjerps et al. 2018
- **Hexa(methoxymethyl)melamine** RIWA Rhine 2017
- **Melem (triazine)** Sjerps et al. 2018
- **Methoxymethyltriphenylphosphonium** Schlüsener et al. 2017
- **Oxipurinol** ARW 2017
- **Trifluoromethanesulfonic acid (F3-MSA)** Vughs et al. 2018
- **Trifluoroacetic acid (TFA)** RIWA Rhine 2017
- **Vigabatrin** RIWA Meuse database

In 2017, the “GenX-compounds” received a lot of media attention in the Netherlands. GenX is a technology which is applied by Chemours in Dordrecht to produce fluoropolymers. Compounds that are respectively formed and applied during this process are ammonium, 2,3,3,3,-tetrafluoro-2-(heptafluorpropoxy)-propanoate (FRD-902) and 2,3,3,3,-tetrafluoro-2-(heptafluorpropoxy)propanoic acid (FRD-903). FRD-902 and FRD-903 dissociate in water to the anion **2,3,3,3-tetrafluoro-2-(heptafluorpropoxy)propanoate (HFPO-DA)**. HFPO-DA was detected in several drinking waters in the province of South Holland in the low ng/L range.
HFPO-DA is included in the list of substances that are potentially of very high concern (Chapter **3.3.1**). HFPO-DA does not occur in concentrations above the ERM target value, but since its pGLV is low (118 ng/L), the compound was included in the evaluation as candidate drinking water relevant compound.

3.3.4 Considerations

For the next evaluation of the Lists of (candidate) drinking water compounds, it would be recommended to include or consider the following points:

- Since most drinking water laboratories are now performing screening studies for the Meuse and have developed strategies for the evaluation of the screening data, it would be recommended to revive the meetings to compare and discuss the results from these screening studies. This could then serve as an input for the list of candidate drinking water relevant compounds. Also, the possibility of developing target methods could be discussed.

- One of the barriers for monitoring candidate drinking water relevant compounds is the lack of available analytical methods. This is logically often the case when compounds are selected based on screening data or based on emission data (e.g. NGI 2018). It would be good if the drinking water companies would discuss/agree about a strategy on how to decide if and who will develop an analytical method.

- One of the criteria in the ranking methodology is “public perception”. At the moment only pharmaceutical residues and pesticides are given points because it is assumed that the presence of these kind of compounds in drinking water is perceived more negative than other compounds. However, in the last couple of years it was mostly the presence of industrial compounds that gained a lot of media attention (GenX; melamine; pyrazole), which raises the question if this is still a valid parameter.

4. Conclusions

The RIWA lists of relevant drinking water compounds (List 1) and candidate relevant drinking water compounds (List 2) have been updated based on new monitoring data from the period 2013-2017 and new candidate compounds have been selected based on a literature study. Based on the evaluation, 12 compounds are newly included on List 1.

Industrial compounds	Pharmaceutical residues
1,4-dioxane	gabapentin
bisphenol A	hydrochlorothiazide
melamine + melem	lamotrigin
pyrazole	tramadol
X-ray contrast agent	valsartan and valsartanic acid
ioxitalamic acid	

Four compounds from List 1 are no longer drinking water relevant, namely acetone; ibuprofen, isoproturon and nicosulfuron. Also the bioassay for estrogenic activity, the ER-CALUX, does no longer fulfil the criteria for List 1.

Based on a literature study, it is proposed to add the following 15 new compounds to List 2:

Industrial compounds	Pharmaceutical residues
1,2,4-triazole	cetirizine
2,2,6,6-tetramethyl-4-oxopiperidinonoxy	citalopram
4-aminophenol	fexofenadine
4-mesyl-2-nitrotoluene	oxipurinol
ethylsulphate	ritalinic acid
hexa(methoxymethyl)melamine	vigabatrin
HFPO-DA	**Pesticide**
methoxymethyltriphenylphosphonium	sebuthylazine

Eight compounds from the former List 2 are no longer drinking water relevant, namely amoxicillin; ciprofloxacin; clarithromycin; clindamycin; erythromycin; methenamine; oxadiazon and propyphenazone. Also the bioassay for glucocorticoid activity, the GR-CALUX, does not fulfil the criteria for List 1.

The main sources for pharmaceutical residues, X-ray contrast agents and pesticides on List 1 and 2 are the emissions via effluent of WWTP. Industrial compounds can more often be related to specific industries.

5. Recommendations

It is recommended to use the new lists of 2018 as input for a joint monitoring program of the drinking water companies along the river Meuse. For 2019 the proposal is to monitor the following compounds:

List 1: Drinking water relevant compounds		
Industrial compounds	**Pharmaceutical residues**	**X-ray contrast agents**
1,4-dioxane	Gabapentin + gabapentin lactam	Amidotrizoic acid
Benzo(a)pyrene	Hydrochlorothiazide	Iohexol
Bisphenol A	Lamotrigin	Iomeprol
Bis(2-ethylhexyl)phthalate (DEHP)	Metformin + guanylurea	Iopamidol
Diethylenetriaminepentaacetic acid (DTPA)	Metoprolol	Iopromide
Diisopropylether (DIPE)	Paroxetine	Ioxitalamic acid
Ethylenediaminetetraacetic acid (EDTA)	Sotalol	**Pesticides**
Fluoride	Tramadol	Desphenylchloridazon
Melamine +	Valsartan +	Diethyltoluamide (DEET)
Melem	Valsartanic acid	Glyphosate +
Nitriloacetic acid (NTA)		Aminomethylphosphonic acid AMPA
Pyrazole		N,N-dimethylsulfamid (DMS)
		Terbuthylazine
List 2: Candidate drinking water relevant compounds		
Industrial compounds	**Pharmaceutical residues**	**Pesticides**
Ethylsulphate	Cetirizine	3,5,6-TCP
Hexa(methoxymethyl)melamine	Citalopram	Sebuthylazine
HFPO-DA (GenX)*	Fluconazole	**Hormone disrupting compounds**
Methoxymethyltriphenylphosphonium	Oxipurinol	Anti-AR-Calux
	Telmisartan	
	Venlafaxine +	
	O-Desmethylvenlafaxine	
	Vigabatrin	

For the compounds 1,2,4-triazole; 2,2,6,6-tetramethyl-4-oxopiperidinonoxy; 4-aminophenol; 4-mesyl-2-nitrotoluene; fexofenadine and ritalinic acid it is not known if an analytical method is available. It is recommended to develop an analytical method for these compounds (or check the possibilities of adding these compounds to an existing method). Additionally, it would be good to initiate the development of suitable analytical techniques in general for the monitoring of polar compounds in water in order to bridge the existing analytical data gap that makes it difficult to monitor and prioritize PMT compounds from the REACH database.

A recommendation for the future is that the drinking water companies develop an aligned strategy for the evaluation of screening data for the Meuse. The screening process is qualitative rather than quantitative: substances can be detected, but the exact concentrations cannot be directly known. This makes the list of potential relevant compounds very long and it is difficult to prioritize and select compounds from the screening.

It is recommended to reconsider if “public perception” should be included in the ranking methodology or if all compounds are equally undesirable (also the industrial compounds).

Although industries have to have a discharge permit which allows them to emit compounds into surface waters, it is too often not clear which compounds are emitted. In order to get more grip on these compounds, members of RIWA have initiated several research projects emissions (e.g. “Grip on substances” by Evides/KWR and the evaluation of 70 discharge permits by RWS). It is recommended to use the results of these studies in the next evaluation of drinking water relevant substances in the Meuse.

