



LIFE Integrated Projects 2016
Optimising the implementation of the 2nd RBMP in the Malta River Basin District
LIFE 16 IPE MT 0008



Action C.18
Monitoring for emerging pollutants of potential concern

Result 3: Proposal for Focused Monitoring

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1.0 Introduction. Purpose, objective and context of this document

1.1 Since 2000, the Water Framework Directive 2000/60/EC (WFD) has been the primary legal instrument for water protection within the EU. Its objective is to achieve good Ecological and Chemical status within inland surface, transitional and coastal surface waters, and good qualitative and quantitative status in groundwaters. The Ecological status - within the context of the WFD - takes into account biological, hydromorphological, physico-chemical (including nutrients) and general quality standards. To achieve good Chemical status, Member States must monitor and meet minimum quality standards for selected pollutants and reduce or phase out the emissions of those substances to water. Subsequent to the WFD, the Groundwater Directive (2006/118/EC) was drawn up specifically to prevent and combat groundwater pollution, providing the criteria for assessing chemical status, assessing trends, and limiting contamination.

1.2 One of the main mechanisms used to monitor and control water pollution is the 'River Basin Management Plan' (RBMP) which oversees the quality of all controlled waters within river basins. The WFD (specifically, its Annexes) documents monitoring requirements, the criteria for assessing water body status, the contents of the RBMPs, and the significance of 'priority substances' - contaminants that Member States must monitor and control at levels lower than their specific Environmental Quality Standards (EQS). Additionally, the WFD also requires Member States to set and meet EQS for substances of national concern, i.e. river basin specific pollutants; the monitoring of which contributes to the assessment of chemical status.

1.3 Subsequent directives have been created to augment the WFD. Firstly, there was Directive 2008/105/EC, which identified the EQSs for 33 priority substances and some other notable pollutants, and then Directive 2013/39/EU, which updated the EQSs for seven of the priority substances - in line with the latest scientific and technical knowledge – as well as adding 12 newly identified priority substances. It also required the European Commission to establish a 'Watch List' of substances for which EU-wide monitoring data are to be gathered to inform future prioritisation. Member States must monitor controlled waters for the substances on the list at least once per year and the chemicals can remain on the list for a maximum of two successive editions. The first watch list was established in 2015, updated in 2018 and 2020 and again in 2022. The latest watch list is due to be published between September-Oct 2024. A groundwater watch list was first endorsed in 2019 and successive iterations are still ongoing.

1.4 Under the obligations of the WFD and associated RBMPs, the Environment and Resources Authority (ERA) commissioned AquaBio Tech Ltd. (ABT) to develop and implement a monitoring strategy of Malta's water resources in terms of contaminants of emerging concern and pollutants attributed to diffuse sources of pollution. The investigation is part of a project funded by the LIFE Programme under the Project Policy Area LIFE Integrated Project Environment (LIFE16/IPE/MT0008, Action C.18).

1.5 The objectives of Action C.18 are as follows:

Objective 1: To update the monitoring strategy developed as part of LIFE16/IPE/MT0008 (Action A.6) to address gaps related to the characterisation and quantification of diffuse sources of pollution in Malta.

Objective 2: To implement an initial screening monitoring exercise of the contaminants of emerging concern and diffuse sources of pollution for a period of two years.

Objective 3: To update the monitoring strategy on the basis of the results of the initial screening monitoring exercise to enable focused monitoring of CECs and their sources, and diffuse sources of pollution.

1.6 This document is presented pursuant to Result 3 of Tender SPD8/2021/066; namely:

1.6.1 To propose a focused monitoring strategy based on monitoring data and relevant legislation identifying and quantifying presence of specific contaminants.

1.6.2 To undertake the sample collection and analysis for said contaminants

1.6.3 To present a report summarizing the results and conclusions of the monitoring campaign.

Name and Surname of Key Expert 1: Nicolas Kalogerakis

Signature:



Date: 06 May 2025

Name and Surname of Key Expert 2: Adrian Love

Signature:



Date: 06 May 2025

2.0 Sampling strategy

The sampling strategy will develop from the best practices and outcomes of previous investigations of Malta's water resources.

2.1 Sampling locations

The two-year sampling of Maltese waters from 2023-2025 (Tender SPD8/2021/066), outlined in section 1.4 and hereafter referred to as ERA12, categorised Maltese water resources according to their origin:

Groundwater: all subsurface water contained in the pores and interstices of rock and substrate.

Stormwater: water drained from surface of conurbation immediately after substantial precipitation

Inland surface water: water bodies found at the surface fed largely, or sometimes entirely, from drainage.

Transitional water: water bodies that, while technically inland, are majorly influenced by sea water influx

Coastal water: Sea water sampled adjacent to the coastline

New water: wastewater that, after standard secondary sewage treatment, undergoes further extensive cleaning and purification using ozone and UV.

Additional monitoring sites: A primary objective of ERA12 was the characterisation and quantification of contaminants from diffuse urban, industrial, and agricultural sources of pollution that pose a risk to Malta's natural water resources. To this end, eight monitoring stations, additional to those representing the aforementioned water types, were identified. These were considered as representative of potential sources of diffuse pollution and were complimentary to sites proposed as part of LIFE16/IPE/MT008 Action A.6 for inland surface waters.

These categories are useful for distinguishing which water bodies are more heavily contaminated and direct a strategy of further focused monitoring which better reflects the hydrology and pressures within the Maltese islands. It is proposed that for future monitoring the degree of contamination of these water sources should dominate in their selection (rather than abundance of sampling sites, for example). Though arguably presenting a 'worst-case' scenario, this approach highlights true areas of concern as well as being capable of revealing improvements.

Other sample locations whose results can inform future monitoring are from the sewage network; these were sampled for the LIFE IP Action C.10 project. The location of all sampling sites – C.10 and ERA12 - are given in figure 1.

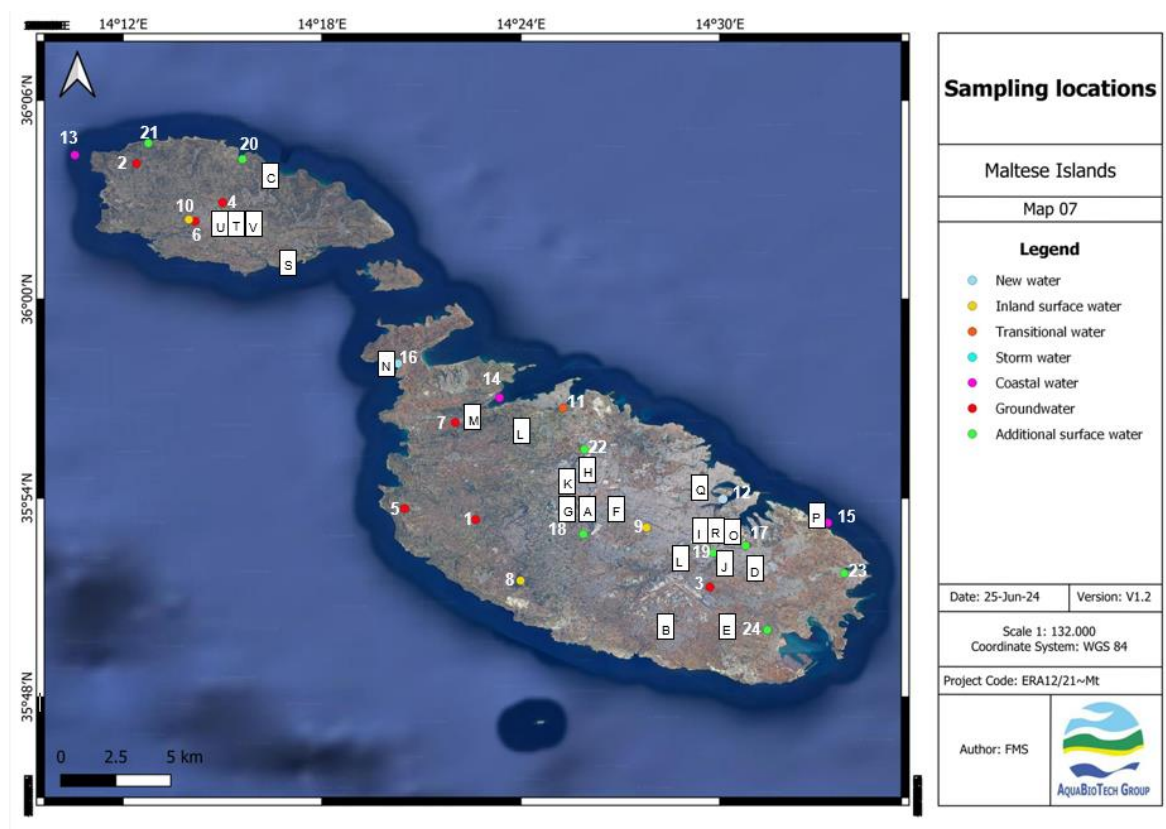


Figure 1 Map of sample sites

Table 1 Identification of sample sites

Label	Study	Identification	Type
1	ERA12	Fiddien Station	Groundwater
2		Ta' Pinu	Groundwater
3		Ġnien	Groundwater
4		Sellun	Groundwater
5		Baħrija	Groundwater
6		Victoria Station	Groundwater
7		Pwales Station	Groundwater
8		Wied il-Luq	Inland surface
9		Wied is-Sewda	Inland surface
0		Wied il-Lunzjata	Inland surface
11		Is-Salini	Transitional
12		Ta' Xbiex	Stormwater
13		Off Ta' Barkat STP (sewage treatment plant)	Coastal water
14		Xemxija Bay	Coastal water

15		San Dimitri Point	Coastal water
16		Ċumnija STW	New water
17		Wied Blandun	Additional surface
18		Wied Inċita	Additional surface
19		Marsa Storm water catchment	Additional surface
20		Marsalforn	Additional surface
21		Wied il Mielat	Additional surface
22		Burmarrad, Mosta	Additional surface
23		IL-Magħluq ta' Marsaskala	Additional surface
24		Wied Qoton	Additional surface
A	C:10	B1 Attard Res	Sewage network
B		B2 Zurrieq Res	Sewage network
C		B3 Xaghra Gozo Res	Sewage network
D		MT 1 Bulebel South	Sewage network
E		MT 2 Hal Far PS	Sewage network
F		MT 3 Mriehel	Sewage network
G		MT 4 Attard	Sewage network
H		MT 5 Wied Il-Ghasel	Sewage network
I		MT 6 Marsa GSD	Sewage network
J		MT 7 Marsa Garibaldi	Sewage network
K		MT 8 Mosta Tech'park	Sewage network
L		MT 9 Handaq	Sewage network
M		MT 10 Pwales PS	Sewage network
N		MT 11 Ċumnija STW	Sewage network
O		MT 12 Corradino PS	Sewage network
P		MT 13 Ta' Barkat	Sewage network
Q		MT 14 Gzira PS	Sewage network

R		MT 15 Marsa PS	Sewage network
S		GZ 1 Ras Il-Hobz	Sewage network
T		GZ 2 Xewkija West	Sewage network
U		GZ 3 Xewkija East	Sewage network
V		GZ 4 Xewkija Old DP	Sewage network

For ERA12, water sources were tested for compounds of emerging concern (CECs), indicators of diffuse pollution in surface waters, and Tentatively Identified Compounds (Table 2).

Table 2 Details of the ERA12 monitoring activities per each water category

Water category	CEC ¹	Diffuse ²	TIC ³	Monitoring Stations	Replicates	Frequency per year ⁴	Screening duration (years)
Groundwater	ü		ü	7	2	4	2
Inland Surface Waters	ü	ü	ü	3	2	2	2
Transitional	ü		ü	1	2	2	2
Stormwater	ü		ü	1	2	2	2
Coastal	ü		ü	3	2	4	2
New Water	ü		ü	1	2	4	2
Additional Monitoring Stations	ü	ü	ü	8	2	2	2

¹CEC= Compounds of Emerging Concern (See appx, Table 13), ²Diffuse = characterisation of diffuse sources of pollutants (see appx. Table 14), ³TIC= Tentatively Identified Compound (see appx. Table 15)

A summary of results from two years of monitoring Malta's water resources for project ERA12 is given in table 3. The number of contaminants, column C, describes how many different contaminants (diffuse pollution and CECs) were detected at each sample location (columns A/B); column D enumerates the contaminants (i.e. column C) that were found at levels higher than their specified EQS (see 1.3). A contaminant may have been recorded on multiple sampling occasions, so columns E and F enumerate the total number of times (frequency) an indicator of diffuse pollution (E) or CEC (F) (**Error! Reference source not found.**) was detected. In ERA12, samples from the same category of water were pooled before being screened for TIC; the values in column G reflect the total number of TIC detected in the pooled samples, and the number of these that were found at levels greater than their EQS (column H).

Table 3 Contaminants of Maltese waters tested in project ERA12

A. Map reference (Figure 1)	B. Sample location	C. Total Number of different contaminants detected	D. No. of detected contaminants > EQS (if EQS available)	E. Frequency of 'indicators of diffuse pollution' detected	F. Frequency of CEC detected	G. Number of TIC detected in Screening	H. Number of TIC detected in Screening > EQS
Groundwater							
1	Fiddien Station	0	0	n/a	0	61	0
2	Ta' Pinu	1	0		1		
3	Ġnien	0	0		0		
4	Sellun	2	0		2		
5	Baħrija	0	0		0		
6	Victoria Station	6	0		24		
7	Pwales Station	0	0		0		
Inland surface water							
8	Wied il-Luq	11	2	24	4	69	1
9	Wied is- Sewda	17	4	26	10		
10	Wied il- Lunzjata	20	6	38	13		
Transitional water							
11	Is-Salini	3	0	n/a	3	54	0
Stormwater							
12	Xatt Ta' Xbiex	10	2	n/a	24	78	1
Coastal							
13	Off Ta' Barkat STP*	1	0	n/a	1	51	0

14	Xemxija Bay	1	0		1		
15	San Dimitri Point	1	0		1		
New water							
16	Ċumnija STP*	7	0	n/a	12	57	1
Additional surface water							
17	Wied Blandun	18	3	30	13	75	0
18	Wied Inċita	16	2	29	4		
19	Marsa Storm water catchment	33	6	46	13		
20	Marsalforn	28	3	43	17		
21	Wied il Mielah	15	6	26	12		
22	Burmarrad, Mosta	17	7	24	7		
23	IL-Magħluq ta' Marsaskala	15	5	24	6		
24	Wied Qoton	18	4	26	13		

* STP = Sewage Treatment Plant

Table 3 suggests there may be a correlation between water type and contamination level, though if the waters are connected the link is not direct. When averaged, the average number of total contaminants (CEC and Diffuse pollution) increases from 1 across Coastal and Groundwater sites, to 3, 7, 10, 16 and 20 in Transitional, New water, Stormwater, Inland Surface and Additional surface sites respectively. Even if Diffuse pollutants are excluded (since they were only analysed in Inland Surface and Additional Surface samples) the average number of CECs shows a similar pattern. This may be coincidental, though when proximate sample sites are compared the pattern is repeated. Ta' Pinu (groundwater), and Wied il-Mielah (Additional Surface water) are only 1.7km apart and share the same aquifer (figure 2), but whilst only one CEC was detected in the former, 6 were

detected in the latter. Similarly, Ġnien (groundwater) and Marsa Stormwater (Additional surface) are only 2.7km apart, but no contamination was detected at the former, compared to 12 contaminants at the latter – though in different catchments, the proximity of sites might suggest similar pressures and potential contamination.

This is elucidated in Figure 2, which shows the prevalence of contaminants across the sites sampled in ERA12. There might be some indication that there is a higher incidence of contaminants around the more heavily urbanised catchments, however this may be an artefact of the distribution of sampling sites – the less urbanised areas in the north of Malta happened to be dominated by sample sites of (less contaminated) Ground, Coastal and Transitional waters, for example.