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7. Appendices

Appendix 1 — Calculation of compound score

The scoring system used was earlier described in (Fischer et al., 2011).

The list of compounds that are relevant to the drinking water function of the River Meuse are proposed to be scored, according to the following principles:

1. The main chemical properties that influence the removal by water treatment; polarity, volatility and removal by powdered activated carbon are ranked:

a) For polarity the log K_{ow} of the compound is used.

b) For volatility the vapor pressure of the compound is used.

c) For biodegradability of the compound the primary biodegradation model (BioWIN3, in EPI Suite 4.1) is used.

2. The toxicological benchmark quotient (BQ) is derived for each compound. BQ is the maximum concentration found in the river (C_{max} water) divided by the (provisional) toxicological drinking water guideline value (pGLV):

$$pGLV = \frac{TDI * m_{adult} * 10\%}{2L/day}$$

Where TDI is the tolerable daily intake in µg (kg body mass)$^{-1}$ day^{-1}, and m_{adult} is the average adult body mass in kg. For the calculations a m_{adult} of 70 kg is assumed.

Table 1. *Point attribution for polarity, volatility, biodegradability, and toxicity.*

Polarity		**Volatility** Vapor pressure		**Biodegradability**		**Toxicity**	
Log K_{ow}	Score	(mm Hg)	Score	BioWIN3	Score	BQ	Score
>6	0	>52,5	0	>4,75 – 5	0	<0,01	0
>3 - 6	1	>35 – 52,5	1	>3,25 – 4,75	1	0,01 – 0,1	6
0 – 3	2	17,5 – 35	2	2,25 – 3,25	2	>0,1 – 1	12
<0	3	<17,5	3	<2,25	3	>1	18

3. If the odor/taste threshold is breached by C_{max} water, 3 points are awarded.

4. If the compound belongs to one of the following categories: pharmaceutical, pesticide, hormone, or hormone disruptor, or is a metabolite of a compound from one of these categories, it is considered harmful to the public perception of the drinking water consumers and 3 points are awarded.

Appendix 2 — Background information on compounds List 1

Table 2a. Information on the drinking water relevant compounds (List 1). Information is given on the ERM value used for the compound, the Dutch drinking water standard if available, the exemption value given in the exemptions, the number of monitoring stations were the compound was monitored, the total number of measurements in the period 2013-2017, the number and percentage of measurements above the ERM, an indication if a REACH dossier is available for the compound and the place where it was during the last evaluation in 2015.

Compound name	CAS	ERM (µg/L)	Dutch DW norm (µg/L)	Exemption value (µg/L)	# monitoring stations	# measurements	# measurements > ERM	% > ERM	REACH file available	Former list 2015	Remark
melamine	108-78-1	1		5	4	122	94	77%	x	2	Monitoring data available for < 5 years
1,4-dioxane	123-91-1	0,1		3	5	425	174	41%	x	New	
amidotrizoic acid	117-96-4	0,1			6	350	36	10%	x	1	
benzo(a)pyrene	50-32-8	0,01	0,01		9	575	41	7%		1	
bisphenol A	80-05-7	0,1			7	219	5	2%	x	2	
desphenylchloridazon	6339-19-1	0,1	1		7	396	310	78%		1	
DEHP	117-81-7	0,1			6	328	4	1%		1	< 7% above LOQ, but LOQ > ERM
DTPA	67-43-6	1			8	317	12	4%	x	1	< 7% above LOQ, but LOQ > ERM
DEET	134-62-3	0,1	0,1		8	468	5	1%		1	
DIPE	108-20-3	1		1400	8	716	153	21%	x	1	
EDTA	60-00-4	1		50	8	317	251	79%	x	1	
fluoride	16984-48-8	1000			8	893	13	1%		1	political reasons, score for removal not possible
gabapentin	60142-96-3	0,1			2	52	43	83%		2	Monitoring data available for < 5 years
glyphosate	1071-83-6	0,1	0,1	0,3	9	620	112	18%		1	
AMPA	1066-51-9	0,1	1	3	9	620	568	92%		1	
hydrochlorothiazide	58-93-5	0,1			4	200	12	6%		New	
isoproturon	34123-59-6	0,1	0,1		9	879	13	1%		1	
iohexol	66108-95-0	0,1			6	347	56	16%	x	1	
iomeprol	78649-41-9	0,1			6	351	297	85%		1	
iopamidol	60166-93-0	0,1			6	349	88	25%		1	
iopromide	73334-07-3	0,1			6	385	247	64%		1	
ioxitalamic acid	28179-44-4	0,1			4	231	36	16%	x	New	
lamotrigin	84057-84-1	0,1			2	50	4	8%		2	Monitoring data available for < 5 years
metformin	657-24-9	0,1		196	6	326	313	96%		1	
guanylurea	141-83-3	0,1		20	6	188	184	98%		1	
melamine	108-78-1	1		5	4	122	94	77%	x	2	Monitoring data available for < 5 years
melem	1502-47-2	0,1			0	0	0	0%		New	
metoprolol	37350-58-6	0,1			7	378	10	3%		1	
DMS	3984-14-3	0,1	1		7	238	55	23%		1	
NTA	139-13-9	1			8	317	9	3%	x	1	< 7% above LOQ, but LOQ > ERM
paroxetine	61869-08-7	0,1			6	122	4	3%		1	
pyrazole	288-13-1	1	3		6	372	102	27%	x	2	Monitoring data available for < 5 years
sotalol	3930-20-9	0,1			7	360	8	2%		1	
terbuthylazine	5915-41-3	0,1	0,1		9	730	8	1%		1	
tramadol	27203-92-5	0,1			7	156	17	11%	x	2	Monitoring data available for < 5 years
valsartan	137862-53-4	0,1			4	100	18	18%	x	2	Monitoring data available for < 5 years
valsartanic acid	164265-78-5	0,1			0	0	-	-	x	New	List 2, but coupled to valsartan

Table 2b. Information on the parameters that determine the total score for the drinking water relevant compounds (List 1).