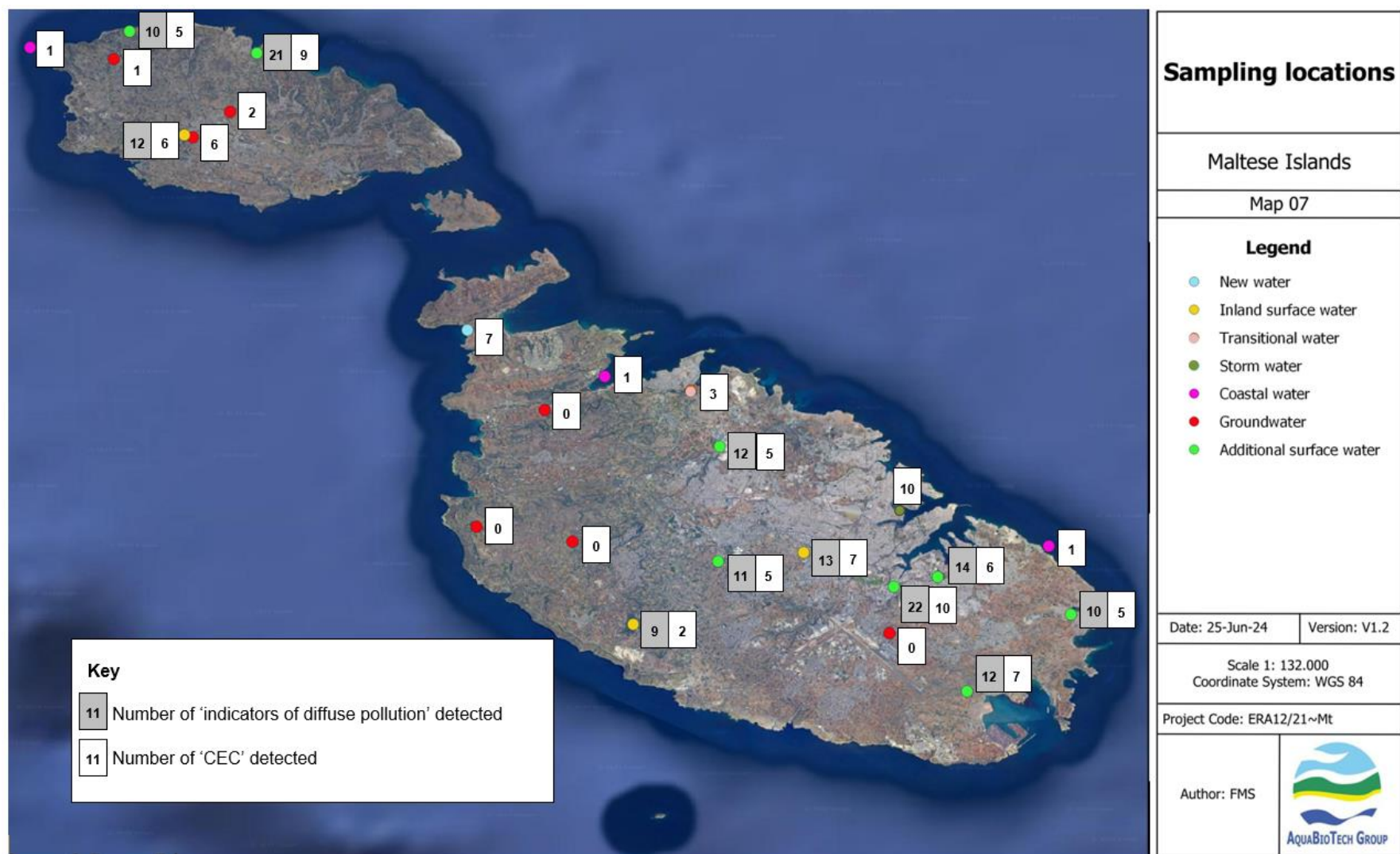


Figure 2 Number of contaminants found across sample sites of ERA12

2.1.1 Groundwater.

There are 15 groundwater bodies found within the Maltese islands occurring in two types of aquifer (Figure 3). Seven of these bodies were sampled for the ERA12 project.

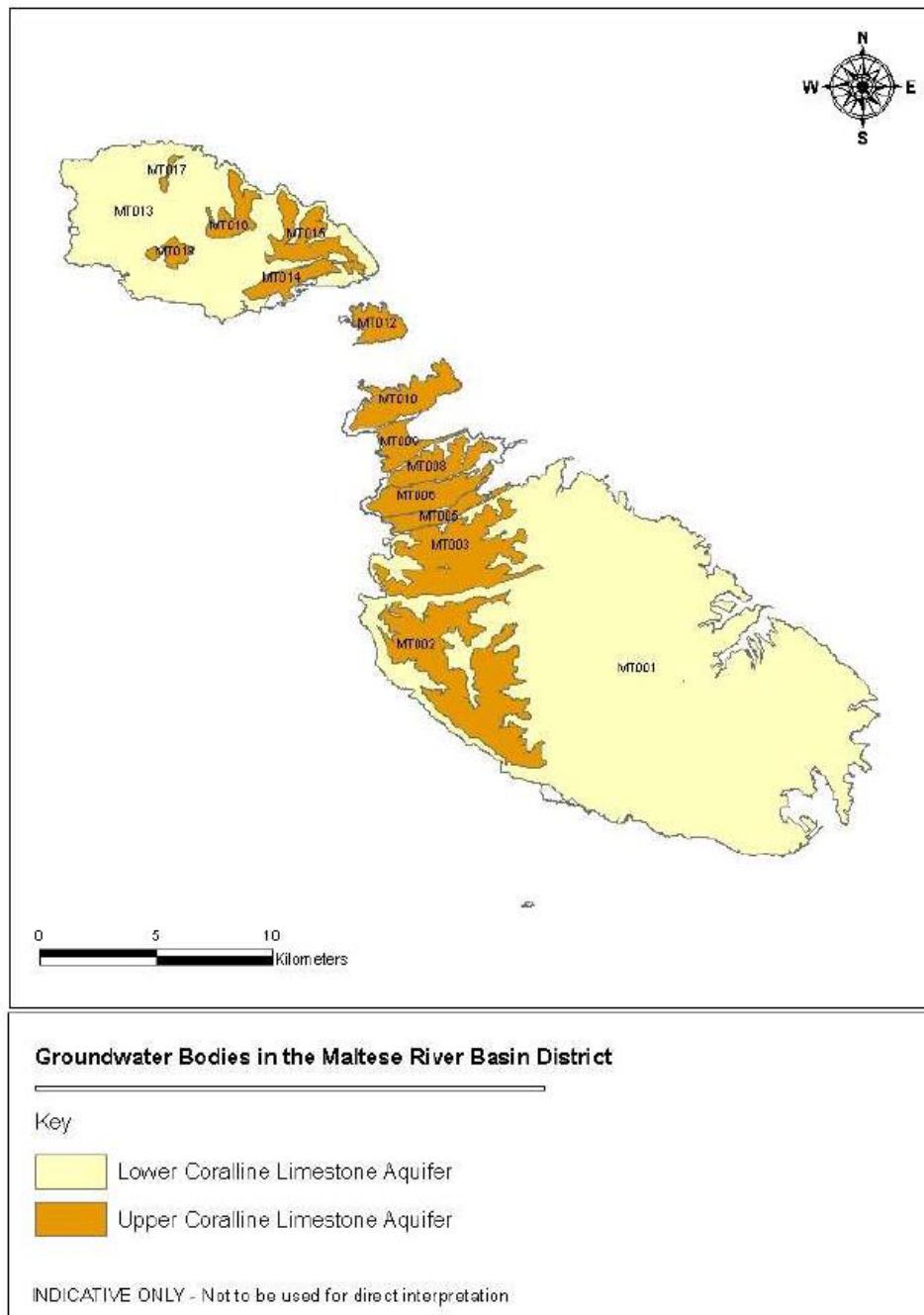


Figure 3 Designated Groundwater bodies in the Maltese Water Catchment District*¹

* MT001 Malta mean sea level¹, MT002 Rabat-Dingli perched¹, MT003 Mgarr-Wardija perched¹, MT005 Pwales coastal¹, MT006 Mizieb mean sea level, MT008 Mellieha perched, MT009 Mellieha coastal, MT010 Marfa coastal¹, MT012 Comino mean sea level, MT013 Gozo mean sea level¹, MT014 Għansielem perched, MT015 Nadur perched, MT016 Xaghra perched, MT017 Zebbug perched, MT018 Victoria-Kercem perched¹ – ¹Sampled for ERA12 project

¹ The Water Catchment Management Plan for the Maltese Islands, March 2011. Available at: https://era.org.mt/wp-content/uploads/2019/05/1st-WCMP_final.pdf

A programme that monitors groundwater can be informative due to its constant availability, wide distribution, and significant usage pressures. However, the ERA12 study found this water source to be relatively uncontaminated (Figure 2), with the singular exception of Fontana (Victoria), Gozo (Table 3) – other water sources were much more evidently contaminated. On this basis, there is little justification for groundwater to be the major focus of investigation in an ongoing monitoring campaign. However, groundwater represents one of the main water sources in Malta and is heavily utilized, so a balanced approach should be taken considering some alternative sites that were not sampled during ERA12. In summary, the following groundwater sites are proposed for sampling:

- Iklin (II) which lies within the Malta mean sea level aquifer (replacing Gnien in ERA12 which occasionally was offline).
- Dingli pumping station which lies within the Rabat, Malta perched aquifer
- Ghattuq which lies within the Gozo mean sea level aquifer (this site was initially proposed for ERA12, but had to be changed due to pump malfunction).
- Fontana, Gozo, which lies within the Gozo perched aquifer and was the most contaminated groundwater sites in ERA12.

2.1.2 Inland surface water.

Malta has very few permanent Inland Surface Waters, but those that were studied for ERA12 contained some of the highest number of detected contaminants. This is evident in the results of analysis of the Inland surface water category and the Additional sample sites - which were predominantly inland surface water. Together, 87% of instances of contamination were found within these sources. Therefore, surface water is proposed to form the majority of sampling sites for an ongoing strategy. Of the surface water sites sampled for ERA12, some - Wied Qoton, Wied Inċita, Wied Blandun and Wied is-Sewda – were found to consist of either surface runoff from a rainfall event, or isolated pools - which, through dilution and evaporation respectively, may obscure the true state of contamination. In addition, one of the Additional sampling sites - Il-Magħluq ta' Marsaskala, is categorized as transitional water. The remaining surface water sites – namely Wied il Luq, Wied il-Lunzjata, Marsa Drain, and Burmarrad (Għasel Catchment) are proposed for future monitoring based on the following credentials: their record of contamination, representation of urban (Marsa), agricultural (Burmarrad) and rural (Wied il-Lunzjata, Wied il-Luq) drainage basins, and probability of containing water. An additional site proposed is Wied tal- Baħrija, which warrants specific monitoring as it is one of the Maltese water bodies delineated under the WFD (with Wied il-Lunzjata and Wied il-Luq) and monitoring CEC contamination of WFD water bodies can be useful in evaluating their status, pressures, and risk. Whilst Baħrija was one of the sampling sites monitored as a groundwater site (where it showed very little evidence of contamination), the

sample point was directly at the spring where the groundwater surfaces and may not completely reflect the status of the whole catchment (as discussed above, ERA12 demonstrated that surface waters were more contaminated than their groundwater counterparts). Therefore the proposed sample point of Wied tal- Baħrija is further along the course of the water body (Table 5).

2.1.3 Coastal

Coastal waters showed very little signs of contamination in the ERA12 project (Table 3); only one contaminant was found, on one occasion, over two years' of sampling. However, for consistency, it is proposed that one of the ERA12 sites is monitored going forward: offshore of ta' Barkat STP, in order to assess potential impacts from STP discharges which are one of the main source of CEC contamination², particularly for pharmaceuticals and personal care products.

2.1.4 Transitional water

The WFD defines transitional waters as “bodies of surface water in the vicinity of river mouths which are partly saline in character as a result of their proximity to coastal waters, but which are substantially influenced by freshwater flows”. There are 5 such water bodies in Malta, two of which were sampled for the ERA12 project. As mentioned in 2.1.2, Il-Magħluq ta' Marsaskala was noted to show signs of contamination (Table 3) and, though grouped as an 'Additional Sampling Station' for that project, it is demonstrably a transitional water. In their 2023 study, Bartolo et al. ³ also found indicators of water pollution at this site which they linked to anthropogenic pressure such as engineering works, chemical run-off from the surrounding fields, and illegal dumping of waste. In contrast, the transitional water sampled in ERA12 (Is-Salini) appeared to be relatively uncontaminated (Table 3) so is not proposed for a focused monitoring campaign and instead replaced by Il-Magħluq ta' Marsaskala as the representative site of transitional water.

2.1.5 Storm and new water

Stormwater is considered as one of the major sources of water pollution⁴ and was found to be one of the most impacted water sources during the ERA12 project (Table 3). The same site, Ta' Xbiex, is proposed for ongoing sampling. It drains an area of over 11.4km² of largely urban utilization, with

² Mumberg, T., Ahrens, L., & Wanner, P. (2024). Managed aquifer recharge as a potential pathway of contaminants of emerging concern into groundwater systems—A systematic review. *Chemosphere*, 143030.

³ Bartolo, D., Bonello, J. J., Gravino, F. S., & Caruana, R. (2022, September). Exploring the Environmental Significance of Il-Magħluq Ta'Marsaskala: A Study on Water Quality Within a Special Area of Conservation. In *International Conference on Energy and Environment Research* (pp. 461-468). Cham: Springer Nature Switzerland.

⁴ Aryal, R., Vigneswaran, S., Kandasamy, J., & Naidu, R. (2010). Urban stormwater quality and treatment. *Korean Journal of Chemical Engineering*, 27, 1343-1359.

a collective population of approximately 43,600 and can collect up to 700,000 cubic meters of water⁵ therefore it is demonstrably a valuable indicator of water quality and anthropogenic impact. Conversely, so-called 'New Water' was notably uncontaminated during the ERA12 project, likely facilitated by its thorough processing including Reverse Osmosis and Ozonation, both of which are processes specifically applied to eradicate any contaminants. However, New Water is identified as one of the water types within the remit of Action C.18 so sampling of the largest New Water production plant at Ċumnija Wastewater Treatment Plant is proposed as part of the focused monitoring strategy.

2.2 Sampling frequency and replication

It is recommended that monitoring sites are sampled twice over the year with two replicate samples taken at each site to corroborate results. Since many sites depend on surface water availability, sampling should be timed when there is a greater likelihood of precipitation (Table 12).

The proposed sampling campaign is summarised in Table 4

Table 4 Proposed sampling programme for each water category.

Water category	Monitoring Stations	Replicates	Frequency per year ¹	Total number of samples
Coastal	1	2	2	4
Transitional	1	2	2	4
Inland Surface Waters	5	2	2	20
Groundwater	4	2	2	16
Stormwater	1	2	2	4
New water	1	2	2	4

¹See Table 12 for sampling schedule

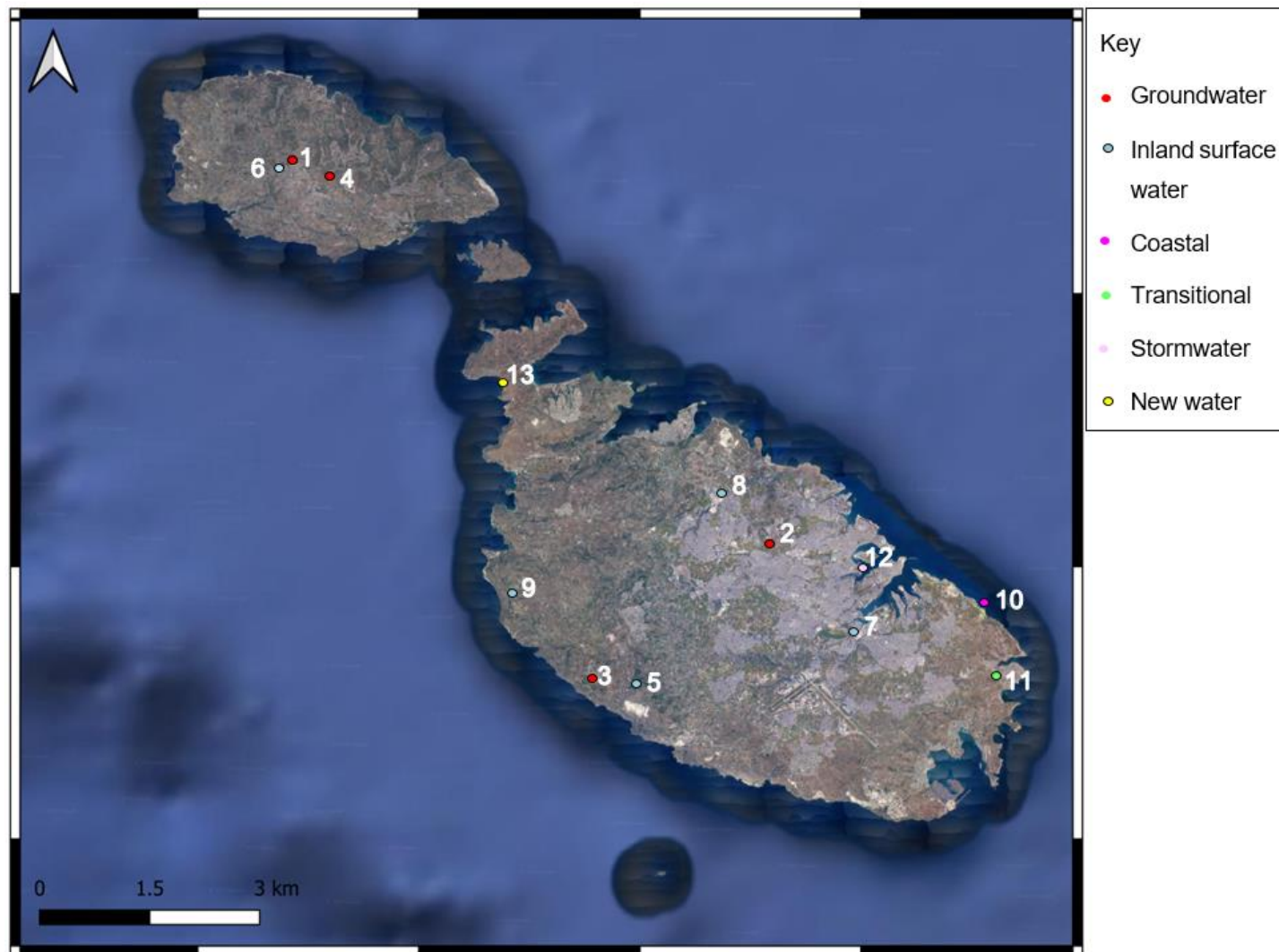
Table 5 Proposed location of sampling sites (see figure 4 for map)

Map point	Station Name, Location	Type of water	Latitude*	Longitude*
1	Fontana, Gozo	Groundwater	36.040055	14.233248

⁵ Pullicino, G. (2012) *Work starts on 11km rainwater tunnel*. Times of Malta, Sept. 21. Available at: <https://timesofmalta.com/article/work-starting-on-11km-rainwater-gallery.437722>

2	Iklin (II)	Groundwater	35.909750	14.455753
3	Dingli	Groundwater	35.873063	14.393868
4	Għattuq	Groundwater	36.04691	14.24957
5	Wied il Luq	Inland Surface water	35.858699	14.400677
6	Wied il-Lunzjata, Gozo	Inland Surface water	36.041124	14.232713
7	Marsa Drain	Inland Surface water	35.877210	14.495686
8	Burmarrad (Għasel Catchment)	Inland Surface water	35.928749	14.429094
9	Wied tal- Baħrija‡	Inland Surface water	35.89350279	14.34007034
10	Off Ta' Barkat STP, Xgħajra	Coastal	35.88578	14.55368
11	Il-Magħluq ta' Marsaskala	Transitional	35.861905	14.562427
12	Ta' Xbiex	Stormwater	35.899487	14.500738
13	Ċumnija STP	New water	35.968138	14.338567

* latitude/longitude values use WGS 84 datum, ‡ coordinates to be verified on site



5 for locations)

Figure 4 Location of sample sites (refer to table

2.3 Selection of contaminants for monitoring

To identify potential candidates for focused monitoring a matrix was developed which evaluated four different criteria (table 6).

Table 6 Criteria used for evaluation of candidate contaminants

Criteria	Sub-criteria	Score
1. Regular monitoring processes	1a. Pollutant constitutes a priority substance for surface water or is listed in the Groundwater Directive and thus already subject to regular monitoring in WFD water bodies	0
	1b. Pollutant is a Chemical of Emerging Concern that is not subject to regular monitoring in WFD water bodies	3
2. Screening Process	2a. Pollutant not detected in screening exercise	0
	2b. Pollutant detected through screening exercise once across water types	1
	2c. Pollutant detected through screening exercise at a frequency of 1-5	2
	2d. Pollutant detected through screening exercise at a frequency of >5	3
3. Use in Malta	3a. Use of pollutant in Malta not verified through presence in sewerage network (LIFE IP Action C.10)	0
	3b. Use of pollutant in Malta verified through presence in sewerage network (LIFE IP Action C.10)	1
4. Watchlist	4a. Pollutant not listed in surface and/or groundwater watch list	0
	4b. Pollutant listed in surface and/or groundwater watch list	2

Criteria 1 deprioritizes contaminants that are already subject to regular monitoring (due to their inclusion in statutory lists such as Priority Substances, see section 1.2) and prioritizes compounds of emerging concern (investigated by ERA 12). Criteria 2 evaluates the number of times the compound was detected through ERA12 - either in the regular monitoring (Table 13 and Table 14) or TIC screening process (Table 15), emphasising contaminants with greater prevalence. Similarly, criteria 3 evaluates whether the contaminants have been detected in the sewerage network

through the LIFE IP Action C10. Finally, criteria 4 prioritises pollutants listed in surface water or groundwater watch lists (see 1.3).

Given the different sub-criteria, it was appropriate to draw up two shortlists: one for groundwater and another for all other 'surface' water sources (inland surface, transitional, new water, stormwater and coastal). In total, 200 compounds were evaluated for surface waters, and 162 for groundwater (Table 7 and Table 8).

Table 7 Evaluation of candidate compounds for focused monitoring of surface waters

<i>Compound</i>	<i>1. Regular monitoring process¹</i>	<i>2. Screening process²</i>	<i>3. Use in Malta³</i>	<i>4. Watch list⁴</i>	<i>Score</i>
<i>1,2,4-trimethyl benzene</i>	3	2	1	0	6
<i>1,2-dichloroethane</i>	0	0	0	0	0
<i>1,3,5-Trimethylbenzene</i>	3	2	0	0	5
<i>1,6-Hexanediol diacrylate</i>	3	2	0	0	5
<i>1-Ethyl-2-pyrrolidone</i>	3	2	0	0	5
<i>2(3H)-Benzothiazolone</i>	3	1	0	0	4
<i>2,4,6-Triallyloxyl-1,3,5-triazine</i>	3	1	0	0	4
<i>2,4,7,9-Tetramethyl-5-decyne-4,7-diol</i>	3	2	0	0	5
<i>2,4-Di-tert-butylphenol</i>	3	1	0	0	4
<i>2,6-Difluorobenzamide</i>	3	1	0	0	4
<i>2-Ethyl-1,3-hexanediol</i>	3	2	0	0	5
<i>2-Ethyl-4-methyl-1,3-dioxolane</i>	3	1	0	0	4
<i>2-Ethylhexanoic acid</i>	3	2	0	0	5
<i>2-Ethylhexyl salicylate</i>	3	1	0	0	4
<i>2-Methoxynaphthalene</i>	3	1	0	0	4
<i>2-Methylnaphthalene</i>	3	2	0	0	5
<i>2-tert-Butylcyclohexanone</i>	3	1	0	0	4
<i>4-chloro-3-methylphenol</i>	3	0	1	0	4
<i>6PPD (quinone)</i>	3	0	0	2	5
<i>Acesulfame K</i>	3	3	1	0	7
<i>Acetone*</i>	0	0	1	2	3
<i>Acetophenone</i>	3	2	0	0	5
<i>Acronifen</i>	0	0	0	0	0
<i>Alachlor</i>	0	0	0	0	0
<i>Ammonium nitrogen*</i>	0	3	1	0	4
<i>Amoxicillin</i>	3	0	1	2	6
<i>Aniline</i>	3	2	1	0	6
<i>Anthracene</i>	0	2	0	0	2
<i>Arsenic</i>	3	3	1	0	7
<i>Atenolol</i>	3	2	1	0	6
<i>Atrazine</i>	0	0	0	0	0
<i>Avermectin B1a</i>	3	0	0	2	5
<i>Avermectin B1b</i>	3	0	0	2	5
<i>Azobenzene</i>	3	2	0	0	5
<i>Benzene</i>	0	0	1	0	1
<i>Benzenesulfonamide, N-butyl</i>	3	2	0	0	5
<i>Benzenesulfonanilide</i>	3	2	0	0	5

<i>Benzo(a)pyrene</i>	0	1	0	0	1
<i>Benzo(b)fluoranthene</i>	0	1	0	0	1
<i>Benzo(ghi)perylene</i>	0	1	0	0	1
<i>Benzo(ghi)perylene</i>	0	1	0	0	1
<i>Benzo(k)fluoranthene</i>	0	1	0	0	1
<i>Benzophenone</i>	3	3	0	2	8
<i>Benzotriazole</i>	3	3	1	0	7
<i>Benzyl alcohol</i>	3	1	0	0	4
<i>Beta-estradiol</i>	3	0	0	2	5
<i>Bifenox</i>	0	0	0	0	0
<i>Biphenyl</i>	3	1	0	0	4
<i>Bis(2-ethylhexyl) adipate</i>	3	3	0	0	6
<i>bis(2-ethylhexyl) phthalate (DEHP)</i>	0	1	0	0	1
<i>Bisphenol A</i>	3	2	1	0	6
<i>Brominated diphenylethers</i>	0	0	0	0	0
<i>Bromuconazole</i>	3	0	0	2	5
<i>Butyl methoxydibenzoyl-methane</i>	3	0	0	2	5
<i>Butylated hydroxyanisole</i>	3	1	0	0	4
<i>Butylated hydroxytoluene</i>	3	1	0	0	4
<i>Cadmium*</i>	0	1	0	0	1
<i>Caffeine*</i>	0	2	0	0	2
<i>Caprolactam</i>	3	1	0	0	4
<i>Carbamazepine</i>	3	2	1	0	6
<i>Carbofuran-3-keto</i>	3	1	0	0	4
<i>Chlorfenvinphos</i>	0	0	0	0	0
<i>Chloroalkanes, C₁₀₋₁₃</i>	0	0	0	0	0
<i>Chloroneb</i>	3	1	0	0	4
<i>Chlorophene (2-Benzyl-4-chlorophenol)</i>	3	1	0	0	4
<i>Chloroxylenol</i>	3	2	0	0	5
<i>Chlorpyrifos (Chlorpyrifos-ethyl)</i>	0	0	0	0	0
<i>Cholesterol*</i>	0	1	0	0	1
<i>Cinnamal</i>	3	1	0	0	4
<i>Citronellol</i>	3	1	0	0	4
<i>Climbazole</i>	3	0	0	2	5
<i>Clindamycin</i>	3	0	0	2	5
<i>Cyazofamid</i>	3	0	0	2	5
<i>Cybutryne</i>	0	0	0	0	0
<i>cyclohexanone</i>	3	0	0	0	3
<i>Cypermethrin</i>	0	0	0	0	0
<i>Deltamethrin</i>	3	0	0	0	3
<i>Decahydronaphthalene (trans)</i>	3	1	0	0	4
<i>Dichloromethane</i>	0	3	0	0	3
<i>Dichlorvos</i>	0	0	0	0	0
<i>Diclofenac</i>	3	0	1	2	6
<i>Dicofol</i>	0	0	0	0	0
<i>Dicyclohexyl phthalate</i>	3	2	0	0	5
<i>Diethyl phthalate</i>	3	2	1	0	6
<i>Difenoconazole</i>	3	0	0	2	5
<i>Diisobutyl phthalate</i>	3	1	0	0	4
<i>Dimethomorph</i>	3	1	0	0	4
<i>Dimethyl phthalate</i>	3	2	0	0	5
<i>di-n-butyl phthalate</i>	3	2	0	0	5
<i>Dioxins and dioxin-like compounds</i>	0	0	0	0	0
<i>Diphenyl ether</i>	3	1	0	0	4
<i>Diphenyl sulfone</i>	3	2	0	0	5

<i>Diuron</i>	0	2	0	0	2
<i>d-Limonene</i>	3	2	0	0	5
<i>EDTA (EthylenDiaminoTetracetyc Acid)</i>	3	2	0	0	5
<i>Endosulfan</i>	0	0	0	0	0
<i>Epoxiconazole</i>	3	0	0	2	5
<i>Ethylbenzene</i>	3	2	1	0	6
<i>Etoxazole</i>	3	0	0	2	5
<i>Fenpiclonil</i>	3	2	0	0	5
<i>Fipronil</i>	3	0	0	2	5
<i>Fluoranthene</i>	0	2	0	0	2
<i>Fluoxetine</i>	3	0	0	2	5
<i>Flurenol-methylester</i>	3	2	0	0	5
<i>Formaldehyde</i>	3	0	1	0	4
<i>Furfuryl alcohol</i>	3	1	0	0	4
<i>Glutaraldehyde</i>	3	1	0	0	4
<i>Glyphosate</i>	3	3	1	0	7
<i>Guanylurea</i>	3	0	0	2	5
<i>Heptachlor</i>	0	0	0	0	0
<i>heptachlor epoxide</i>	0	0	0	0	0
<i>Hexabromocyclododecanes (HBCDD)</i>	0	0	0	0	0
<i>Hexachlorobenzene</i>	0	0	0	0	0
<i>Hexachlorobutadiene</i>	0	1	0	0	1
<i>Hexachlorobutadiene</i>	0	0	0	0	0
<i>Hexachlorocyclohexane</i>	0	0	0	0	0
<i>Hexadecane</i>	3	1	0	0	4
<i>Homosalate</i>	3	1	0	0	4
<i>Imidacloprid</i>	3	0	0	2	5
<i>Indane</i>	3	2	0	0	5
<i>Indeno(1,2,3-c,d)pyrene</i>	0	0	0	0	0
<i>Isobornyl thiocynoacetate</i>	3	1	0	0	4
<i>Isopropylbenzene</i>	3	1	0	0	4
<i>Isoproturon</i>	0	0	0	0	0
<i>Isopropyl palmitate</i>	3	1	0	0	4
<i>Itraconazole</i>	3	0	0	2	5
<i>Ketoconazole</i>	3	0	0	2	5
<i>Lead*</i>	0	3	1	0	4
<i>Mefentrifluconazole</i>	3	0	0	2	5
<i>Mercury and its compounds*</i>	0	0	0	0	0
<i>Metformin</i>	3	0	0	2	5
<i>Methomyl</i>	3	1	0	0	4
<i>Methyl tert-butyl ether (MTBE)</i>	3	1	0	0	4
<i>Methylbenzotriazole</i>	3	3	1	0	7
<i>Methylparaben</i>	3	1	0	0	4
<i>n-Butylbenzene</i>	3	1	0	0	4
<i>N,N-Diethyl-m-toluamide</i>	3	2	0	0	5
<i>N-1,3-Dimethylbutyl-N'-phenyl-p-phenylenediamine (6PPD)</i>	3	0	0	2	5
<i>Naphthalene</i>	0	1	0	0	1
<i>Naproxen</i>	3	1	0	0	4
<i>Neodecanoic acid-ethenyl ester</i>	3	2	0	0	5
<i>Nickel*</i>	0	3	1	0	4
<i>N-methyl-2-pyrrolidone</i>	3	0	1	0	4

<i>Nonylphenols</i>	0	0	0	0	0
<i>n-Propylbenzene</i>	3	2	0	0	5
<i>Octisalate (2-ethylhexyl salicylate)</i>	3	0	0	2	5
<i>Octocrylene</i>	3	2	0	2	7
<i>Octyl-methoxycinnamate</i>	3	1	0	0	4
<i>Octylphenols</i>	0	0	0	0	0
<i>Ofloxacin</i>	3	0	0	2	5
<i>o-Phenylphenol</i>	3	1	0	0	4
<i>o-Toluidine</i>	3	1	0	0	4
<i>Oxacyclohexadecan-2-one</i>	3	2	0	0	5
<i>o-Xylene</i>	3	1	0	0	4
<i>Oxytetracycline</i>	3	0	0	2	5
<i>P- Chloro-M-Cresol</i>	3	0	0	0	3
<i>Paracetamol</i>	3	0	1	0	4
<i>Pentachlorobenzene</i>	0	0	0	0	0
<i>Pentachlorophenol</i>	0	0	0	0	0
<i>Perfluorooctanesulfonic acid (PFOS)</i>	0	2	1	0	3
<i>Perfluorooctanoic acid (PFOA)</i>	0	3	1	0	4
<i>Phenanthrene</i>	3	2	0	0	5
<i>Phenol</i>	3	2	0	0	5
<i>Polyaromatic hydrocarbons (PAH)</i>	0	0	0	0	0
<i>Promecarb</i>	3	1	0	0	4
<i>Propamocarb</i>	3	0	0	0	3
<i>propan-1,2-diol</i>	3	0	0	0	3
<i>Propiconazole</i>	3	0	0	2	5
<i>Propranolol</i>	3	0	0	2	5
<i>Propylparaben</i>	3	1	0	0	4
<i>Pyrene</i>	3	1	0	0	4
<i>Quinoxifen</i>	0	0	0	0	0
<i>Simazine</i>	0	0	0	0	0
<i>Squalane</i>	3	2	0	0	5
<i>Styrene</i>	3	2	0	0	5
<i>Sulfamethoxazole</i>	3	3	1	0	7
<i>Sulfolane</i>	3	2	0	0	5
<i>Sulphate*</i>	3	3	0	0	6
<i>Terbucarb</i>	3	1	0	0	4
<i>Terbutryn</i>	0	0	0	0	0
<i>Terpineol</i>	3	1	0	0	4
<i>tert-butyl methyl ether; methoxy-2- methylpropane</i>	3	0	0	0	3
<i>Tetrachloroethylene</i>	0	1	0	0	1
<i>Tetracycline</i>	3	0	0	2	5
<i>Toluene</i>	3	0	1	0	4
<i>Tri-(2-chloroethyl) phosphate</i>	3	1	0	0	4
<i>Tributyl acetylcitrate</i>	3	2	0	0	5
<i>Tributyl phosphate</i>	3	2	0	0	5
<i>Tributyltin compounds</i>	0	0	0	0	0

<i>Trichlorobenzenes</i>	0	0	0	0	0
<i>Trichloromethane*</i>	0	3	1	0	4
<i>Tridiphane</i>	3	1	0	0	4
<i>Trifluralin</i>	0	0	0	0	0
<i>Triisobutylphosphate</i>	3	3	0	0	6
<i>Trimethoprim</i>	3	0	1	0	4
<i>Triphenyl phosphate</i>	3	0	0	0	3
<i>Tris-(1,3-dichloroisopropyl) phosphate</i>	3	2	0	0	5
<i>Triticonazole</i>	3	0	0	2	5
<i>Vanillin*</i>	3	1	0	0	4
<i>Xylenes</i>	3	0	1	0	4