Compound name	Total score	Max (µg/L)	(p)GLV (µg/L)	BQ	BQ Score	Log K_{ow}		VP (mm Hg)		BIOWIN3 score		Exceedance taste/odor threshold	Public perception	Reference (p)GLV
1,4-dioxane	18	1,1	3	3,7E-01	12	**-0,42**	3	3,81E+01	1	2,99	2	0	0	RIVM (exemption)
amidotrizoic acid	11	0,2	250000	9,6E-07	0	1,37	2	3,57E-15	3	1,69	3	0	3	Leerdam et al (2018)
benzo(a)pyrene	18	0,09	0,7	1,2E-01	12	6,13	0	5,49E-09	3	1,84	3	0	0	WHO (2011)
bisphenol A	18	3,1	14	2,2E-01	12	**3,40**	1	**3,10E-09**	3	2,60	2	0	0	Smit en Wuijts (2012)
desphenylchloridazon	11	2,4	700	3,4E-03	0	-1,59	3	4,23E-06	3	2,73	2	0	3	BTO2015.056
DEHP	17	3,1	8	3,8E-01	12	7,60	0	1,42E-07	3	3,21	2	0	0	WHO (2011)
DTPA	13	18,1	350	5,2E-02	6	-4,91	3	1,21E-16	3	3,39	1	0	0	Schriks et al (2010)
DEET	10	0,4	6250	7,0E-05	0	2,18	2	2,00E-03	3	2,65	2	0	3	Schriks et al (2010)
DIPE	13	28,1	1400	2,0E-02	6	**2,40**	2	1,49E+02	0	2,96	2	3*	0	RIVM (exemption)
EDTA	12	48,0	600	8,0E-02	6	**0,13**	2	1,50E-12	3	3,50	1	0	0	RIVM (exemption)
fluoride	0	1,3	1500	8,7E-04	0	-	-	-	-	-	-	0	0	WHO (2011)
gabapentin	11	0,7	100	7,0E-03	0	**-1,10**	3	2,94E-10	3	3,00	2	0	3	Leerdam et al (2018)
glyphosate	11	1,1	1500	7,3E-04	0	-3,40	3	1,58E-08	3	3,21	2	0	3	RIVM (exemption)
AMPA	11	7,9	1500	5,3E-03	0	-4,00	3	5,76E-05	3	2,98	2	0	3	RIVM (exemption)
hydrochlorothiazide	12	0,3	87,5	3,4E-03	0	-0,07	3	1,78E-10	3	2,2	3	0	3	Based on ADI in Khan and Nicell (2015)
iohexol	12	0,2	375000	6,4E-07	0	**-0,50**	3	4,06E-29	3	2,05	3	0	3	Leerdam et al (2018)
iomeprol	12	0,7	1000000	7,1E-07	0	-2,79	3	3,04E-29	3	1,98	3	0	3	Leerdam et al (2018)
iopamidol	12	0,3	415000	8,0E-07	0	-2,79	3	1,33E-30	3	1,98	3	0	3	Leerdam et al (2018)
iopromide	12	0,7	250000	2,8E-06	0	-2,05	3	1,59E-28	3	1,78	3	0	3	Versteegh et al (2007)
ioxitalamic acid	11	0,2	500000	3,8E-07	0	0,50	2	2,85E-20	3	1,78	3	0	3	Leerdam et al (2018)
lamotrigin	23	0,1	0,53	2,4E-01	12	**2,57**	2	9,41E-09	3	1,95	3	0	3	Based on ADI in Khan and Nicell (2015)
melamine	20	6,6	50	1,3E-01	12	**-1,22**	3	**8,93E-08**	3	2,27	2	0	0	RIVM (exemption)
melem	27	0,17	0,10	1,7	18	-1,22	3	1,09E-08	3	2,06	3	0	0	TTC
metformin	17	2,8	196	1,4E-02	6	-2,64	3	7,58E-05	3	2,91	2	0	3	RIVM (exemption)
guanylurea	23	3,5	20	1,8E-01	12	-1,22	3	8,68E-04	3	2,97	2	0	3	RIVM (exemption)
metoprolol	16	0,2	9,8	2,0E-02	6	1,88	2	2,88E-07	3	2,65	2	0	3	Leerdam et al (2018)
DMS	11	0,5	700	6,6E-04	0	**-0,80**	3	**1,35E-06**	3	2,92	2	0	3	Based on ADI in ECHA (2016)
NTA	13	8,0	200	4,0E-02	6	**-3,81**	3	7,16E-09	3	3,62	1	0	0	WHO (2011)
paroxetine	22	0,5	5	1,0E-01	12	3,95	1	4,79E-08	3	1,89	3	0	3	Leerdam et al (2018)
pyrazole	26	7,4	3	2,5E+00	18	**0,33**	2	**1,58E-01**	3	2,11	3	0	0	RIVM (exemption)
sotalol	10	0,2	80	2,4E-03	0	0,24	2	1,34E-09	3	2,78	2	0	3	Leerdam et al (2018)
terbuthylazine	16	0,5	7	6,9E-02	6	3,21	1	1,12E-06	3	1,76	3	0	3	WHO (2011)
tramadol	17	0,2	4,9	4,8E-02	6	**2,51**	2	4,57E-07	3	2,09	3	0	3	Based on ADI in Khan and Nicell (2015)
valsartan	28	0,9	0,20	4,5E+00	18	**1,20**	2	8,18E-16	3	2,85	2	0	3	Based on ADI in Khan and Nicell (2015)
valsartanic acid	28	*0,15**	0,10	1,5E+00	18	**1,83**	2	8,51E-11	3	2,70	2	0	3	TTC-value

Max = maximum concentration in the Meuse in 2013-2017; (p)GLV=provisional guideline value; BQ = benchmark quotiënt; VP= vapor pressure; TTC = threshold of toxicological concern
Log Kow and VP values in bold are experimental values, otherwise they are estimated. Values are black are from the EPI Suite database, values in blue from the REACH dossier. For DMS experimental values are taken from EFSA (2016). DIPE is the only compound with an exceedance of its odor threshold of <10 µg/L (Smit and Wuijts 2012)

Appendix 3 — Background information on new compounds List 2

Table 3a. Information on the candidate drinking water relevant compounds (List 2). Source refers to either literature, monitoring data or screening data from where the candidate compound was selected.

Compound name	CAS	Source	REACH file available	Remark
1,2,4-triazole	288-88-0	NGI (2018)	x	
2,2,6,6-tetramethyl-4-oxopiperidinonoxy	2896-70-0	NGI (2018)	x	
3,5,6-Trichloro-2-pyridinol (TCP)	6515-38-4	Current list 2 compound		Metabolite of chlorpyrifos and triclopyr
4-aminophenol	123-30-8	NGI (2018)	x	
4-mesyl-2-nitrotoluene	1671-49-4	NGI (2018)	x	
anti-AR-Calux	not applicable	Monitoring data		
cetirizine	83881-51-0	Monitoring data		Now only measured in NAM en LUI, several times > 0,1 µg/L
citalopram	59729-33-8	Current list 2 compound		
ethylsulphate	540-82-9	BTO report 2018.023		Metabolite of ethanol
fexofenadine	83799-24-0	Screening	x	
fluconazole	86386-73-4	Current list 2 compound		
hexa(methoxymethyl)melamine	68002-20-0	Monitoring data	x	
HFPO-DA (GenX)*	62037-80-3	Report antropogenic compounds		Clear emitting source
methoxymethyltriphenylphosphonium	4009-98-7	Schlüsener et al. 2015		
O-desmethylvenlafaxine	93413-62-8	Current list 2 compound		
oxipurinol	2465-59-0	Monitoring data		
ritalinic acid	19395-41-6	Screening		Metabolite of methylphenidate
sebuthylazine	7286-69-3	Screening		Pesticide, but not registered in NL
telmisartan	144701-48-4	Current list 2 compound		
venlafaxine	93413-69-5	Current list 2 compound		
vigabatrin	60643-86-9	Monitoring data	x	Now only measured in HAV/STEL and KEI, detected above LOQ (0,5 µg/L)

Table 3b. Information on the parameters that determine the total score for the candidate drinking water relevant compounds (List 2).

Compound name	Total score	Max (µg/L)	(p)GLV (µg/L)	BQ	BQ Score	Log K_{ow}		VP (mm Hg)		BIOWIN3 score		Exceedance taste/odor threshold	Public perception	Reference (p)GLV
1,2,4-triazole	**>8**	?	280	?	?	**-0,58**	3	6,27E-02	3	3,05	2	0	0	Based on DNEL in REACH file
2,2,6,6-tetramethyl-4-oxopiperidinonoxy	**>7**	?	10500	?	?	**0,28**	2	3,71E-06	3	2,37	2	0	0	Based on NOAEL in REACH file
3,5,6-TCP	**>10**	?	0,35	?	?	**3,21**	1	1,03E-03	3	1,98	3	0	3	WHO 2011; EFSA 2014*[1]
4-aminophenol	**>8**	?	70	?	?	**-0,09**	3	3,27E-05	3	2,88	2	0	0	Based on NOAEL in REACH file
4-mesyl-2-nitrotoluene	**>7**	?	263	?	?	**0,93**	2	1,64-05	3	2,48	2	0	0	Based on DNEL in REACH file
anti-AR-Calux	**NA**	220	?	?	?	**-**	-	-	-	-	-	0	3	Guideline value will be established in 2018 by KWR
cetirizine	**29**	0,24	0,25	1,0	18	**1,7**	2	2,98-11	3	2,00	3	0	3	Based on ADI in Khan en Nicell (2015)
citalopram	**>10**	?	0,05	?	?	3,74	1	1,13E-07	3	1,52	3	0	3	Based on ADI in Khan en Nicell (2015)
ethylsulphate	**26**	0,53	0,10	5,3	18	-2,49	3	1,37E-03	3	2,92	2	0	0	TTC
fexofenadine	**>11**	?	60	?	?	2,81	2	9,51E-19	3	1,98	3	0	3	DDD of 1200 mg/day and UF=100 (www.whocc.no)
fluconazole	**>11**	?	1,02	?	?	**0,50**	2	6,78E-09	3	1,50	3	0	3	Based on ADI in Khan en Nicell (2015)
hexa(methoxymethyl)melamine	**27**	0,11	0,10	1,1	18	-0,66	3	2,17E-06	3	2,21	3	0	0	TTC, no tox data in REACH file
HFPO-DA (GenX)	**22**	0,012	0,12	0,10	12	3,36	1	6,30E-11	3	1,17	3	0	3	RIVM (2018)
methoxymethyltriphenyl-phosphonium	**26**	0,56	0,10	5,6	18	**-1,17**	3	1,24E-07	3	2,50	2	0	0	TTC
O-desmethylvenlafaxine	**>11**	?	0,95	?	?	2,72	2	6,85E-08	3	2,13	3	0	3	Based on ADI in Khan en Nicell (2015)
oxipurinol	**20**	0,60	4,90	0,12	12	-0,28	3	9,91E-08	3	2,98	2	0	0	Based on ADI in Khan en Nicell (2015)
ritalinic acid	**>11**	?	0,13	?	?	-1,07	3	6,23E-10	3	3,05	2	0	3	DDD of 2 g/day and UF=100 (www.farmacotherapeutischkompas.nl)
sebuthylazine	**>11**	?	0,10	?	?	2,61	2	5,10E-05	3	1,97	3	0	3	TTC
telmisartan	**>9**	?	20,00	?	?	8,42	0	9,33E-20	3	2,00	3	0	3	DDD of 40 mg/day and UF=100 (www.whocc.no)
venlafaxine	**>10**	?	0,95	?	?	**3,2**	1	2,46E-07	3	1.99	3	0	3	Based on ADI in Khan en Nicell (2015)
vigabatrin	**10**	1,00	500	0,002	0	**-2,16**	3	6,09E-09	3	3,30	1	0	3	Based on the therapeutic dose for children with an UF of 100 (www.farmacotherapeutischkompas.nl)

Max = maximum concentration in the Meuse; (p)GLV=provisional guideline value; BQ = benchmark quotiënt; VP= vapor pressure; TTC = threshold of toxicological concern
Log Kow and VP values in bold are experimental values, otherwise they are estimated. Values are black are from the EPI Suite database, values in blue from the REACH dossier.
**[1] WHO gives a GLV of 30 µg/L for chlorpyrifos, but this is based on an ADI of 0,01 mg/kg/day, which was adjusted by EFSA in 2014 to 0,001 mg/kg/day. TCP is less toxic than chlorpyrifos, to be safe the pGLV of the mother compound is used*

Appendix 4 — Considered candidate compounds with a score below 10

Table 4. Information on the parameters that determine the total score for the candidate drinking water relevant compounds.

Compound name	Total score	Max (µg/L) *[1]	(p)GLV (µg/L)	BQ	BQ Score	Log K_{ow}		VP (mm Hg)		BIOWIN3 score		Exceedance taste/odor threshold	Public perception	Reference (p)GLV
1,2-Benzisothiazol-3(2H)-one	**7**	?	210	<0,01	0	**0,7**	2	**4,72E-07**	3	2,87	2	0	0	Ctgb
1,3-Diethyldiphenylurea	**6**	-	0,18	<0,01	0	4,2	1	6,45E-06	3	2,65	2	0	0	Based on NOAEL in REACH file
1,3-Diphenylguanidine	**7**	0,24	298	8E-04	0	**2,42**	2	3,97E-06	3	2,51	2	0	0	Based on DNEL in REACH file
Azelaic acid	**9**	0,03	8750	3E-06	0	**1,57**	2	2,29E-05	3	3,51	1	0	3	Based on DNEL in REACH file
F3-MSA	**7**	>0,1	11900	8E-06	0	**0,3**	2	5,45E-01	3	2,55	2	0	0	Vughs et al. 2018
TCA	**7**	0,3	200	2E-03	0	**1,33**	2	**6,00E-02**	3	2,47	2	0	0	WHO (2011)
TCPP	**8**	?	1820	<0,01	0	2,59	2	5,64E-05	3	2,11	3	0	0	Based on DNEL in REACH file
TFA	**5**	2,5	35	7E-02	0	-0,5	3	1,16E+02	0	2,80	2	0	0	RIVM (exemption)
TPPO	**7**	0,12	28	4E-03	0	**2,83**	2	2,82E-07	3	2,65	2	0	0	Schriks et al. 2010

Max = maximum concentration in surface water in the Netherlands in literature or from monitoring data in case of TCA and TFA; (p)GLV=provisional guideline value; BQ = benchmark quotiënt; VP= vapor pressure; TTC = threshold of toxicological concern. Log Kow and VP values in bold are experimental values, otherwise they are estimated. Values are black are from the EPI Suite database, values in blue from the REACH dossier.

Appendix 5 — Candidate compounds to keep in sight

Table 5. Candidate relevant compounds for which an analytical technique is not available yet. "Screening" indicates that the compounds can be monitored with analytical screening techniques og HWL, ALZ and/or Water-link