Key:

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2 Pollutant not detected in screening exercise: 0 OR Pollutant detected through screening exercise once across water types: 1 OR Pollutant detected through screening exercise at a frequency of 1-5: 2 OR Pollutant detected through screening exercise at a frequency of >5: 3

3 Use of pollutant in Malta not verified through presence in sewerage network (Action C.10): 0 OR Use of pollutant in Malta verified through presence in sewerage network (Action C.10): 2

4 Pollutant not listed in surface and/or groundwater watchlist: 0 OR Pollutant listed in surface and/or groundwater watchlist: 1

* Compound already monitored through other ERA/EWA projects

Table 8 Evaluation of candidate compounds for focused monitoring of groundwater

<i>Compound</i>	<i>1. Regular monitoring process¹</i>	<i>2. Screening process²</i>	<i>3. Use in Malta³</i>	<i>4. Watch list⁴</i>	<i>Score</i>
<i>1,1,1-Trichloroethane</i>	3	0	0	2	5
<i>1,1,2-Trichloroethane</i>	3	0	0	2	5
<i>1,1-Dichloroethane</i>	3	0	0	2	5
<i>1,1-Dichloroethene</i>	3	0	0	2	5
<i>1,2,3-Trichlorobenzene</i>	3	0	0	2	5
<i>1,2,4-Trichlorobenzene</i>	3	0	0	2	5
<i>1,2,4-trimethyl benzene</i>	3	0	0	0	3
<i>1,2-Dichlorobenzene</i>	3	0	0	2	5
<i>1,2-Dichloroethane*</i>	0	0	0	2	2
<i>1,2-dichloropropane</i>	3	0	0	2	5
<i>1,4-Dioxane</i>	3	0	0	2	5
<i>1-Decanol</i>	3	1	0	0	4
<i>1-Ethyl-2-pyrrolidone</i>	3	1	0	0	4
<i>2,4-Di-tert-butylphenol</i>	3	1	0	0	4
<i>2-Ethoxy-2-methylpropane</i>	3	0	0	2	5
<i>2-Ethyl-1,3-hexanediol</i>	3	1	0	0	4
<i>2-Ethylhexanoic acid</i>	3	2	0	0	5
<i>2-Ethylhexyl diphenyl phosphate</i>	3	1	0	0	4
<i>2-Ethylhexyl salicylate</i>	3	1	0	0	4
<i>3-Chlorophenol</i>	3	1	0	0	4
<i>4,4'-Methylenebis (phenyl isocyanate)</i>	3	1	0	0	4
<i>4-chloro-3-methylphenol</i>	3	0	1	0	4
<i>4-Chlorophenol</i>	3	1	0	0	4
<i>4-Methylanisole</i>	3	1	0	0	4
<i>Acesulfame K</i>	3	2	1	0	6
<i>Acetone</i>	3	0	1	0	4
<i>Amidotrizoic Acid</i>	3	0	0	2	5

<i>Ammonium *</i>	0	0	0	0	0
<i>Amoxicillin</i>	3	0	1	0	4
<i>Aniline</i>	3	0	1	0	4
<i>Arsenic *</i>	0	0	0	0	0
<i>Atenolol</i>	3	0	1	0	4
<i>Azoxystrobin</i>	3	0	0	0	3
<i>Benzene</i>	0	0	0	2	2
<i>Benzenesulfonanilide</i>	3	2	0	0	5
<i>Benzophenone</i>	3	3	0	0	6
<i>Benzotriazole</i>	3	2	1	0	6
<i>Benzyl alcohol</i>	3	1	0	0	4
<i>Beta-estradiol</i>	3	0	0	0	3
<i>Bis(2-ethylhexyl) adipate</i>	3	1	0	0	4
<i>Bisphenol A *</i>	0	0	1	0	1
<i>Bromdichloromethane</i>	0	0	0	2	2
<i>Bromoform</i>	3	1	0	0	4
<i>Butylated hydroxytoluene</i>	3	3	0	0	6
<i>Cadmium *</i>	0	0	0	0	0
<i>Caffeine</i>	3	3	0	0	6
<i>Carbamazepine*</i>	0	2	0	2	4
<i>Cedrol</i>	3	1	0	0	4
<i>Chloride *</i>	0	0	0	0	0
<i>Chlorobenzene</i>	3	0	0	2	5
<i>Chloroethane</i>	3	0	0	2	5
<i>Chloromethane/chloroform</i>	0	0	0	2	2
<i>Chloroneb</i>	3	1	0	0	4
<i>Chlorpyrifos-methyl *</i>	0	0	0	0	0
<i>Cholesterol</i>	3	1	0	0	4
<i>cis-1,2-Dichloroethene</i>	3	0	0	2	5
<i>Clarithromycin</i>	3	0	0	2	5
<i>Clopidol</i>	3	0	0	2	5
<i>Coumarin</i>	3	1	0	0	4
<i>Crotamiton</i>	3	0	0	2	5
<i>cyclohexanone</i>	3	0	0	0	3
<i>Bis(2-ethylhexyl) phthalate (DEHP)</i>	3	0	1	0	4
<i>Deltamethrin</i>	3	0	0	0	3
<i>Dibromochloromethane *</i>	0	0	0	2	2
<i>Dichloromethane *</i>	0	0	0	2	2
<i>Diclofenac</i>	3	0	1	0	4
<i>Diethyl phthalate</i>	3	0	1	0	4
<i>Diethylene glycol dimethyl ether</i>	3	0	0	2	5
<i>Diisobutyl phthalate</i>	3	1	0	0	4
<i>Diisopropylether</i>	3	0	0	2	5
<i>Dimethomorph</i>	3	0	0	0	3
<i>Dimethyl phthalate</i>	3	2	0	0	5
<i>Diphenyl ether</i>	3	1	0	0	4
<i>Diphenyl sulfone</i>	3	2	0	0	5
<i>d-Limonene</i>	3	2	0	0	5
<i>EDTA</i>	3	0	0	2	5
<i>Erythromycin</i>	3	0	0	2	5
<i>Ethylbenzene</i>	3	1	0	2	6
<i>Ethylparaben</i>	3	1	0	0	4
<i>Fipronil</i>	3	0	0	0	3
<i>Flurenol-methylester</i>	3	1	0	0	4
<i>Formaldehyde</i>	3	0	1	0	4
<i>Glyphosate *</i>	0	0	1	0	1

Hexadecane	3	1	0	0	4
Ibuprofen *	0	0	0	2	2
Imidacloprid	3	0	0	0	3
Isopropyl myristate	3	1	0	0	4
Isopropylbenzene	3	2	0	2	7
Lead *	0	3	0	0	3
Linalool	3	1	0	0	4
m-Cresol (3-methylphenol)	3	1	0	0	4
Mercury *	0	0	0	0	0
Methylbenzotriazole	3	2	1	0	6
Methylparaben	3	2	0	0	5
Methyltertbutylether (MTBE) *	0	0	1	0	1
m-Xylene	3	1	0	0	4
N,N-Diethyl-m-toluamide	3	2	0	0	5
Naphthalene	0	2	0	0	2
Nitrilotriacetic Acid (NTA)	3	0	0	2	5
N-methyl-2-pyrrolidone	3	0	0	0	3
N-nitrosopiperidine (1-nitrosopiperidin)	3	1	0	0	4
n-Propylbenzene	3	2	0	0	5
o-Cresol (2-methylphenol)	3	1	0	0	4
Octocrylene	3	2	0	0	5
o-Toluidine	3	2	0	0	5
Oxacyclohexadecan-2-one	3	1	0	0	4
o-Xylene	3	1	0	0	4
P- Chloro-M-Cresol	3	0	0	0	3
Paracetamol	3	0	1	0	4
p-Cresol (4-methylphenol)	3	1	0	0	4
Perfluorobutane Sulfonate PFBS *	0	0	0	2	2
Perfluorobutanoic Acid PFBA *	0	0	0	2	2
Perfluorodecanoic Acid PFDA *	0	0	0	2	2
Perfluorododecanoic Acid *	0	0	0	2	2
Perfluoroheptanoic Acid PFHpA *	0	0	0	2	2
Perfluorohexane Sulfonate PFHxS *	0	0	0	2	2
Perfluorohexanoic Acid PFHxA	0	0	0	2	2
Perfluorononanoic Acid PFNA *	0	0	0	2	2
Perfluorooctane Sulfonate PFOS *	0	0	0	2	2
Perfluorooctanoic Acid PFOA *	0	0	0	2	2
Perfluoropentanoic Acid PFPeA *	0	0	0	2	2
Perfluoroundecanoic Acid *	0	0	0	2	2
Phenol	3	2	0	0	5
Primidone	3	0	0	2	5
Promecarb	3	1	0	0	4
Propamocarb	3	0	0	0	3
propan-1,2-diol	3	0	0	0	3
Propylparaben	3	1	0	0	4
p-Xylene	3	1	0	0	4
Sotalol *	0	0	0	2	2
Styrene	3	2	0	0	5
Sulfadiazine	0	0	0	2	2
Sulfamethoxazole *	0	1	1	2	4
Sulfolane	3	2	0	0	5
Sulphate *	0	3	1	0	4
Tert-butanol	3	0	0	2	5
tert-butyl methyl ether; methoxy-2-methylpropane	3	0	0	2	5

<i>Tetrachloroethene</i>	0	0	0	0	0
<i>Tetrachloroethylene</i>	3	1	0	0	4
<i>Tetrachloromethane / Carbon tetrachloride</i>	3	0	0	2	5
<i>Tetraglyme</i>	3	0	0	2	5
<i>Tetrahydrofuran *</i>	0	0	0	2	2
<i>Toluene</i>	3	0	1	2	6
<i>trans-1,2-Dichloroethene</i>	3	0	0	2	5
<i>Tribromomethane</i>	3	0	0	2	5
<i>Tributyl acetylacrylate</i>	3	2	0	0	5
<i>Tributyl phosphate</i>	3	2	0	0	5
<i>Trichloroethylene</i>	0	0	0	2	2
<i>Trichloromethane</i>	3	0	1	0	4
<i>Tridiphenyl</i>	3	1	0	0	4
<i>Trifluoroacetic Acid</i>	3	0	0	2	5
<i>Triisobutylphosphate</i>	3	0	0	0	3
<i>Trimethoprim</i>	3	0	1	0	4
<i>Triphenyl phosphate</i>	3	0	0	0	3
<i>Tris (2,3-epoxypropyl) isocyanate</i>	3	1	0	0	4

Key:

1 Pollutant constitutes a priority substance for surface water or is listed in the Groundwater Directive and thus already subject to regular monitoring in WFD water bodies: 0 OR Pollutant is a Chemical of Emerging Concern that is not subject to regular monitoring in WFD water bodies: 3

2 Pollutant not detected in screening exercise: 0 OR Pollutant detected through screening exercise once across water types: 1 OR Pollutant detected through screening exercise at a frequency of 1-5: 2 OR Pollutant detected through screening exercise at a frequency of >5: 3

3 Use of pollutant in Malta not verified through presence in sewerage network (Action C.10): 0 OR Use of pollutant in Malta verified through presence in sewerage network (Action C.10): 2

4 Pollutant not listed in surface and/or groundwater watchlist: 0 OR Pollutant listed in surface and/or groundwater watchlist: 1

* Compound already monitored through other ERA/EWA projects

The results of Table 7 and Table 8 (hereafter referred to as the Priority Short Lists) evaluated all contaminants that could be considered for monitoring; the lists required further refinement to develop a focused monitoring strategy that considered and matched the specific requirements of Malta. This refinement should take into consideration whether:

- the contaminant is already monitored through official monitoring programmes.
- the contaminant is known to be associated with significant environmental or human health impact.
- other shortlisting is appropriate based on the representativeness of sources (e.g. the same type of contaminants with the same sources can be represented by a few such contaminants).

With respect to point (a), all contaminants that are monitored in other programmes were removed from the selection process. Point (b) required a criterion or formula for evaluating significant environmental or human health impact. The NORMAN⁶ prioritization (referred to in Action A6) is a comprehensive review in evaluating environmental risk of contaminants which uses such a formula.

⁶ Dulio, V., Alygizakis, N., Ng, K., Schymanski, E. L., Andres, S., Vorkamp, K., ... & von der Ohe, P. C. (2024). Beyond target chemicals: updating the NORMAN prioritisation scheme to support the EU chemicals strategy with semi-quantitative suspect/non-target screening data. *Environmental Sciences Europe*, 36(1), 113.

It applies a Risk Quotient (RQ), calculated as $RQ = MEC_{95}/\text{lowest PNEC}$, where MEC is the measured Maximum Environmental Concentration and PNEC is the Predicted No-Effect Concentration. The PNEC is calculated from toxicity values – LC50⁷s – ‘corrected’ to allow for environmental relevance (by multiplying by 10, for example). However, this formula could not be directly applied to the Priority Short Lists because MECs in Malta are not consistently known.

An alternative approach is that taken by the Voluntary Groundwater Watch List⁸, which assessed the likelihood for a contaminant to be in groundwater from its ‘leaching potential’ and combined this with a Hazard Score - based on whether the compound was Persistent, Bio-accumulative, Toxic, Carcinogenic, Mutagenic, Reprotoxic, and/or Endocrine Disrupting. However, the formula used by the Groundwater Watch List could not be used to narrow down the Priority Short Lists because leaching potential only applies to the movement of contaminants from soils to groundwater/surface waters. Furthermore, many chemicals in the Priority Short Lists have not been fully assessed for their modes of toxicity (carcinogenicity etc) - even in drawing up the Voluntary Groundwater Watch List the Hazard Score was not applicable to 58% of the compounds assessed. Therefore, there was a requirement for a new formula that should incorporate an assessment of the likelihood for contamination (equivalent to the MECs and leaching scores) and a measurement of the toxicity (equivalent to the PNEC and Hazard Scores). This led to the development of the following formula:

$$\text{Risk Quotient (RQ)} = \sqrt{(\text{solubility}) \times (1 \div (\text{LC50}_{\text{fish}} \times \text{LC}_{\text{daphnia}}))}$$

The water solubility indicated the likely prevalence in the aquatic environment. Toxicity was assessed through LC50 values of aquatic vertebrates (fish) and invertebrates (daphnia). The LC50 has the advantage of always being available (unlike carcinogenicity (etc) values) and it is an empirical, not derivative, value (unlike PNEC, which is derived from LC50s). The inverse of the LC50s was used because a high LC50 value indicates low toxicity and it was more appropriate for a Risk score to be intuitive (i.e. a high RQ is a higher risk), the square root was taken to narrow down the range of scores which otherwise would range several orders of magnitude (due to differences in toxicity and solubility).

To investigate whether the RQ could be a useful tool in ranking the Priority Short Lists, the RQ was calculated for compounds with a score equal to or greater than 5 for surface waters and 4 for groundwaters (toluene and isopropylbenzene, though scoring 4, were also included in the RQ calculations of surface waters because they were proposed for groundwater monitoring). This allowed for a comparable number of contaminants of both water categories to be assessed. Thus,

⁷ The value of LD₅₀ for a substance is the dose required to kill half the members of a tested population after a specified test duration. LD₅₀ figures are frequently used as a general indicator of a substance's acute toxicity. A lower LD₅₀ is indicative of higher toxicity

⁸ Common Implementation Strategy For The Water Framework Directive And The Floods Directive Voluntary Groundwater Watch List Concept & Methodology Technical Report. https://circabc.europa.eu/sd/a/d3fa0178-0134-4316-a11c-dcfd71efca69/Watch-List_Concept_Final.pdf

the RQ of 85 and 74 compounds was calculated for contaminants of surface and groundwater respectively (Table 16 and Table 17). The data indicates that the RQ is effective in ranking compounds effectively in respect to their likelihood in water and potential impact once there. However, any results from the exercise must be then proposed for analysis at environmentally relevant, or legislated, concentrations and currently analytical technology was only able to specifically test for 34% and 44% of the contaminants assessed for toxicity in surface and groundwater respectively. Nevertheless, analytical techniques are continually improving and therefore the RQ is a useful tool for future selection of the most critical contaminants.

With respect to point (c) of the considerations to select or deselect contaminants for focused monitoring, although compounds share similar uses and therefore potentially similar origins, potentially valuable information may be lost if only representative contaminants are monitored. For instance, the incidence of all 12 pharmaceuticals proposed for surface water testing provides a useful overview of how widespread this category of contaminant is. Therefore, similarity of use has not been applied as a selection criterion.