#	Compound	CAS number	Application	Monitoring
Industrial compounds				
1	1,2,4-Triazole	288-88-0	Industrial compound	
2	2,2,6,6-Tetramethyl-4-oxopiperidinonoxy	2896-70-0	Industrial compound	
3	4-Aminophenol	123-30-8	Industrial compound	
4	4-Mesyl-2-nitrotoluene	1671-49-4	Industrial compound	
5	4,4-Sulfonyldifenol	80-09-1	Industrial compound	Screening
6	Capric acid	334-48-5	Industrial compound	Screening
7	Propiophenone	93-55-0	Industrial compound	Screening
8	Dichloroaniline	-	Industrial compound	Screening
9	Dichlorobenzene	-	Industrial compound	Screening
10	Tetra-acetyl-ethylene-diamine (TAED)	1054305-70-4	Industrial compound	Screening
11	Tri-phenyl-phosphine oxide (TPPO)	791-28-6	Industrial compound	Screening
12	Tetramethylbutanedinitrile	3333-52-6	Industrial compound	Screening
13	Tributylamine	102-82-9	Industrial compound	Screening
14	3'-(Trifluoromethyl)acetophenone	349-76-8	Industrial compound	Screening
Pesticides/biocides				
15	Dettol (chloroxylenol)	88-04-0	Biocide	Screening
16	Sebuthylazine	7286-69-3	Pesticide	
Veterinary pharmaceuticals				
17	Ivermectin	70288-86-7	Veterinary parasiticide	
Pharmaceuticals				
18	3,4-Dimethoxyphenethylamine	120-20-7	Neurotransmitter	Screening
19	3,4-Methylenedioxyethylamphetamine	82801-81-8	Amphetamine	Screening
20	Butetamate	14007-64-8	Bronchodilator	Screening
21	Celiprolol	57470-78-7	Beta-blocker	Screening
22	Certomycin	56391-57-2	Antibiotic	
23	Cetobemidone	5965-49-1	Analgesic	Screening
24	Ciclacilline	3485-14-1	Antibiotic	
25	Cimetidine	51481-61-9	H_2-receptor antagonist	
26	Codein	76-57-3	Analgesic	
27	Cyclopentamine	102-45-4	Decongestant	Screening
28	Eprosartan	133040-01-4	Antihypertensive	Screening
29	Etilefrine	709-55-7	Antihypotensive	Screening
30	Fexofenadine	83799-24-0	Antihistamine	
31	Flecainide	54143-55-4	Antiarrhythmic agent	Screening
32	Meperidine/pethidine	57-42-1	Analgesic	Screening
33	Mirtazapine	61337-67-5	Antidepressant	
34	N-methyl-1-(1,3-benzodioxol-5-yl)-2-aminobutane	103818-46-8	Amphetamine	Screening
35	Nortramadol (metabolite tramadol)	80456-81-1	Analgesic	
36	Oxilofrine	365-26-4	Antihypotensive	Screening
37	Ritalic acid	19395-41-6	Stimulant	
38	Sulpiride	15676-16-1	Anti-psychotic	Screening
39	Thymopentin	177966-81-3	Immunostimulant	Screening
Unknown application				
40	1,2,3-Propanetriol, 1-nitrate	?	?	Screening
41	1,2-Ethanediol, dinitrate	?	?	Screening
42	3-Hexanone-2.5-dimethyl-4-nitro	?	?	Screening
43	5-Methyl-1-hexeen	?	?	Screening
44	Cyclotetradecane	?	?	Screening

Appendix 6 — List of no longer drinking water relevant compounds

Table 6. Complete list of no longer drinking water relevant compounds (including the compounds from Van der Hoek et al. 2015)

Compound	CAS	Compound	CAS
1,2-Benzisothiazol-3(2H)-one	2634-33-5	Lincomycin	154-21-2
1,3-Diethyldiphenylurea	85-98-3	MCPA (4-chloro-2-methylphenoxyacetic acid)	94-74-6
1,3-Diphenylguanidine	102-06-7	Mecoprop (MCPP)	93-65-2
2,4-D (2,4-dichlorophenoxyacetic Acid)	94-75-7	Metazachlor	67129-08-2
4-n-Nonyl phenol	104-40-5	Methenamine/urotropine/hexamine	100-97-0
Acesulfame-K	55589-62-3	Methyl-desfenylchloridazon	17254-80-7
Acetone	67-64-1	Metolachlor	51218-45-2
AHTN (6-acetyl-1,1,2,4,4,7-hexamethyltetraline)	1506-02-01	MTBE (methyl-tert-butylether)	1634-04-04
Amoxicillin	26787-78-0	Musk (ketone)	81-14-1
Aspirin (acetylsalicylic acid)	50-78-2	Musk (xylene)	81-15-2
Azelaic acid	123-99-9	Naproxen	22204-53-1
BAM (2,6-dichlorobenzamide)	2008-58-4	N-butylbenzenesulphonamide	3622-84-2
Barbital	57-44-3	NDMA (nitrosodimethylamine)	62-75-9
BBP (butylbenzylphtalate)	85-68-7	Nicosulfuron	111991-09-4
Benzotriazole	95-14-7	Oxadiazon	19666-30-9
BPS (4,4'-sulfonyldiphenol)	80-09-1	Pentobarbital	76-74-4
Caffeine	58-08-2	PFBA (perfluorobutanoic acid)	375-22-4
Carbamazepine	298-46-4	PFBS (perfluorobutane sulfonate)	29420-49-3
Carbendazim	10605-21-7	PFHxS (perfluorohexane sulfonate)	432-50-7
Chloridazon	1698-60-8	PFOA (perfluorooctanoic acid)	335-67-1
Chlorotoluron	15545-48-9	PFOS (perfluorooctanoic sulfonate)	1763-23-1
Ciprofloxacin	85721-33-1	Phenanthrene	85-01-8
Clarithromycin	81103-11-9	Phenazone	60-80-0
Clindamycin	18323-44-9	Phenobarbital	50-06-6
DBP (dibutyl phthalate)	84-74-2	Salicylic Acid	69-72-7
DEP (diethyl phthalate)	84-66-2	Sucralose	56038-13-2
DIBP (di-(2-methyl-propyl)phthalate)	84-69-5	Sulfamethoxazole	723-46-6
Diclofenac	15307-86-5	Surfynol 104	126-86-3
Diglyme (bis(2-methoxyethyl)ether)	111-96-6	TBP (tributylphosphate)	126-73-8
Dimethenamid	87674-68-8	TCEP (tris(2-chloroethyl) phosphate)	115-96-8
Diuron (DMCU)	330-54-1	TCPP (tri-(2-chloroisopropyl) phosphate)	13674-84-5
DMSA (N,N-dimethylaminosulfanilide)	4710-17-2	Tolyltriazole (5-methyl-1-H-benzotriazole)	29385-43-1
ER-CALUX	not applicable	Triamcinolonehexacetonide	5611-51-8
Erythromycin	114-07-8	Trichloroacetic acid (TCA)	76-03-9
Estrone	53-16-7	Trifluoroacetic acid (TFA)	76-05-1
ETBE (ethyl-tertiairy-butyl-ether)	637-92-3	Trifluoroacetic acid (TFA)	76-05-1
Galaxolide (HHCB)	1222-05-5	Trifluoromethanesulfonic acid (F3-MSA)	1493-13-6
GR-CALUX	not applicable	Trifluoromethanesulfonic acid (F3-MSA)	1493-13-6
Ibuprofen	15687-27-1	Triphenylphosphine oxide (TPPO)	791-28-6
Ioxaglic acid	59017-64-0	Tris(1-chloro-2-propyl)phosphate (TCPP)	13674-84-5
Isoproturon	34123-59-6	Vinylchloride	75-01-4

Appendix 7 — Available analytical techniques for compounds List 2

Table 7. Complete list of no longer drinking water relevant compounds (including the compounds from Van der Hoek et al. 2015)

Compound name	CAS-number	Vivaqua	Water-link	ALZ	HWL	KWR	Remark
1,2,4-Triazole	288-88-0						
2,2,6,6-Tetramethyl-4-oxopiperidinonoxy	2896-70-0						
3,5,6-Trichloro-2-pyridinol (TCP)	6515-38-4						TZW
4-AAA (metabolite metamizol)	83-15-8						
4-Aminophenol	123-30-8						
4-FAA (metabolite metamizol)	1672-58-8						
4-Mesyl-2-nitrotoluene	1671-49-4						
anti-AR-CALUX	-						
Aniline	62-53-3						
Benzylalcohol	100-51-6						
Cetirizine	83881-51-0						
Citalopram	59729-33-8						
Ethylsulphate	540-82-9						
Fexofenadine	83799-24-0						
Fluconazole	86386-73-4						TZW
Hexa(methoxymethyl)melamine	68002-20-0						
HFPO-DA	62037-80-3						IVM/RIKILT
Irbesartan	138402-11-6						
Metazachlor ethane sulfonic acid	172960-62-2						
Metazachlor oxalic acid	1231244-60-2						
Methoxymethyltriphenylphosphonium	4009-98-7						BfG
Metolachlor ethane sulfonic acid	171118-09-5						
O-desmethylvenlafaxine	*93413-62-8*						*Not separable from tramadol*
Oxipurinol	2465-59-0						
Ritalinic acid	19395-41-6						
Sebuthylazine	7286-69-3						
Telmisartan	144701-48-4						
Tert-butyl alcohol (metabolite MTBE)	75-65-0						
Venlafaxine	93413-69-5						
Vigabatrin	60643-86-9						
Quantitative analytical technique available							
Screening method available							

Appendix 8 — Literature list

Table 8a. List of articles on emerging compounds

Auteur	Year	Title	Link
Adamson et al.	2017	1,4-Dioxane drinking water occurrence data from the third unregulated contaminant monitoring rule	http://www.sciencedirect.com/science/article/pii/S0048969717309221
Altenburger et al.	2015	Future water quality monitoring — Adapting tools to deal with mixtures of pollutants in water resource management	http://www.sciencedirect.com/science/article/pii/S0048969714017598
Aparico et al.	2017	Stir bar sorptive extraction and liquid chromatography-tandem mass spectrometry determination of polar and non-polar emerging and priority pollutants in environmental waters	https://www.ncbi.nlm.nih.gov/pubmed/28416215
Bade et al.	2015	Suspect screening of large numbers of emerging contaminants in environmental waters using artificial neural networks for chromatographic retention time prediction and high resolution mass spectrometry data analysis.	https://www.ncbi.nlm.nih.gov/pubmed/26363605
Bader et al.	2016	Application of Non-Target Analysis with LC-HRMS for the Monitoring of Raw and Potable Water: Strategy and Results	http://pubs.acs.org/doi/pdf/10.1021/bk-2016-1242.ch003
Baz Lomba et al.	2016	Comparison of pharmaceutical, illicit drug, wastewater with sale, seizure and consumption data for 8 European cities	https://www.ncbi.nlm.nih.gov/pubmed/27716139
Benson et al.	2017	Human health screening and public health significance of contaminants of emerging concern detected in public water supplies.	https://www.ncbi.nlm.nih.gov/pubmed/28040195
Bertelkamp et al.	2016	Verwijdering van Pyrazool in drinkwaterzuiveringsprocessen	https://www.h2owaternetwerk.nl/vakartikelen/548-verwijdering-van-pyrazool-in-drinkwaterzuiveringsprocessen
Bieber et al.	2016	Polarity-extended chromatographic separations: a novel view on trace organic compounds in environmental samples	http://pubs.acs.org/doi/abs/10.1021/bk-2016-1241.ch007
Bletsou et al.	2015	Targeted and non-targeted liquid chromatography-mass spectrometric workflows for identification of transformation products of emerging pollutants in the aquatic environment	http://www.sciencedirect.com/science/article/pii/S0165993615000035
Blum et al.	2017	Non-target screening and prioritization of potentially persistent, bioaccumulating and toxic domestic wastewater contaminants and their removal in on-site and large-scale sewage treatment plants	http://www.sciencedirect.com/science/article/pii/S0048969716320654
Boix et al.	2016	Biotransformation of pharmaceuticals in surface water and during waste water treatment: Identification and occurrence of transformation products	http://dx.doi.org/10.1016/j.jhazmat.2015.09.053
Bopp et al.	2015	Approaches, experiences and future directions in assessing human and environmental health	http://dx.doi.org/10.1016/j.toxlet.2015.08.988
Brack et al.	2017	Towards the review of the European Union Water Framework management of chemical contamination in European surface water resources	http://dx.doi.org/10.1016/j.scitotenv.2016.10.104
Busch et al.	2016	Micropollutants in European rivers: A mode of action survey to support the development of effect-based tools for water monitoring.	https://www.ncbi.nlm.nih.gov/pubmed/27299692
Causanilles et al.	2017	Occurrence and fate of illicit drugs and pharmaceuticals in wastewater	http://dx.doi.org/10.1016/j.scitotenv.2017.04.202

Auteur	Year	Title	Link
Chibwe et al.	2017	Integrated Framework for Identifying Toxic Transformation Products in Complex Environmental Mixtures	http://pubs.acs.org/doi/abs/10.1021/acs.estlett.6b00455
Daughton	2016	Pharmaceuticals and the Environment (PiE): Evolution and impact of the published literature revealed by bibliometric analysis	http://www.sciencedirect.com/science/article/pii/S0048969716305320
Dimzon et al.	2017	Sampling and simultaneous determination of volatile per- and polyfluoroalkyl substances in wastewater treatment plant air and water	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5258797/
Du et al.	2014	Comparison of contaminants of emerging concern removal, discharge, and water quality hazards among centralized and on-site wastewater treatment system effluents receiving common wastewater influent	http://www.sciencedirect.com/science/article/pii/S0048969713009108
Escher et al.	2013	Benchmarking Organic Micropollutants in Wastewater, Recycled Water and Drinking Water with In Vitro Bioassays	https://www.ncbi.nlm.nih.gov/pubmed/24369993
Fischer et al.	2015	Beslissingsondersteuning: Wat te doen met milieuvreemde stoffen in water?	http://edepot.wur.nl/364866
Fischer et al.	2017	Decision support for water quality management of contaminants of emerging concern	http://dx.doi.org/10.1016/j.jenvman.2017.02.002
Furlong et al.	2017	Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States: Pharmaceuticals.	https://www.ncbi.nlm.nih.gov/pubmed/28040194
Gago-Ferrero et al.	2015	Extended Suspect and Non-Target Strategies to Characterize Emerging Polar Organic Contaminants in Raw Wastewater with LC-HRMS/MS	http://pubs.acs.org/doi/abs/10.1021/acs.est.5b03454
Gago-Ferrero et al.	2016	Chapter 13 - Nontarget Analysis of Environmental Samples Based on Liquid Chromatography Coupled to High Resolution Mass Spectrometry (LC-HRMS)	http://www.sciencedirect.com/science/article/pii/S0166526X16300125
Glassmeyer et al.	2017	Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States	http://www.sciencedirect.com/science/article/pii/S0048969716326894
Gros et al.	2017	Screening and prioritization of micropollutants in wastewaters from on-site sewage treatment facilities	http://www.sciencedirect.com/science/article/pii/S0304389416311967
Han en Lee	2017	Significance of metabolites in the environmental risk assessment of pharmaceuticals consumed by human.	https://www.ncbi.nlm.nih.gov/pubmed/28318699
Hannemann et al.	2016	HRMS Approaches for Evaluating Transformations of Pharmaceuticals in the Aquatic Environment	http://pubs.acs.org/doi/abs/10.1021/bk-2016-1241.ch003
Hopkins en Blaney	2016	An aggregate analysis of personal care products in the environment: Identifying the distribution of environmentally-relevant concentrations	http://www.sciencedirect.com/science/article/pii/S0160412016301556
Hüffer et al.	2017	Microplastic Exposure Assessment in Aquatic Environments: Learning from Similarities and Differences to Engineered Nanoparticles	http://pubs.acs.org/doi/abs/10.1021/acs.est.6b04054?src=recsys
Inostroza et al.	2016	Body burden of pesticides and wastewater-derived pollutants on freshwater invertebrates: Method development and application in the Danube River	http://www.sciencedirect.com/science/article/pii/S0269749116302457
Kaserzon et al.	2017	Rapid screening and identification of chemical hazards in surface and drinking water using high resolution mass spectrometry and a case-control filter	http://www.sciencedirect.com/science/article/pii/S0045653517307750
Kay et al.	2017	Widespread, routine occurrence of pharmaceuticals in sewage effluent, combined sewer overflows and receiving waters	http://dx.doi.org/10.1016/j.envpol.2016.10.087
Khan en Nicell	2015	Human Health Relevance of Pharmaceutically Active Compounds in Drinking Water	https://www.ncbi.nlm.nih.gov/pubmed/25739816
Kinyua et al.	2016	Qualitative screening of new psychoactive substances in pooled urine samples from Belgium and United Kingdom	http://dx.doi.org/10.1016/j.scitotenv.2016.08.124