In conclusion, for focused monitoring, all contaminants with scores equal to or greater than 5 and 4 in the Priority Short lists for Surface and Groundwaters respectively (that aren't already tested in another project) are proposed for analysis. The difference in threshold is due to the number of contaminants in each category. Due to analytical limitations, some of the contaminants can only be assessed as part of the TIC screening (see Appx Table 15), however this offers the advantage of assessing the presence of 1020 compounds, not only those on the Priority Short Lists. For clarification, analysing for a specific compound initially requires that the sample is prepared using various methods specific to the chemical of interest, which isolates the compound before it is measured (it is the developments in these pre-treatments that determines the range of contaminants that can be analysed). In the TIC screening, there is no pre-treatment of the samples; all contaminants within it are measured against a library of known signatures. If the result of the screening shares sufficient similarity with the library signature (50% similarity being the threshold, and 100% being identical) then the identity of the compound is confirmed.

Two compounds that scored '4' in the surface water Priority Short List: Isopropyl benzene and Toluene, will be monitored in surface waters because they are also being monitored in groundwater. Along with other common contaminants being monitored in both water categories, this approach is being taken in order to link any potential connection between surface and groundwater.

Finally, technology doesn't currently permit the analysis of a few contaminants in the short list at environmentally relevant levels. The final list of contaminants for focused monitoring, along with their use, LODs and LOQs are provided in Table 9 and Table 10.

Table 9 Compounds for analysis in focused monitoring of surface waters¹

Compound	Analysis ²	Use	LOD ³ (µg/L)	Surface water LOQ ⁴ (µg/L)	Seawater LOQ ⁴ (µg/L)
1,2,4-trimethyl benzene	GC/MS	solvent	0.3	1	5
1,3,5-Trimethylbenzene	GC/MS	solvent	0.3	1	5
1-Ethyl-2-pyrrolidone	TIC	manufacture	0.1	-	-
1,6-Hexanediol diacrylate	TIC	manufacture	0.1	-	-
2-Ethyl-1,3-hexanediol	TIC	solvent	0.1	-	-
2,4,7,9-Tetramethyl-5-decyne-4,7-diol	TIC	PPP	0.1	-	-
2-Ethylhexanoic acid	TIC	manufacture	0.1	-	-
2-Methylnaphthalene	TIC	manufacture	0.1	-	-
Acesulfame K	GC/MS	food	0.02	0.04	0.1
Acetophenone	TIC	manufacture	0.1	-	-
Amoxicillin	GC/MS	pharmaceutical	0.5	1	1
Aniline	GC/MS	dyes and pigments	0.006	0.02	0.02
Arsenic	GC/MS	manufacture	0.05	1	3
Atenolol	GC/MS	pharmaceutical	0.02	0.04	0.4
Azobenzene	TIC	dyes and pigments	0.1	-	-
Benzenesulfonanilide	TIC	manufacture	0.1	-	-
Benzenesulfonamide, N-butyl	TIC	pharmaceutical	0.1	-	-
Benzophenone	TIC	manufacture	0.1	-	-
Benzotriazole	GC/MS	corrosion inhibitor	0.02	0.05	0.5
Beta-estradiol	GC/MS	manufacture	0.02	0.05	0.5
Bis(2-ethylhexyl) adipate	TIC	plastics	0.1	-	-
Bisphenol A	GC/MS	manufacture	100	300	300
Carbamazepine	GC/MS	pharmaceutical	0.01	0.02	0.15
Chloroxylonol	TIC	pharmaceutical	0.1	-	-
Diclofenac	GC/MS	pharmaceutical	0.025	0.05	0.05
Dicyclohexyl phthalate	TIC	plastics	0.1	-	-
Diethyl phthalate	GC/MS	plastics	0.03	0.1	0.1
Dimethyl phthalate	GC/MS	pharmaceutical	0.03	0.1	0.1
di-n-butyl phthalate	GC/MS	plastics	0.03	0.1	0.1
Diphenyl sulfone	TIC	solvent	0.1	-	-
d-Limonene	GC/MS	manufacture	0.03	0.1	0.1
EDTA	GC/MS	chelating agent	500	1500	1500
(EthylenDiaminoTetracetyc Acid)					
Epoxiconazole	TIC	PPP	0.1	-	-
Ethylbenzene	GC/MS	manufacture	0.001	0.02	0.1
Etoxazole	TIC	PPP	0.1	-	-
Fenpiclonil	TIC	PPP	0.1	-	-
Fipronil	GC/MS	PPP	0.03	0.1	0.1
Fluoxetine	TIC	pharmaceutical	0.1	-	-
Flurenol-methylester	TIC	pharmaceutical	0.1	-	-

<i>Glyphosate</i>	GC/MS	PPP	0.1	-	-
<i>Imidacloprid</i>	GC/MS	PPP	0.1	0.05	0.5
<i>Indane</i>	TIC	Fuels	0.1	-	-
<i>Isopropilbenzene</i>	GC/MS	manufacture	0.001	0.02	0.1
<i>Methylbenzotriazole</i>	GC/MS	corrosion inhibitor	0.02	0.05	0.5
<i>N,N-Diethyl-m-toluamide</i>	TIC	pharmaceutical	0.1	-	-
<i>Neodecanoic acid-ethenyl ester</i>	TIC	dyes and pigments	0.1	-	-
<i>n-Propylbenzene</i>	GC/MS	dyes and pigments	0.001	0.02	0.1
<i>Octocrylene</i>	TIC	cosmetic	0.1	-	-
<i>Oxacyclohexadecan-2-one</i>	TIC	pharmaceutical	0.1	-	-
<i>Phenanthrene</i>	GC/MS	dyes and pigments	0.1	0.05	0.3
<i>Phenol</i>	GC/MS	manufacture	0.01	0.05	0.5
<i>Propiconazole</i>	TIC	PPP	0.1	-	-
<i>Squalane</i>	TIC	cosmetic	0.1	-	-
<i>Styrene</i>	GC/MS	plastics	0.1	1	10
<i>Sulfamethoxazole</i>	GC/MS	pharmaceutical	0.004	0.02	0.03
<i>Toluene</i>	GC/MS	solvent	0.1	0.05	0.3
<i>Tributyl acetylcitrate</i>	TIC	manufacture	0.1	-	-
<i>Tributyl phosphate</i>	TIC	plastics	0.1	-	-
<i>Triisobutylphosphate</i>	GC/MS	manufacture	0.01	0.025	0.025
<i>Tris-(1,3-dichloroisopropyl) phosphate</i>	TIC	plastics	0.1	-	-
<i>6PPD (quinone)</i>	NP	Tyres	-	-	-
<i>Avermectin B1a</i>	NP	manufacture	-	-	-
<i>Avermectin B1b</i>	NP	manufacture	-	-	-
<i>Bromuconazole</i>	NP	PPP	-	-	-
<i>Butyl methoxydibenzoyl-methane</i>	NP	pharmaceutical	-	-	-
<i>Climbazole</i>	NP	pharmaceutical	-	-	-
<i>Clindamycin</i>	NP	pharmaceutical	-	-	-
<i>Cyazofamid</i>	NP	PPP	-	-	-
<i>Difenoconazole</i>	NP	PPP	-	-	-
<i>Guanylurea</i>	NP	manufacture	-	-	-
<i>Itraconazole</i>	NP	pharmaceutical	-	-	-
<i>Ketoconazole</i>	NP	pharmaceutical	-	-	-
<i>Mefentrifluconazole</i>	NP	PPP	-	-	-
<i>Metformin</i>	NP	pharmaceutical	-	-	-
<i>N-1,3-Dimethylbutyl-N'-phenyl-p-phenylenediamine (6PPD)</i>	NP	fuels	-	-	-
<i>Octisalate (2-ethylhexyl salicylate)</i>	NP	cosmetic	-	-	-
<i>Ofloxacin</i>	NP	pharmaceutical	-	-	-
<i>Oxytetracycline</i>	NP	pharmaceutical	-	-	-
<i>Propranolol</i>	NP	pharmaceutical	-	-	-
<i>Sulfolane</i>	NP	solvent	-	-	-

<i>Triticonazole</i>	NP	PPP	-	-	-
<i>Tetracycline</i>	NP	pharmaceutical	-	-	-

1. Surface waters in this context refer to Inland Surface, Stormwater, Transitional, New waters and Coastal waters. 2 Method of analysis: GC/MS – specific analysis, TIC Water screening, NP Analysis not possible. 3. LOD = Limit of Detection (the typical LOD of the screening process is 0.1µg/L) 4. LOQ = Limit of Quantification

Table 10 Compounds for analysis in focused monitoring of groundwater

Compound	Analysis ¹	Use	LOD ² (µg/L)	LOQ ³ (µg/L)
<i>1,1,1-Trichloroethane</i>	TIC	solvent	0.1	-
<i>1,1,2-Trichloroethane</i>	TIC	solvent	0.1	-
<i>1,1-Dichloroethane</i>	NP	solvent	0.1	-
<i>1,1-Dichloroethene</i>	GC/MS	solvent	0.03	0.1
<i>1,2,3-Trichlorobenzene</i>	GC/MS	solvent	0.3	1
<i>1,2,4-Trichlorobenzene</i>	GC/MS	solvent	0.3	1
<i>1,2-Dichlorobenzene</i>	GC/MS	solvent	0.3	1
<i>1,2-dichloropropane</i>	GC/MS	solvent	0.3	1
<i>1,4-Dioxane</i>	TIC	solvent	0.1	-
<i>1-Decanol</i>	TIC	solvent	0.1	-
<i>1-Ethyl-2-pyrrolidone</i>	TIC	manufacture	0.1	-
<i>2,4-Di-tert-butylphenol</i>	TIC	manufacture	0.1	-
<i>2-Ethoxy-2-methylpropane</i>	NP	solvent	0.1	-
<i>2-Ethyl-1,3-hexanediol</i>	TIC	solvent	0.1	-
<i>2-Ethylhexanoic acid</i>	TIC	manufacture	0.1	-
<i>2-Ethylhexyl diphenyl phosphate</i>	TIC	plastics	0.1	-
<i>2-Ethylhexyl salicylate</i>	TIC	cosmetic	0.1	-
<i>3-Chlorophenol</i>	TIC	manufacture	0.1	-
<i>4,4'-Methylenebis (phenyl isocyanate)</i>	TIC	manufacture	0.1	-
<i>4-chloro-3-methylphenol</i>	GC/MS	pharmaceutical	0.3	1
<i>4-Chlorophenol</i>	TIC	dyes and pigments	0.1	-
<i>4-Methylanisole</i>	TIC	manufacture	0.1	-
<i>Acesulfame K</i>	GC/MS	food	0.02	0.04
<i>Acetone</i>	GC/MS	solvent	10	25
<i>Amidotrizoic Acid</i>	NP	pharmaceutical	0.1	-
<i>Amoxicillin</i>	GC/MS	pharmaceutical	0.3	1
<i>Aniline</i>	GC/MS	dyes and pigments	0.006	0.02
<i>Atenolol</i>	TIC	pharmaceutical	0.02	0.04
<i>Benzenesulfonanilide</i>	TIC	manufacture	0.1	-
<i>Benzophenone</i>	TIC	manufacture	0.1	-
<i>Benzotriazole</i>	GC/MS	corrosion inhibitor	0.02	0.05
<i>Benzyl alcohol</i>	TIC	solvent	0.1	-
<i>Bis(2-ethylhexyl) adipate</i>	TIC	plastics	0.1	-
<i>Bis(2-ethylhexyl) phthalate (DEHP)</i>	GC/MS	plastics	0.03	0.1
<i>Butylated hydroxytoluene</i>	TIC	fuels	0.1	-
<i>Caffeine</i>	TIC	food	0.1	-
<i>Cedrol</i>	TIC	pharmaceutical	0.1	-
<i>Chlorobenzene</i>	TIC	solvent	0.1	-
<i>Chloroethane</i>	GC/MS	fuels	0.1	-
<i>Chloroneb</i>	TIC	PPP	0.1	-
<i>Cholesterol</i>	TIC	food	0.1	-

<i>cis</i> -1,2-Dichloroethene	GC/MS	solvent	0.03	0.1
Clarithromycin	NP	pharmaceutical	0.1	-
Clopidol	NP	pharmaceutical	0.1	-
Coumarin	TIC	pharmaceutical	0.1	-
Crotamiton	TIC	pharmaceutical	0.1	-
Diclofenac	GC/MS	pharmaceutical	0.025	0.05
Diethyl phthalate	GC/MS	plastics	0.03	0.1
Diethylene glycol dimethyl ether	TIC	solvent	0.1	-
Diisobutyl phthalate	TIC	plastics	0.1	-
Diisopropylether	NP	solvent	0.1	-
Dimethyl phthalate	GC/MS	pharmaceutical	0.03	0.1
Diphenyl ether	NP	manufacture	0.1	-
Diphenyl sulfone	TIC	solvent	0.1	-
d-Limonene	TIC	manufacture	0.1	-
EDTA	GC/MS	chelating agent	500	1500
Erythromycin	TIC	pharmaceutical	0.1	-
Ethylbenzene	GC/MS	manufacture	0.3	1
Ethylparaben	TIC	food	0.1	-
Flurenol-methylester	TIC	pharmaceutical	0.1	-
Formaldehyde	GC/MS	manufacture	0.1	-
Hexadecane	TIC	pharmaceutical	0.1	-
Isopropyl myristate	TIC	pharmaceutical	0.1	-
Isopropylbenzene	GC/MS	fuels	0.1	-
Linalool	TIC	manufacture	0.1	-
m-Cresol (3-methylphenol)	TIC	manufacture	0.1	-
Methylbenzotriazole	GC/MS	corrosion inhibitor	0.02	0.05
Methylparaben	TIC	cosmetic	0.1	-
m-Xylene	GC/MS	solvent	0.1	1
N,N-Diethyl-m-toluamide	TIC	pharmaceutical	0.1	-
Nitrilotriacetic Acid (NTA)	NP	detergent	0.1	-
N-nitrosopiperidine (1-nitrosopiperidin)	TIC	PPP	0.1	-
n-Propylbenzene	GC/MS	dyes and pigments	0.001	0.02
o-Cresol (2-methylphenol)	GC/MS	PPP	0.006	0.02
Octocrylene	TIC	cosmetic	0.1	-
o-Toluidine	TIC	PPP	0.1	-
Oxacyclohexadecan-2-one	TIC	pharmaceutical	0.1	-
o-Xylene	GC/MS	solvent	0.1	1
Paracetamol	NP	pharmaceutical	-	-
p-Cresol (4-methylphenol)	GC/MS	PPP	0.006	0.02
Phenol	GC/MS	manufacture	0.01	0.05
Primidone	TIC	pharmaceutical	-	-
Promecarb	TIC	PPP	-	-
Propylparaben	TIC	pharmaceutical	-	-
p-Xylene	GC/MS	solvent	0.1	1
Styrene	GC/MS	plastics	2	1
Sulfolane	NP	solvent	-	-
Tert-butanol	NP	solvent	-	-
tert-butyl methyl ether; methoxy-2-methylpropane	GC/MS	fuels	0.1	1
Tetrachloroethylene	GC/MS	detergent	0.03	0.1
Tetrachloromethane / Carbon tetrachloride	NP	manufacture	-	-
Tetraglyme	NP	manufacture	-	-
Toluene	GC/MS	solvent	0.1	0.05

<i>trans-1,2-Dichloroethene</i>	NP	solvent	-	-
<i>Tribromomethane</i>	GC/MS	solvent	0.003	0.01
<i>Tributyl acetylcitrate</i>	TIC	manufacture	-	-
<i>Tributyl phosphate</i>	TIC	plastics	-	-
<i>Trichloromethane</i>	GC/MS	solvent	0.003	0.01
<i>Tridiphane</i>	TIC	PPP	-	-
<i>Trifluoroacetic Acid</i>	NP	manufacture	-	-
<i>Trimethoprim</i>	TIC	pharmaceutical	-	-
<i>Tris (2,3-epoxypropyl) isocyanate</i>	TIC	plastics	-	-

1. Method of analysis: GC/MS – specific analysis, TIC Water screening, NP Analysis not possible. 2. LOD = Limit of Detection (the typical LOD of the screening process is 0.1µg/L) 3. LOQ = Limit of Quantification

3.0 Sample Collection, Laboratory Analysis and Reporting

Before collection of samples, the relevant stakeholders (e.g. WSC) will be contacted and ERA will be notified. Monitoring sites will be grouped geographically to minimize time in transit. Samples will be collected following ISO 5667-1:2020 into clean, new vessels depending on the volume and material of container required by the type of analysis (Table 11).

Table 11 Container type for different parameters

Compound Class	Volume	Container Type	Acid Volume
PFOA/S + Alkylphenols + Pesticide (LC amenable) + Glyphosate + Un-ionized ammonia (NH ₃) + Anions,	500mL	PP PFOA/S free	
POPs + Pesticide (GC amenable), PAH + SVOC Dioxins and dioxin-like compounds (HRMS). TIC screening	6 x 1 L	Dark Glass	
VOC	2 x 40 mL	Glass	2 drops HCl
Metal	50mL	Falcon or PP	2 drops HNO ₃

For samples taken from a tap (e.g. groundwater), to ensure a representative sample is taken (rather than standing water in the pipework), the water will be purged by running the tap for approximately 5 minutes while measuring both pH and conductivity - only taking samples once these parameters are stable. Sampling will be otherwise conducted as per ISO5667-1:2020. Once collected and prepared, samples will be boxed in specialized secure boxes, and ice blocks added. Samples will then be couriered to the analysing laboratory as soon as possible.

All analyses will be carried out by Biochemie Lab SRL (Accredited by Accredia No. 0195, see Annex 1) This laboratory is accredited to UNI CEI EN ISO IEC 17025:2017 to analyze the required parameters in accordance with MSA EN ISO/IEC-17025:2005 (see Appx 1).

Results will be collated and sorted into sample type (coastal, new water etc) and sent to stakeholders at ERA and EWA when available. The final report will summarise findings, noting any compounds that were found in excess of EQS, and providing recommendations for future monitoring. This report will be submitted to stakeholders once all results are compiled (Table 12)

Table 12 Sampling schedule and report deadlines

Months	M27	M28	M29	M30
Date	Sep-24	Oct	Nov	Dec
Updated monitoring strategy - DRAFT				
Updated monitoring Strategy - FINAL				

Months	M31	M32	M33	M34	M35	M36	M37	M38	M39	M40	M41	M42	M43
Date	Jan-25	Feb	Mar	Apr	May	Jun	Jul	Aug	Sept	Oct	Nov	Dec	Jan-26
Updated monitoring Strategy - FINAL													
Surveying													
Draft report on the Focused Monitoring													

Months	M44	M45
Date	Feb-26	Mar-26
Approval of Final report on the Focused Monitoring		

Annex 1.0 Accreditation certificate



DL0195L/006

CERTIFICATO DI ACCREDITAMENTO Accreditation Certificate

ACCREDITAMENTO N.
ACCREDITATION N. **0195L REV. 06**

EMESSO DA
ISSUED BY **DIPARTIMENTO LABORATORI DI PROVA**

SI DICHIARA CHE
WE DECLARE THAT **BIOCHEMIE LAB S.r.l.**
Sede/Headquarters:
- Via di Limite 27/G - 50013 Campi Bisenzio FI

MD-CAL rev. 06

È CONFORME AI REQUISITI
DELLA NORMA **UNI CEI EN ISO/IEC 17025:2018**

MEETS THE REQUIREMENTS
OF THE STANDARD **ISO/IEC 17025:2017**

QUALE **Laboratorio di Prova**
AS **Testing Laboratory**

Data di 1ª emissione
1st issue date
29-10-1998

Data di revisione
Review date
15-11-2022

Data di scadenza
Expiring date
10-12-2026

L'accertamento attesta la competenza tecnica, l'imparzialità e il costante e coerente funzionamento del Laboratorio relativamente al campo di accreditamento riportato nell'elenco Prove allegato al presente certificato di accreditamento.
Il presente certificato non è da ritenersi valido se non accompagnato dagli Elenchi Prove, che possono variare nel tempo e può essere sospeso o revocato o ridotto in qualsiasi momento nel caso di inadempienza accertata da parte di ACCREDIA.
La validità dell'accertamento può essere verificata sul sito web (www.accredia.it) o richiesta al Dipartimento di competenza.
I requisiti di sistema della ISO/IEC 17025 sono scritti in un linguaggio attinente alle attività di laboratorio e sono generalmente in accordo con i principi della norma ISO 9001 (si veda comunicato congiunto ISO-ILAC-IAF dell'Aprile 2017).
The accreditation attests competence, impartiality and consistent operation in performing laboratory activities, limited to the scope detailed in the attached Enclosure.
The present certificate is valid only if associated to the annexed Lists and can be suspended, withdrawn or reduced at any time in the event of non fulfilment as ascertained by ACCREDIA.
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The management system requirements in ISO/IEC 17025 are written in language relevant to laboratories operations and generally operate in accordance with the principles of ISO 9001 (refer joint ISO-ILAC-IAF Communiqué dated April 2017).

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Sede operativa, legale e amministrativa: Via Guglielmo Salice to, 7/9 | 00161 Roma - Italy
Tel. +39 06 8440991 | Fax +39 06 8841199
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Appendices

Appx 1. Testing parameters of ERA12

Table 13 Compound of Emerging Concern (CEC)

Aniline	Propamocarb
Fipronil	Imidacloprid
Chlorpyrifos-methyl	Acesulpham k
Deltamethrin	Carbamazepine
Triisobutyl phosphate	Beta-estradiol (50-28-2)
Triphenyl phosphate	Atenolol
P- Chloro-M-Cresol	Sulfamethoxazole
DEHP	Amoxicillin
Diethyl phthalate (DEP)	Methylbenzotriazole
1,2,4-trimethyl benzene	Benzotriazole
Cyclohexanone	Bisphenol A
Tert-butyl methyl ether; MTBE; 2- methoxy-2-methylpropane	N-methyl-2-pyrrolidone
Styrene	Propan-1,2-diol
Azoxystrobin	Glyphosate
Dimethomorph	EDTA

Table 14 Indicators of diffuse pollution

Alachlor	Heptachlor
Atrazine	Heptachlor epoxide
Chlorfenvinphos	Brominated diphenylethers
Chlorpyrifos or Chlorpyrifos-ethyl	Chloroalkanes, C10-13
Endrin	Hexabromocyclododecane
Isodrin	<i>Benzo(b)fluoranthene + Benzo(k)fluoranthene + Benzo(a)pyrene + Benzo(g,h,i)perylene + Indeno(1,2,3-cd)pyrene</i>
Aldrin	Anthracene
Dieldrin	Fluoranthene (PHC)
p,p'-DDD	Hexachlorobenzene
p,p'-DDE	Naphthalene
DDT Total o,p' + p,p'	Pentachlorobenzene
p,p'-DDT	Pentachlorophenol
o,p'-DDD	Benzo(a)pyrene
o,p'-DDE	Benzo(b)fluoranthene
<i>o,p'-DDT</i>	Benzo(ghi)perylene
Chlordane	Benzo(k)fluoranthene
Cis-chlordane	Indeno(1,2,3-cd)pyrene
Trans-chlordane	Trichlorobenzenes
Endosulfan	Di(2-ethylhexyl)phthalate
<i>Alpha-endosulfan (endosulphan I)</i>	Benzene
<i>Beta-endosulfan (endosulphan II)</i>	Carbon tetrachloride
Endosulfan sulfate	1,2- Dichloroethane

Hexachlorocyclohexanes	Dichloromethane
<i>Alpha-hexachlorocyclohexane (alfa-HCH)</i>	Hexachlorobutadiene
<i>Beta-hexachlorocyclohexane(beta-HCH)</i>	Tetrachloroethylene
<i>Delta hexachlorocyclohexane (delta-HCH)</i>	Trichloroethylene
<i>Gamma-hexachlorocyclohexane (Lindane)</i>	Trichloromethane
Methoxychlor	Diuron
o,p-methoxychlor	Famphur
p,p-methoxychlor	Fensulfotion
Isoproturon	Nonylphenols
Simazine	4-nonylphenol (CAS: 104-40-5)
Trifluralin	Octylphenols
Dicofol	Cadmium
Quinoxifen	Lead
Aclonifen	Mercury and its compound as Total Mercury
Bifenox	Nickel and its compounds as Total Nickel
Cybutryne	Arsenic
Cypermethrine	Dioxins and dioxin-like compounds HRMS
Dichlorvos	Ammonium (Un-ionized ammonia (NH3))
Terbutryn	Chloride
Ametryn	Sulphate
Azinphos-ethyl	Tributyltin compounds
Azinphos-methyl	PFOA and its compounds
Chlordecone	<i>Benzo(b)fluoranthene + Benzo(k)fluoranthene + Benzo(a)pyrene + Benzo(g,h,i)perylene + Indeno(1,2,3-cd)pyrene</i>
Coumafos	Anthracene
Crotoxyfos	Fluoranthene (PHC)
Cyanazine	Hexachlorobenzene
Desmetryn	Naphthalene
Diazinone	Pentachlorobenzene
Dimethoate	Pentachlorophenol
Fenitrothion	Benzo(a)pyrene
Fenthion	Benzo(b)fluoranthene
Leptofos	Benzo(ghi)perylene
Malathion	Benzo(k)fluoranthene
Methidation	Indeno(1,2,3-cd)pyrene
Metolachlor	Trichlorobenzenes
Mevinfos	Di(2-ethylhexyl)phthalate
Mirex	Benzene
Molinate	Carbon tetrachloride
Parathion-ethyl	1,2- Dichloroethane
Parathion-methyl	Triazophos
Pendimethalin	Heptachlor
Phorate	Heptachlor epoxide
Prometryn	Brominated diphenylethers
Propazine	Chloroalkanes, C10-13
Terbutylazine	Hexabromocyclododecane
Tetrachlorvinphos	

Table 15 Chemicals tested for within 'Tentatively Identified Compounds' Screening Assay

Compound List	
Name	CAS#
1(3H)-Isobenzofuranone	87-41-2
1,1,1,2-Tetrachloroethane	630-20-6
1,1,2,2-Tetrachloroethane	79-34-5
1,1,2-Trichloroethane	79-00-5
1,2,3,4,6,7,8-Heptachlorodibenzofuran	67562-39-4
1,2,3,4,6,7,8-Heptachlorodibenzo-p-diox	35822-46-9
1,2,3,4,7,8-Hexachlorodibenzofuran	70648-26-9
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	39227-28-6
1,2,3,7,8-Pentachlorodibenzofuran	57117-41-6
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	40321-76-4
1,2,3-Trichlorobenzene	87-61-6
1,2,3-Trichloropropane	96-18-4
1,2,4,5-Tetrachlorobenzene	95-94-3
1,2,4-Trichlorobenzene	120-82-1
1,2,4-Trimethylbenzene	95-63-6
1,2-Dibromoethane	106-93-4
1,2-Dichlorobenzene	95-50-1
1,2-Dichloropropane	78-87-5
1,3,5-Triallyl-1,3,5-triazine-2,4,6	1025-15-6
1,3,5-Trichlorobenzene	108-70-3
1,3,5-Trimethylbenzene	108-67-8
1,3,5-Trinitrobenzene	99-35-4
1,3-Dichlorobenzene	541-73-1
1,3-Dichloropropane	142-28-9
1,4-Dichlorobenzene	106-46-7
1,4-Dioxane	123-91-1
1,4-Naphthoquinone	130-15-4
1,6-Hexanediol diacrylate	13048-33-4
17a-Ethynylestradiol	57-63-6
1-Decanol	112-30-1
1-Ethyl-2-pyrrolidone	2687-91-4
1H-Benzotriazole	95-14-7
1H-Benzotriazole-5-methyl	136-85-6
1-Isocyanato-3-methyl-Benzene	621-29-4
1-Naphthylamine	134-32-7
2-(1-naphthyl)acetamide	86-86-2
2-(2-Butoxyethoxy)ethyl thiocyanate	112-56-1
2(3H)-Benzothiazolone	934-34-9
2-(Octylthio)ethanol	3547-33-9
2,2',3,3',4,4',5,5',6-nonachlorobiphenyl	40186-72-9
2,2',3,3',4,4',5-Heptachlorobiphenyl	35065-30-6
2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3
2,2',3,4,4',5',6-Heptachlorobiphenyl	52663-69-1

Name	CAS#
Epichlorhydrin	106-89-8
EPN	2104-64-5
Epoxiconazole	133855-98-8
Epsilon-HCH	6108-10-7
EPTC	759-94-4
Erbon	136-25-4
Esfenvalerate	66230-04-4
Esprocarb	85785-20-2
Estazolam	29975-16-4
Etaconazole	71245-23-3
Ethalfuralin	55283-68-6
Ethiofencarb	29973-13-5
Ethiolate	2941-55-1
Ethion	563-12-2
Ethofumesate	26225-79-6
Ethoprophos	13194-48-4
Ethoxyquin	91-53-2
Ethyl methanesulfonate	62-50-0
Ethylbenzene	100-41-4
Ethylene thiourea	96-45-7
Ethylparaben	120-47-8
Etoxazole	153233-91-1
Etridiazole	2593-15-9
Etrimfos	38260-54-7
Eugenol	97-53-0
Famoxadone	131807-57-3
Famphur	52-85-7
Farnesol	4602-84-0
Fenarimol	60168-88-9
Fenazaflor	14255-88-0
Fenazaquin	120928-09-8
Fenbuconazole	11961-10-0
Fenchlorphos	299-84-3
Fenfuram	24691-80-3
Fenhexamide	126833-17-8
Fenitrothion	122-14-5
Fenobucarb	3766-81-2
Fenoprop	93-72-1
Fenoprop methyl ester	4841-20-7
Fenoxaprop-ethyl	82110-72-3
Fenoxycarb	79127-80-3
Fenpiclonil	74738-17-3
Fenpropathrin	64257-84-7
Fenpropidin	67306-00-7

2,2',3,4,4',5'-Hexachlorobiphenyl	35065-28-2
2,2',3,4',5,5',6-Heptachlorobiphenyl	52663-68-0
2,2',3,4,5,5'-Hexachlorobiphenyl	52712-04-6
2,2',3,4,5'-Pentachlorobiphenyl	38380-02-8
2,2',3,5,5',6-Hexachlorobiphenyl	52663-63-5
2,2',3,5'-Tetrachlorobiphenyl	41464-39-5
2,2',4,4',5,5'-Hexabromodiphenyl	68631-49-2
2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1
2,2',4,4',5,6'-Hexabromodiphenyl ether	207122-15-4
2,2',4,4',5-Pentabromodiphenyl ether	60348-60-9
2,2',4,4',6-Pentabromodiphenyl ether	189084-64-8
2,2',4,5,5'-Pentachlorobiphenyl	37680-73-2
2,2',5,5'-Tetrachlorobiphenyl	35693-99-3
2,2',5-Trichlorobiphenyl	37680-65-2
2,3,3',4',6-Pentachlorobiphenyl	38380-03-9
2,3',4,4'-Tetrachlorobiphenyl	32598-10-0
2,3,4,5-Tetrachlorophenol	4901-51-3
2,3,4,6-Tetrachlorophenol	58-90-2
2,3,4-Trichloroanisole	54135-80-7
2,3,5,6-Tetrachloroaniline	3481-20-7
2,3,5,6-Tetrachlorophenol	935-95-5
2,3,5,6-Tetrachlorothioanisole	68671-90-9
2,3,5-Trichlorophenol	933-78-8
2,3,5-Trimethacarb	2655-15-4
2,3,5-Trimethylphenyl methyl carbamate	2655-15-4
2,3,6-TBA	50-31-7
2,3,7,8-Tetrachlorodibenzofuran	51207-31-9
2,3,7,8-Tetrachlorodibenzo-p-dioxin	1746-01-6
2,3-Dichlorobiphenyl	16605-91-7
2,3-Dimethylphenol	526-75-0
2,4,4'-Tribromodiphenyl ether	41318-75-6
2,4,5-T methyl ester	1928-37-6
2,4',5-Trichlorobiphenyl	16606-02-3
2,4,5-Trichlorophenol	95-95-4
2,4,6-Triallyloxy-1,3,5-triazine	101-37-1
2,4,6-Tribromoanisole	607-99-8
2,4,6-Tribromophenol	118-79-6
2,4,6-Trichloroanisole	87-40-1
2,4,6-trichlorophenol	88-06-2
2,4,7,9-Tetramethyl-5-decyne-4,7-diol	126-86-3
2,4-Dichlorophenoxyacetic acid	94-75-7
2,4-D methyl ester	1928-38-7
2,4-D sec-butyl ester	000000-00-3
2,4-DB methyl ester	18625-12-2
2,4-Dichlorobenzamide	2447-79-2
2,4-Dichlorophenol	120-83-2

Fenpropimorph	67306-03-0
Fenson	80-38-6
Fensulfothion	115-90-2
Fenthion	55-38-9
Fenthion sulfoxide	000000-00-4
Fenuron	101-42-8
Fenvalerate I	51630-58-1
Fenvalerate II	51630-58-1
Fipronil	120068-37-3
Flamprop-isopropyl	52756-22-6
Flamprop-methyl	52756-25-9
Flonicamid	158062-67-0
Florfenicol	73231-34-2
Fluazifop-P-butyl	79241-46-6
Fluazinam	79622-59-6
Flubenzimine	37893-02-0
Fluchloralin	33245-39-5
Flucythrinate I	70124-77-5
Flucythrinate II	70124-77-5
Fludioxonil	131341-86-1
Flufenacet	142459-58-3
Flumetralin	62924-70-3
Flumioxazin	103361-09-7
Fluometuron	2164-17-2
Fluopicolide	239110-15-7
Fluoranthene	206-44-0
Fluorene	86-73-7
Fluorodifen	15457-05-3
Fluotrimazole	31251-03-3
Fluoxastrobilin	361377-29-9
Fluoxetine (Prozac)	54910-89-3
Fluquinconazole	136426-54-5
Flurbiprofen	5104-49-4
Flurenol-butyl ester	2314-09-2
Flurenol-methylester	1216-44-0
Fluridone	59756-60-4
Flurochloridone I	61213-25-0
Flurochloridone II	61213-25-0
Fluroxypyr-1-methylheptyl ester	81406-37-3
Flurtamone	96525-23-4
Flusilazole	85509-19-9
Flutolanil	66332-96-5
Flutriafol	76674-21-0
Fluvalinate-tau-I	10285-10-6
Fluvalinate-tau-II	10285-10-6
Folione	111-12-6