Auteur	Year	Title	Link
Loos et al.	2017	Analysis of emerging organic contaminants in water, fish and suspended particulate matter (SPM) in the Joint Danube Survey using solid-phase extraction followed by UHPLC-MS-MS and GC–MS analysis	http://www.sciencedirect.com/science/article/pii/S0048969717317424
Luo et al.	2014	A review on the occurrence of micropollutants in the aquatic environment and their fate and removal during wastewater treatment	http://www.sciencedirect.com/science/article/pii/S0048969713015465
Markus et al.	2016	Modelling the transport of engineered metallic nanoparticles in the river Rhine	http://dx.doi.org/10.1016/j.watres.2016.01.003
Mastroianni et al.	2016	Occurrence of drugs of abuse in surface water from four Spanish river basins: Spatial and temporal variations and environmental risk assessment	http://www.sciencedirect.com/science/article/pii/S0304389416304563
Meffe et al.	2014	Emerging organic contaminants in surface water and groundwater: A first overview of the situation in Italy	http://www.sciencedirect.com/science/article/pii/S0048969714002277
Mestankova et al.	2016	Transformation of Contaminant Candidate List (CCL3) compounds during ozonation and advanced oxidation processes in drinking water: Assessment of biological effects	http://www.sciencedirect.com/science/article/pii/S0043135415304462
Montes-Grajales et al.	2017	Occurrence of personal care products as emerging chemicals of concern in water resources: A review	http://www.sciencedirect.com/science/article/pii/S0048969717308161
Munthe et al.	2017	An expanded conceptual framework for solution-focused management of chemical pollution in European waters	http://enveurope.springeropen.com/articles/10.1186/s12302-017-0112-2
Newton et al.	2017	Suspect screening and non-targeted analysis of drinking water using point-of-use filters	https://www.sciencedirect.com/science/article/pii/S026974911732691X
Padhye et al.	2013	Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant	http://www.sciencedirect.com/science/article/pii/S0043135413008968
Pal et al.	2014	Emerging contaminants of public health significance as water quality indicator compounds in the urban water cycle	http://www.sciencedirect.com/science/article/pii/S0160412014001767
Petrie et al.	2014	A review on emerging contaminants in wastewaters and the environment: Current knowledge, understudied areas and recommendations for future monitoring	http://www.sciencedirect.com/science/article/pii/S0043135414006307
Pochodylo en Helbling	2017	Emerging investigators series: prioritization of suspect hits in a sensitive suspect screening workflow for comprehensive micropollutant characterization in environmental samples	http://pubs.rsc.org/en/Content/ArticleLanding/2017/EW/c6ew00248j#!divAbstract
Poste et al.	2014	Amines and amine-related compounds in surface waters: a review of sources, concentrations and aquatic toxicity.	https://www.ncbi.nlm.nih.gov/pubmed/24602912
Reemtsma et al.	2016	Mind the Gap: Persistent and Mobile Organic Compounds-Water Contaminants That Slip Through	https://www.ncbi.nlm.nih.gov/pubmed/27571393
Rivetti et al. 2017	2017	Integrated environmental risk assessment of chemical pollution in a Mediterranean floodplain by combining chemical and biological methods.	https://www.ncbi.nlm.nih.gov/m/pubmed/28119008/
Robles-Molina et al.	2014	Multi-residue method for the determination of over 400 priority and emerging pollutants in water and wastewater by solid-phase extraction and liquid chromatography-time-of-flight mass spectrometry	http://www.sciencedirect.com/science/article/pii/S0021967314007225
Rozas et al.	2016	Organic micropollutants (OMPs) in natural waters: Oxidation by UV/H2O2 treatment and toxicity assessment	http://www.sciencedirect.com/science/article/pii/S0043135416301944

Auteur	Year	Title	Link
Ryu et al.	2016	Comparative measurement and quantitative risk assessment of alcohol consumption through wastewater-based epidemiology: An international study in 20 cities	http://dx.doi.org/10.1016/j.scitotenv.2016.04.138
Schlüsener et al.	2015	Quaternary Triphenylphosphonium Compounds: A New Class of Environmental Pollutants	http://pubs.acs.org/doi/abs/10.1021/acs.est.5b03926
Schollée et al.	2015	Prioritizing Unknown Transformation Products from Biologically-Treated Wastewater Using High-Resolution Mass Spectrometry, Multivariate Statistics, and Metabolic Logic	http://pubs.acs.org/doi/abs/10.1021/acs.analchem.5b02905
Schröder et al.	2016	Status of hormones and painkillers in wastewater effluents across several European states-considerations for the EU watch list concerning estradiols and diclofenac	https://www.ncbi.nlm.nih.gov/pubmed/27023823
Singer et al.	2016	Rapid Screening for Exposure to “Non-Target” Pharmaceuticals from Wastewater Effluents by Combining HRMS-Based Suspect Screening and Exposure Modeling	http://pubs.acs.org/doi/pdf/10.1021/acs.est.5b03332
Sjerps et al.	2016	Data-driven prioritization of chemicals for various water types using suspect screening LC-HRMS	http://dx.doi.org/10.1016/j.watres.2016.02.034
Struijs et al.	2016	Adapting SimpleTreat for simulating behaviour of chemical substances during industrial sewage treatment	http://dx.doi.org/10.1016/j.chemosphere.2016.06.063
Tang et al.	2014	Which chemicals drive biological effects in wastewater and recycled water?	http://dx.doi.org/10.1016/j.watres.2014.04.043
Tousova et al.	2017	European demonstration program on the effect-based and chemical identification and monitoring of organic pollutants in European surface waters	http://www.sciencedirect.com/science/article/pii/S0048969717314365
Tuerk et al.	2016	Target Analysis, Suspected-Target, and Non-Target Screening for Evaluation and Comparison of Full-Scale Ozonation at Three Wastewater Treatment Plants	http://pubs.acs.org/doi/abs/10.1021/bk-2016-1242.ch002
van Wezel et al.	2017	Mitigation options for chemicals of emerging concern in surface waters; operationalising solutions-focused risk assessment	http://pubs.rsc.org/en/content/articlelanding/2017/ew/c7ew00077d#!divAbstract
Vergeynst et al.	2014	Suspect screening and target quantification of multi-class pharmaceuticals in surface water based on large-volume injection liquid chromatography and time-of-flight mass spectrometry	https://link.springer.com/article/10.1007/s00216-014-7672-4
Wang et al.	2016	Evaluating a Tap Water Contamination Incident Attributed to Oil Contamination by Nontargeted Screening Strategies	http://pubs.acs.org/doi/abs/10.1021/acs.est.5b05755
Yamamoto et al.	2016	Identification of Anthropogenic Compounds in Urban Environments and Evaluation of Automated Methods for Reading Fragmentation-A Case of River Water	https://www.ncbi.nlm.nih.gov/pubmed/27313978
Yang et al.	2017	Occurrences and removal of pharmaceuticals and personal care products (PPCPs) in drinking water and water/sewage treatment plants: A review	http://www.sciencedirect.com/science/article/pii/S0048969717309373
Zahn et al.	2016	Halogenated methanesulfonic acids: A new class of organic micropollutants in the water cycle	http://dx.doi.org/10.1016/j.watres.2016.05.082