2,4-Dichlorophenyl benzenesulfonate	97-16-5
2,4-Dimethylaniline	95-68-1
2,4-Dimethylphenol	105-67-9
2,4-Dinitrophenol	51-28-5
2,4-Dinitrotoluene	121-14-2
2,4-Di-tert-butylphenol	96-76-4
2,6-Dichlorobenzamide	2008-58-4
2,6-Dichlorobenzonitrile	1194-65-6
2,6-Dichlorophenol	87-65-0
2,6-Difluorobenzamide	18063-03-1
2,6-Dimethylaniline	87-62-7
2,6-Dimethylphenol	576-26-1
2,6-Dinitrotoluene	606-20-2
2,6-Di-tert-butylphenol	128-39-2
2-[3-Chlorophenoxy]propionamide	5825-87-6
2-Acetylaminofluorene	53-96-3
2-Chloro-4-nitrotoluene	121-86-8
2-Chloro-5-nitrotoluene	13290-74-9
2-Chloro-6-nitrotoluene	83-42-1
2-Chlorobiphenyl	2051-60-7
2-Chloronaphthalene	91-58-7
2-Chlorophenol	95-57-8
2-Chlorophenyl isocyanate	3320-83-0
2-Chlorotoluene	95-49-8
2-Ethyl-1,3-hexanediol	94-96-2
2-Ethyl-4-methyl-1,3-dioxolane	4359-46-0
2-Ethyl-5,5-dimethyl-1,3-dioxane	768-58-1
2-Ethylhexanoic acid	149-57-5
2-Ethylhexyl diphenyl phosphate	1241-94-7
2-Ethylhexyl salicylate	118-60-5
2H-Indol-2-one, 1,3-dihydro	59-48-3
2-Hydroxyestradiol	362-05-0
2-Methoxynaphthalene	93-04-9
2-Methyl-4,6-dinitrophenol	534-52-1
2-Methylnaphthalene	91-57-6
2-Naphthylamine	91-59-8
2-Nitroaniline	88-74-4
2-Nitrophenol	88-75-5
2-Octyl-4-isothiazolin-3-one	26530-20-1
2-Phenoxypropionic acid	940-31-8
2-Picoline	109-06-8
2-tert-Butylcyclohexanone	1728-46-7
3,3'-Dichlorobenzidine	91-94-1
3,3'-Dimethylbenzidine	119-93-7
3,4,5-Trimethacarb	2686-99-9
3,4-Dichloroaniline	95-76-1

Folpet	133-07-3
Fonofos	944-22-9
Formothion	2540-82-1
Fosthiazate	98886-44-3
Fuberidazole	3878-19-1
Furalaxyl	57646-30-7
Furathiocarb	65907-30-4
Furfural	98-01-1
Furfuryl alcohol	98-00-0
Furmecyclox	60568-05-0
Gabapentin	60142-96-3
gamma-BHC (lindane)	58-89-9
Gemfibrozil	25812-30-0
Geraniol	106-24-1
Glutaraldehyde	111-30-8
Griseofulvin	126-07-8
Heptachlor	76-44-8
Heptachlor epoxide -isomer B	1024-57-3
Heptachlor exo-epoxide isomer B	28044-83-9
Heptenophos	23560-59-0
Heroin Hydrochloride	1502-95-0
Hexabromobenzene	87-82-1
Hexachlorobenzene	118-74-1
Hexachlorobutadiene	87-68-3
Hexachlorocyclopentadiene	77-47-4
Hexachloroethane	67-72-1
Hexachlorophene	70-30-4
Hexachloropropene	1888-71-7
Hexaconazole	79983-71-4
Hexadecane	544-76-3
Hexametapol	680-31-9
Hexazinone	51235-04-2
Hexestrol	84-16-2
Hexyl Cinnamaldehyde	101-86-0
Hexyl salicylate	6259-76-3
Homosalate	118-56-9
Hydroxy Citronellal	107-75-5
Ibuprofen	15687-27-1
Imazalil	35554-44-0
Imazapyr	81334-34-1
Imidacloprid	138261-41-3
Indane	496-11-7
Indene	95-13-6
Indeno[1,2,3-cd]pyrene	193-39-5
Indosulfuron methyl Na (breakdown product)	144550-36-7
Indoxacarb	173584-44-6

3,5-Dichloroaniline	626-43-7
3,5-Dimethylphenol	108-68-9
3-Chloro-1,2-dibromopropane	96-12-8
3-Chloroaniline	108-42-9
3-Chlorophenol	108-43-0
3-Hydroxycarbofuran	16655-82-6
3-Iodo-2-propynyl butylcarbamate	55406-53-6
3-Methylcholanthrene	56-49-5
3-nitroaniline	99-09-2
4,4'-DDD	72-54-8
4,4'-DDE	72-55-9
4,4'-DDT	50-29-3
4,4'-Dichlorobenzophenone	90-98-2
4,4'-Methylenebis (phenyl isocyanate)	101-68-8
4-Aminobiphenyl	92-67-1
4-Bromophenyl phenyl ether	101-55-3
4-Chloro-2-methylphenol	1570-64-5
4-Chloro-2-nitrotoluene	89-59-8
4-Chloro-3-methylphenol	59-50-7
4-Chloro-3-nitrotoluene	89-60-1
4-Chloroaniline	106-47-8
4-Chlorophenol	106-48-9
4-Chlorophenyl phenyl ether	7005-72-3
4-Chlorotoluene	106-43-4
4-Methylanisole	104-93-8
4-Methyl-benzylidene camphor	36861-47-9
4-Nitroaniline	100-01-6
4-Nitrophenol	100-02-7
4-Nitroquinoline-1-oxide	56-57-5
4-Nonylphenol	104-40-5
4-Octyne	1942-45-6
4-tert-Butyltoluene	98-51-1
4-tert-Octylphenol	140-66-9
5,7-Dihydroxy-4'-methoxyisoflavone	491-80-5
5-Nitro-o-toluidine	99-55-8
7,12-Dimethylbenz[a]anthracene	57-97-6
9,10-Anthraquinone	84-65-1
a,a-Dimethylphenethylamine	122-09-8
acenaphthene	83-32-9
Acenaphthylene	208-96-8
Acephate	30560-19-1
Acetamiprid	160430-64-8
Acetochlor	34256-82-1
Acetophenone	98-86-2
Acifluorfen methyl ester	050594-67-7
Aclonifen	74070-46-5
Alachlor	15972-60-8

loxynil	1689-83-4
Ipconazole	125225-28-7
Iprobenfos	26087-47-8
Iprodione	36734-19-7
Irgarol	28159-98-0
Isazophos	42509-80-8
Isobenzan	297-78-9
Isobornyl thiocynoacetate	115-31-1
Isocarbamide	30979-48-7
Isodecyl diphenyl phosphate	29761-21-5
Isodrin	465-73-6
Isoeugenol	97-54-1
Isufenphos	25311-71-1
Isomethiozin	57052-04-7
Isophorone	78-59-1
Isoprocab	2631-40-5
Isopropalin	33820-53-0
Isopropyl myristate	110-27-0
Isopropyl palmitate	142-91-6
Isopropylbenzene	98-82-8
Isoprothiolane	50512-35-1
Isoproturon	34123-59-6
Isopyrazam	881685-58-1
Isosafrole	120-58-1
Isoxaben	82558-50-7
Isoxaflutole	141112-29-0
Isoxathion	18854-01-8
Jodfenphos	18181-70-9
Kepone	143-50-0
Ketoprofen	22071-15-4
Kinoprene	43588-37-4
Kresoxim-methyl	143390-89-0
Lenacil	2164-08-1
Leptophos	21609-90-5
Leptophos oxon	25006-32-0
Lidocaine	137-58-6
Lilial	80-54-6
Linalool	78-70-6
Linuron	330-55-2
Malathion	121-75-5
Malathion-o-analog	1634-78-2
MCPA	94-74-6
MCPA methyl ester	2436-73-9
MCPB	94-81-5
MCPB methyl ester	57153-18-1
m-Cresol (3-methylphenol)	108-39-4
m-Dinitrobenzene	99-65-0

Aldrin	309-00-2
Allidochlor	93-71-0
alpha Isomethyl Ionone	127-51-5
alpha-BHC (alpha-HCH)	319-84-6
Alprazolam	28981-97-7
Ambroxol	18683-91-5
Ametryn	834-12-8
Amidithion	919-76-6
Aminocarb	2032-59-9
Aminopyralid	150114-71-9
Amitraz	33089-61-1
Amitrole	61-82-5
Amyl Cinnamal	122-40-7
Amylcinnamyl Alcohol	101-85-9
Ancymidol	12771-68-5
Androstadienedione	897-06-3
Anilazine	101-05-3
Aniline	62-53-3
Anisyl Alcohol	105-13-5
Anthracene	120-12-7
Aramite	140-57-8
Atraton	1610-17-9
Atrazine	1912-24-9
Atrazine desethyl	6190-65-4
Atrazine desisopropyl	1007-28-9
Azaconazole	60207-31-0
Azamethiphos	35575-96-3
Azinphos-ethyl	2642-71-9
Azinphos-methyl	86-50-0
Aziprotryne	4658-28-0
Azobenzene	103-33-3
Azoxystrobin	131860-33-8
Barban	101-27-9
Benalaxyl	71626-11-4
Benazolin-ethyl	25059-80-7
Bendiocarb	22781-23-2
Benfluralin	1861-40-1
Benfuracarb	82560-54-1
Benfuresate	68505-69-1
Benodanil	15310-01-7
Bentazone	25057-89-0
Bentazone methyl derivative	61592-45-8
Benthocarb	28249-77-6
Benz[a]anthracene	56-55-3
Benzenepropanoic acid	501-52-0
Benzenesulfonamide	98-10-2

Mecarbam	2595-54-2
Mecoprop	93-65-2
Mecoprop methyl ester	23844-56-6
Mefenacet	73250-68-7
Mefluidide	53780-34-0
Menazon	78-57-9
Mephosfolan	950-10-7
Mepronil	55814-41-0
Mesosulfuron methyl (breakdown product)	208465-21-8
Metalaxyl	57837-19-1
Metaldehyde	108-62-3
Metamitron	41394-05-2
Metasystox thiol	919-86-8
Metazachlor	67129-08-2
Methabenzthiazuron	18691-97-9
Methacrifos	62610-77-9
Methamidophos	10265-92-6
Methapyrilene	91-80-5
Methaqualone	72-44-6
Methfuroxam	2873-17-8
Methidathion	950-37-8
Methiocarb	2032-65-7
Methiocarb sulfone	2179-25-1
Methiocarb sulfoxide	2635-10-1
Methomyl	16752-77-5
Methoprene I	40596-69-8
Methoprene II	40596-69-8
Methoprotryne	841-06-5
Methoxychlor	72-43-5
Methyl Methacrylate	80-62-6
Methyl methanesulfonate	66-27-3
Methyl paraoxon	950-35-6
methyl Parathion	298-00-0
Methyl-1-naphthalene acetate	2876-78-0
Methylcyclohexanone	108-87-2
Methyldymron	42609-73-4
Methylparaben	99-76-3
Metobromuron	3060-89-7
Metolachlor	51218-45-2
Metolcarb	1129-41-5
Metribuzin	21087-64-9
Metronidazole	443-48-1
Mevinphos	7786-34-7
Midazolam	59467-70-8
Mirex	2385-85-5
Molinate	2212-67-1

Benzenesulfonamide, 4-methyl-	70-55-3
Benzenesulfonamide, N-butyl	3622-84-2
Benzenesulfonanilide	1678-25-7
Benzo[a]pyrene	50-32-8
Benzo[b]fluoranthene	205-99-2
Benzo[ghi]perylene	191-24-2
Benzo[k]fluoranthene	207-08-9
Benzonitrile	100-47-0
Benzophenone	119-61-9
Benzophenone-3	131-57-7
Benzoylprop ethyl	22212-55-1
Benzyl alcohol	100-51-6
Benzyl Benzoate	120-51-4
Benzyl Cinnamate	103-41-3
Benzyl laurate	140-25-0
Benzyl Salicylate	118-58-1
b-Estradiol	50-28-2
beta-BHC (beta-HCH)	319-85-7
Bifenazate	149877-41-8
Bifenox	42576-02-3
Bifenthrin	82657-04-3
Binapacryl	485-31-4
Bioallethrin	584-79-2
Bioallethrin S-cyclopentenyl isomer	28434-00-6
Bioresmethrin	10453-86-8
Biphenyl	92-52-4
Bis (4-chlorophenyl) sulfone	80-07-9
bis(2-chloroethoxy)methane	111-91-1
bis(2-chloroethyl) ether	111-44-4
bis(2-chloroisopropyl) ether	108-60-1
Bis(2-ethylhexyl) adipate	103-23-1
bis(2-ethylhexyl)phthalate (DEHP)	117-81-7
Bisphenol A	80-05-7
Bitertanol I	55179-31-2
Bitertanol II	55179-31-2
Bixafer	581809-46-3
Boscalid	188425-85-6
Bromacil	314-40-9
Bromazepam	1812-30-2
Bromobenzene	108-86-1
Bromobutide	74712-19-9
Bromocyclen	1715-40-8
Bromodichloromethane	75-27-4
Bromoform	75-25-2

Monalide	7287-36-7
Monocrotophos	6923-22-4
Monolinuron	1746-81-2
Monuron	150-68-5
Musk Xylene	81-15-2
m-Xylene	108-38-3
Myclobutanil	88671-89-0
N,N,N',N'-Tetraacetylenediamine	10543-57-4
N,N-Diethyl-m-toluamide	134-62-3
N,N-Dimethylaniline	121-69-7
N-1-Naphthylacetamide	000575-36-0
Nalorphine	62-67-9
Naphthalene	91-20-3
Naphthalic anhydride	81-84-5
Napropamide	15299-99-7
Naproxen	22204-53-1
n-Butylbenzene	104-51-8
Neodecanoic acid-ethenyl ester	51000-52-3
Nerolidol	7212-44-4
Nicotine	54-11-5
Nitralin	4726-14-1
Nitrapyrin	1929-82-4
Nitrazepam	146-22-5
Nitrobenzene	98-95-3
Nitrofen	1836-75-5
Nitrothal-isopropyl	10552-74-6
Nitroxynil	1689-89-0
N-Methyl-N-1-naphthyl acetamide	000000-00-2
N-nitrosodiethylamine	55-18-5
N-nitrosodimethylamine	62-75-9
N-nitrosodi-n-butylamine	924-16-3
N-nitrosodi-n-propylamine	621-64-7
N-nitrosodiphenylamine	86-30-6
N-nitrosomethylethylamine	10595-95-6
N-nitrosomorpholine (4-nitrosomorpholin	59-89-2
N-nitrosopiperidine (1-nitrosopiperidin	100-75-4
N-nitrosopyrrolidine (1-nitrosopyrrolid	930-55-2
Norflurazon	27314-13-2
N-Phenyl-1-naphthylamine	90-30-2
n-Propylbenzene	103-65-1
Nuarimol	63284-71-9
O,O,O-Triethyl phosphorothioate	126-68-1
o,p'-DDD	53-19-0
o,p'-DDE	3424-82-6