Table 8b. List of reports on emerging compounds

Auteur	Jaar	Titel	Rapport
Ahrens et al.	2016	Screening of PFASs in groundwater and surface water	SLU, Vatten och miljö: Rapport 2016:2
Baken	2016	Verdiepende studie naar gezondheidskundige relevantie van Chroom VI in drinkwater	BTO 2016.087
Baken et al.	2015	Toxicologische risicobeoordeling geprioriteerde stoffen	BTO 2015.056
Baken et al.	2016	Signalering van 'overige antropogene stoffen', en dan? De pyrazool-casus	H2O-Online / 11 september 2016
Baken et al.	2017	Grip op opkomende stoffen in drinkwaterbronnen	H2O-Online / 10 mei 2017
Bannink	2017	De kwaliteit van het Maaswater in 2016	RIWA Maas Jaarrapport
Brauch et al.	2016	Wesentliche Ergebnisse aus dem ARW-Untersuchungsprogramm 2015	72. ARW-Jahresbericht 2015, DVGW-Technologiezentrum Wasser (TZW), Karlsruhe, ISSN 0343-0391, 69-79 (2016)
Deltares	2017	Verslag EmissieSymposium Water 6 april 2017	
Fleig et al.	2016	Sonderuntersuchungen auf organische Spurenstoffe im Längsprofil des Mains	72. ARW-Jahresbericht 2015, DVGW-Technologiezentrum Wasser (TZW), Karlsruhe, ISSN 0343-0391, 69-79 (2016)
Hijnen et al.	2016	Pyrazool - inventarisatie full-scale data en verkennend experimenteel onderzoek	BTO 2016.203(s)
ICBR	2016	Rapport over de beoordeling en de ontwikkeling van de kwaliteit van het Rijnwater in de periode 2013-2014	ISBN 978-3-946501-02-2
Methorst	2017	Meetprogramma antropogene stoffen - Pilot naar het risicogestuurd opstellen van het meetprogramma voor de kalksteenwinning IJzeren Kuilen	MSc stageverslag voor WML
Minister van Infrastructuur en Milieu	2017	Regeling van de Minister van Infrastructuur en Milieu, van 7 juli 2017, nr. IENM/BSK-2017/160338, houdende wijziging van de Drinkwaterregeling in verband met het toevoegen van een parameter voor pyrazool aan de kwaliteitseisen voor oppervlaktewater bestemd voor de bereiding van drinkwater	Staatscourant nr. 38058
Moermond	2016	Geneesmiddelen en waterkwaliteit	RIVM Briefrapport 2016-0111
Rörden et al.	2016	Untersuchung zu Vorkommen und Bedeutung von 1,4-Dioxan für die Trinkwassergewinnung aus Rheinuferfiltrat	72. ARW-Jahresbericht 2015, DVGW-Technologiezentrum Wasser (TZW), Karlsruhe, ISSN 0343-0391, 69-79 (2016)
Roskam	2017	Brede Maasscreening - Resultaat van monitoring op drie RWS-locaties	Deltares rapport in opdracht van RWS-WVL, project 1221383-002
Rougoor et al.	2016	Diergeneesmiddelen en waterkwaliteit	STOWA-Rapport 26, ISBN 978.90.5773.733.6
Schoenmakers et al.	2016	Dumping en lozing van synthetisch drugsafval: verschijningsvormen en politieaanpak	In opdracht van: Programma Politie & Wetenschap. ISBN: 978 90 352 4933 2
Sjerps et al.	2015	Signaleren van nieuwe stoffen (2014-2015)	BTO 2015.059
Sjerps et al.	2015	Datamining in non-target chemical screening data	BTO 2015.062

Auteur	Jaar	Titel	Rapport
Sjerps et al.	2015	Data-driven prioritization of chemicals for various water types using suspect screening LC-HRMS	BTO 2015.003
Sjerps et al.	2015	Suspect screening' voor datagestuurde prioritering van stoffen in (bronnen van) drinkwater	H2O-Online / 9 april 2015
Sjerps et al.	2016	Ontwikkeling waterkwaliteit bij innamepunten van oppervlaktewater voor de drinkwatervoorziening	BTO 2016.028
Sjerps et al.	2016	Haalbaarheidsstudie stoffendatabase voor de Nederlandse drinkwatersector	BTO 2016.027
Sjerps et al.	2016	Wateraanvoer van Waal naar Maas: gunstig voor de waterkwaliteit?	H2O-Online / 16 November 2016
Sjerps et al.	2018	Meten is weten: Zeer polaire stoffen in bronnen van drinkwater	BTO 2018.023
Steen	2017	Risicogestuurd Meten Antropogene Stoffen	Verslag workshop 23 oktober 2017
Stroomberg et al.	2017	Jaarrapport 2016 - De Rijn	RIWA Rijn Jaarrapport
Ter Laak en Kools	2016	Quickscan Diergeneesmiddelen in de waterketen	KWR rapport in opdracht van IenM / November 2016
ter Laak et al.	2016	Opkomende stoffen	BTO 2016.067
van der Aa et al.	2017	Evaluatie signaleringsparameter nieuwe stoffen drinkwaterbeleid	RIVM Rapport 2017-0091
van der Meer	2017	Evaluatie uitvoeringspraktijk stoffenbeleid	RHK-DHV rapport WATBE9626R01-I&I-MvdM voor Ministerie van Infrastructuur en Milieu.
van Leerdam et al.	2015	Brede screening van drinkwater: op zoek naar onbekende stoffen	H2O/ NR11/12 -November 2015
van Leerdam et al.	2017	Bevestiging van de identiteit van geprioriteerde suspects	BTO 2017.040
van Leerdam et al.	2017	Non-target screening van kwetsbare winningen van Brabant Water	BTO 2017.203
van Leerdam et al.	2017	Exploring the boundaries of non-target screening with Liquid Chromatography coupled to ESI-MS	BTO 2017.011
Versteegh en de Voogt	2017	Risicoduiding en véérkomen van FRD-903 in drinkwater en drinkwaterbronnen bij een selectie van drinkwaterwinningen in Nederland.	RIVM Briefrapport 2017-0175
Vughs et al.	2015	HILIC screening - analyse van zeer polaire stoffen in water	BTO 2015.076
Vughs et al.	2018	Emerging (per)fluorinated compounds in the watercycle	BTO 2018.061
Weissinger et al.	2016	Screening for Contaminants of Emerging Concern in Waters of the Northern Colorado Plateau Network	Natural Resource Report NPS/NCPN/NRR—2016/1239