Bromophos	2104-96-3
Bromophos-ethyl	4824-78-6
Bromopropylate	18181-80-1
Bromoxynil	1689-84-5
Bromoxynil octanoic acid ester	1689-99-2
Bupirimate	41483-43-6
Buprofezin	69327-76-0
Butabarbital	125-40-6
Butachlor	23184-66-9
Butamifos	36335-67-8
Butanedioic acid, dimethyl ester	106-65-0
Butoxycarboxim	34681-23-7
Butralin	33629-47-9
butyl benzyl phthalate	85-68-7
Butylate	2008-41-5
Butylated hydroxyanisole	25013-16-5
Butylated hydroxytoluene	128-37-0
Butylparaben	94-26-8
Caffeine	58-08-2
Caprolactam	105-60-2
Captafol	2425-06-1
Captan	133-06-2
Carbamazepine	298-46-4
Carbaryl	63-25-2
Carbazole	86-74-8
Carbetamide	16118-49-3
Carbofuran	1563-66-2
Carbofuran-3-keto	016709-30-1
Carbophenothion	786-19-6
Carbosulfan	55285-14-8
Carboxin	5234-68-4
Carfentrazone-ethyl	128639-02-1
Caryophyllene	87-44-5
Cedrol	77-53-2
Cedryl acetate	77-54-3
Chinomethionat	2439-01-2
Chloramben methyl ester	7286-84-2
Chloranocryl	2164-09-2
Chlorbenside	103-17-3
Chlorbromuron	13360-45-7
Chlorbufam	1967-16-4
Chlordimeform	6164-98-3
Chlorfenapyr	122453-73-0
Chlorfenethol	80-06-8
Chlorfenprop-methyl	14437-17-3
Chlorfenson	80-33-1
Chlorfenvinphos	470-90-6

o,p'-DDT	789-02-6
o-Cresol (2-methylphenol)	95-48-7
Octachlorodibenzofuran	39001-02-0
Octachlorodibenzo-p-dioxin	3268-87-9
Octachlorostyrene	29082-74-4
Octocrylene	6197-30-4
Octyl-methoxycinnamate	5466-77-3
Ofurace	58810-48-3
Omethoate	1113-02-6
o-Phenylphenol	90-43-7
Oryzalin	19044-88-3
o-Terphenyl	84-15-1
o-Toluidine	95-53-4
Oxabetrinil	74782-23-3
Oxacyclohexadecan-2-one	106-02-5
Oxadiazon	19666-30-9
Oxadixyl	77732-09-3
Oxamyl	23135-22-0
Oxazepam	604-75-1
Oxycarboxin	5259-88-1
Oxychlordan	27304-13-8
Oxydemeton-methyl	301-12-2
Oxyfluorfen	42874-03-3
o-Xylene	95-47-6
p-(dimethylamino)azobenzene	60-11-7
Paclobutrazol	76738-62-0
Padimate O	21245-02-3
Paraldehyde	123-63-7
Paraoxon	311-45-5
Parathion (ethyl)	56-38-2
p-Benzoquinone	106-51-4
p-Cresol (4-methylphenol)	106-44-5
Pebulate	1114-71-2
Penconazole	66246-88-6
Pencycuron (breakdown product)	66063-05-6
Pendimethalin	40487-42-1
Pentachloroaniline	527-20-8
Pentachloroanisole	1825-21-4
Pentachlorobenzene	608-93-5
Pentachloroethane	76-01-7
Pentachloronitrobenzene	82-68-8
Pentachlorophenol	87-86-5
Pentanochlor	2307-68-8
Pentobarbital	76-74-4
Permethrin I	52645-53-1
Permethrin II	52645-53-1
Perthane	72-56-0

Chlorflurecol-methyl ester	2536-31-4
Chlormefos	24934-91-6
Chlornitrofen	1836-77-7
Chlorobenzene	108-90-7
Chlorobenzilate	510-15-6
Chlorodibromomethane	124-48-1
Chloroneb	2675-77-6
Chlorophacinone	3691-35-8
Chlorophene (2-Benzyl-4-chlorophenol)	120-32-1
Chloropropylate	5836-10-2
Chlorothalonil	1897-45-6
Chlorotoluron	15545-48-9
Chloroxylenol	88-04-0
Chlorpropham	101-21-3
Chlorpyrifos	2921-88-2
Chlorpyrifos Methyl	5598-13-0
Chlorthal-dimethyl	1861-32-1
Chlorthiamid	1918-13-4
Chlorthion	500-28-7
Chlorthiophos	60238-56-4
Chlorthiophos sulfone	025900-20-3
Chlorthiophos sulfoxide	029-21-5
Chlozolate	84332-86-5
Cholesterol	57-88-5
Chrysene	218-01-9
Cinnamal	104-55-2
Cinnamyl Alcohol	104-54-1
cis-1,3-Dichloropropylene	10061-01-5
cis-Chlordane	5103-71-9
Citral	5392-40-5
Citronellol	106-22-9
Clofibrate	637-07-0
Clomazone	81777-89-1
Clomipramine	303-49-1
Clonazepam	1622-61-3
Clopyralid	1702-17-6
Cloquintocet-mexyl	99607-70-2
Clothianidin	210880-92-5
Cocaine	50-36-2
Codeine	76-57-3
Cotinine	486-56-6
Coumaphos	56-72-4
Coumarin	91-64-5
CPA	122-88-3
Cresyl diphenyl phosphate	26444-49-5
Crimidine	535-89-7
Crotamiton	483-63-6

Pethidine	57-42-1
phenacetin	62-44-2
Phenamiphos	22224-92-6
Phenanthrene	85-01-8
Phenkapton	2275-14-1
Phenmedipham	13684-63-4
Phenol	108-95-2
Phenoxyacetic acid	122-59-8
Phenthoate	2597-03-7
Phenylbutazone	50-33-9
phorate	298-02-2
Phosalone	2310-17-0
Phosfolan	947-02-4
Phosmet	732-11-6
Phosphamidon I	13171-21-6
Phosphamidon II	13171-21-6
Phthalide	27355-22-2
Picloram methyl ester	14143-55-6
Picolinafen	137641-05-5
Pindone	83-26-1
Pinoxaden	243973-20-8
Piperalin	3478-94-2
Piperonyl butoxide	51-03-6
Piperonylbutoxide	51-03-6
Piperophos	24151-93-7
Pirimicarb	23103-98-2
Pirimiphos-ethyl	23505-41-1
Pirimiphos-methyl	29232-93-7
p-Isopropyltoluene	99-87-6
Plifenat	21757-82-4
p-Nitrotoluene	99-99-0
p-Phenylenediamine	106-50-3
Prazepam	2955-38-6
Pretilachlor	51218-49-6
Primidone	125-33-7
Probenazole	27605-76-1
Prochloraz	67747-09-5
Procymidone	32809-16-8
Profenofos	41198-08-7
Profluralin	26399-36-0
Promecarb	2631-37-0
Prometon	1610-18-0
Prometryn	7287-19-6
Propachlor	1918-16-7
Propamocarb	24579-73-5
Propanil	709-98-8
Propargite	2312-35-8

Crotoxyphos	7700-17-6
Crufomate	299-86-5
Cyanazine	21725-46-2
Cyanofenphos	13067-93-1
Cyanophos	2636-26-2
Cycloate	1134-23-2
Cyclohexanone	108-94-1
Cycluron	2163-69-1
Cyfluthrin I	68359-37-5
Cyfluthrin II	68359-37-5
Cyfluthrin III	68359-37-5
Cyfluthrin IV	68359-37-5
Cyhalothrin I (lambda)	68085-85-8
Cymoxanil	57966-95-7
Cypermethrin I	52315-07-8
Cypermethrin II	52315-07-8
Cypermethrin III	52315-07-8
Cypermethrin IV	52315-07-8
Cyprazine	22936-86-3
Cyproconazole	113096-99-4
Cyprodinil	121552-61-2
Cyprofuram	69581-33-5
Cyromazine	66215-27-8
d-(cis-trans)-Phenothrin-I	26002-80-2
d-(cis-trans)-Phenothrin-II	26002-80-2
Dapson	80-08-0
Dazomet	533-74-4
Decachlorobiphenyl	2051-24-3
Decahydronaphthalene (cis)	493-01-6
Decahydronaphthalene (trans)	493-02-7
delta-BHC (delta-HCH)	319-86-8
Deltamethrin	52918-63-5
Demephion	8065-62-1
Demeton-S	126-75-0
Demeton-S-methylsulfon	17040-19-6
Desbromo-bromobutide	000000-00-1
Desimpramine	50-47-5
Desmedipham	13684-56-5
Desmetryn	1014-69-3
Dialifos	10311-84-9
Diallate	2303-16-4
Di-allate II	2303-16-4
Diallyl phthalate	131-17-9
Diamyl phthalate	131-18-0
Diazepam	439-14-5
Diazinon	333-41-5

Propazine	139-40-2
Propetamphos	31218-83-4
Propham	122-42-9
Propiconazole-I	60207-90-1
Propiconazole-II	60207-90-1
Propofol	2078-54-8
Propoxur	114-26-1
Propylparaben	94-13-3
Propyzamide	23950-58-5
Prosulfocarb	52888-80-9
Prothioconazole (breakdown product)	178928-70-6
Prothiofos	34643-46-4
Prothoate	2275-18-5
p-Xylene	106-42-3
Pymetrozin	123312-89-0
Pyracarbolid	24691-76-7
Pyrazine	290-37-9
Pyrazon	1698-60-8
Pyrazophos	13457-18-6
Pyrazoxyfen	71561-11-0
Pyrene	129-00-0
Pyributicarb	88678-67-5
Pyridaben	96489-71-3
Pyridaphenthion	119-12-0
Pyridate	55512-33-9
Pyridine	110-86-1
Pyridinitril	1086-02-8
Pyrifenox I	731-27-1
Pyrifenox II	88283-41-4
Pyrimethanil	53112-28-0
Pyroquilon	57369-32-1
Quinalphos	13593-03-8
Quinmerac (breakdown product)	90717-03-6
Quinoclamine	2797-51-5
Quinoxifen	124495-18-7
Quizalofop-ethyl	76578-14-8
Resmethrin	28434-01-7
Rotenone	83-79-4
S,S,S-Tributylphosphorotrithioate	78-48-8
Safrole	94-59-7
Sebuthylazine	7286-69-3
Secbumeton	26259-45-0
sec-Butylbenzene	135-98-8
Silthiofam	175217-20-6
Simazine	122-34-9
Simetryn	1014-70-6

Dibenz[a,h]anthracene	53-70-3
Dibenzofuran	132-64-9
Dibrom (naled)	300-76-5
Dibromomethane	74-95-3
Dibromophenyl ether	5436-43-1
Dicamba	1918-00-9
Dicamba methyl ester	6597-78-0
Dicapthon	2463-84-5
Dichlofenthion	97-17-6
Dichlofluanid	1085-98-9
Dichlone	117-80-6
Dichlormid	37764-25-3
Dichlorophen	97-23-4
Dichlorprop	120-36-5
Dichlorprop methyl ester	57153-17-0
Dichlorvos	62-73-7
Diclobutrazol	75736-33-3
Diclofenac artifact	15362-40-0
Diclofenac-methyl ester	15307-78-5
Diclofop methyl	51338-27-3
Dicloran	99-30-9
Dicofol	115-32-2
Dicrotophos	141-66-2
Dicyclanil	112636-83-6
Dicyclohexyl phthalate	84-61-7
Dicyclopentadiene	77-73-6
Dieldrin	60-57-1
Dienochlor	2227-17-0
Diethatyl ethyl	38727-55-8
Diethofencarb	87130-20-9
Diethyl dithiobis(thionoformate) (EXD)	502-55-6
Diethyl phthalate	84-66-2
Diethylene glycol	111-46-6
Diethylstilbestrol	56-53-1
Difenoconazol I	119446-68-3
Difenoconazol II	119446-68-3
Diflufenican	83164-33-4
Diisobutyl phthalate	84-69-5
Dimefox	115-26-4
Dimethachlor	50563-36-5
Dimethametryn	22936-75-0
Dimethenamid	87674-68-8
Dimethipin	55290-64-7
Dimethoate	60-51-5
Dimethomorph	110488-70-5
Dimethyl adipate	627-93-0
Dimethyl fumarate	624-49-7

Spirodiclofen	148477-71-8
Squalane	111-01-3
Styrene	100-42-5
Suflolane	126-33-0
Sulfadiazine	68-35-9
Sulfamethoxazole	723-46-6
Sulfotepp	3689-24-5
Sulfur (S8)	10544-50-0
Sulprofos	35400-43-2
Swep	1918-18-9
Tamoxifen	10540-29-1
TCMTB	21564-17-0
Tebuconazole	107534-96-3
Tebufenpyrad	119168-77-3
Tebutam	35256-85-0
Tecnazene	117-18-0
Tefluthrin	79538-32-2
Temephos	3383-96-8
Tepraloxymid	149979-41-9
Terbacil	5902-51-2
Terbucarb	191-81-1
Terbufos	13071-79-9
Terbumeton	33693-04-8
Terbutylazine	5915-41-3
Terbutryne	886-50-0
Terpineol	98-55-5
Terpinyl acetate	80-26-2
tert-Butylbenzene	98-06-6
Tetrachloroethylene	127-18-4
Tetrachlorvinphos	961-11-5
Tetraconazole	112281-77-3
Tetradifon	116-29-0
Tetraethylpyrophosphate (TEPP)	107-49-3
Tetramethrin I	7696-12-0
Tetramethrin II	7696-12-0
Tetrapropyl thiodiphosphate	3244-90-4
Tetrasul	2227-13-6
Thenylchlor	96491-05-3
Thiabendazole	148-79-8
Thiacloprid	111988-49-9
Thiamethoxam	153719-23-4
Thiofanox	39196-18-4
Thiometon	640-15-3
Thionazin	297-97-2
Tiocarbazil I	36756-79-3
Tiocarbazil II	36756-79-3
Tolclofos-methyl	57018-04-9

Dimethyl phosphite	868-85-9
Dimethyl phthalate	131-11-3
Dimethylvinphos(z)	2274-67-1
Dimetilan	644-64-4
Dimetridazole	551-92-8
Dimoxystrobin	149961-52-4
di-n-butyl phthalate	84-74-2
Diniconazole	83657-24-3
Dinitramine	29091-05-2
Dinobuton	973-21-7
Dinocap I	39300-45-3
Dinocap II	39300-45-3
Dinocap III	39300-45-3
Dinocap IV	39300-45-3
di-n-octyl phthalate	117-84-0
Dinoseb	88-85-7
Dinoseb acetate	2813-95-8
Dinoseb methyl ether	6099-79-2
Dinoterb	1420-07-1
Dinoterb acetate	3204-27-1
Di-n-propyl phthalate	131-16-8
Dioxacarb	6988-21-2
Dioxathion	78-34-2
Dioxydemeton-S-methyl	17040-19-6
Diphacinone	82-66-6
Diphenamid	957-51-7
Diphenyl ether	101-84-8
Diphenyl sulfone	127-63-9
Diphenylamine	122-39-4
Dipropetryn	4147-51-7
Disulfoton	298-04-4
Ditalimfos	5131-24-8
Dithiopyr	97886-45-8
Diuron	330-54-1
d-Limonene	5989-27-5
Dodemorph I	1593-77-7
Dodemorph II	1593-77-7
Doxepin	1668-19-5
Drazoxolon	5707-69-7
Drometrizole	2440-22-4
Edifenphos	17109-49-8
Endosulfan ether	3369-52-6
Endosulfan I	959-98-8
Endosulfan II	33213-65-9
Endosulfan lactone	3868-61-9

Toltrazuril	69004-03-1
Toltrazuril Sulfone	69004-04-2
Toluene	108-88-3
Tolyfluanid	88283-41-4
Totarol	511-15-9
Tralkoxydim	87820-88-0
trans-1,3-Dichloropropylene	10061-02-6
trans-Chlordane	5103-74-2
trans-Nonachlor	39765-80-5
Tri-(2-chloroethyl) phosphate	115-96-8
Triacetin	102-76-1
Triadimefon	43121-43-3
Triadimenol	55219-65-3
Tri-allate	2303-17-5
Triamiphos	1031-47-6
Triazophos	24017-47-8
Triazoxide	72459-58-6
Tribenuron-methyl (breakdown product)	101200-48-0
Tributyl acetylcitrate	77-90-7
Tributyl phosphate	126-73-8
Tributyl phosphorotrithioite	150-50-5
Tributylamine	102-82-9
Trichlopyr	55335-06-3
Trichlorfon	52-68-6
Trichloroethylene	79-01-6
Trichloronate	327-98-0
Triclopyr methyl ester	060825-26-5
Triclosan	3380-34-5
Triclosan-methyl	4640-01-1
Tricresyl phosphate	78-30-8
Tricyclazole	41814-78-2
Tridiphane	58138-08-2
Trietazine	1912-26-1
Trifloxystrobin	141517-21-7
Triflumizole	68694-11-1
Trifluralin	1582-09-8
Trimethoprim	738-70-5
Trinexapac-ethyl	95266-40-3
Triphenyl phosphate	115-86-6
Triphenylphosphine	603-35-0
Triphenylphosphine oxide	791-28-6
Tris (2,3-epoxypropyl) isocyanate	2451-62-9
Tris-(1,3-dichloroisopropyl) phosphate	13674-87-8
Trixylenyl phosphate	25155-23-1
Tryclopyrbutoxyethyl	64470-88-8

Endosulfan sulfate	1031-07-8
Endrin	72-20-8
Endrin aldehyde	7421-93-4
Endrin ketone	53494-70-5

Tycor (SMY 1500)	64529-56-2
Uniconazole-P	83657-17-4
Vamidothion	2265-23-2
Vanillin	121-33-5
Vernolate	1929-77-7
Vinclozolin	50471-44-8
Zoxamide	156052-68-5

Table 16 Toxicity score of short-listed compounds (Surface waters¹)

Prior -ity list score	Compound	RQ ²	Solubility ³ (g/l)	LC50 fish (mg/L)	LC50 daphni a (mg/L)	References
6	1,2,4-trimethyl benzene	0.0453	0.057	7.72	3.6	https://www.sigmaaldrich.com/MT/en/sds/aldrich/t73601?userType=anonymous
5	1,3,5-Trimethylbenzene	0.4807	2.9	3.48	3.606	https://www.agilent.com/cs/library/msds/RAB-007_NAEnglish.pdf
5	1-Ethyl-2-pyrrolidone	0.0031	1	104	999	https://www.sigmaaldrich.com/MT/en/sds/aldrich/146358?userType=anonymous
5	2,4,7,9-Tetramethyl-5-decyne-4,7-diol	0.0211	1.7	91	42	https://www.sigmaaldrich.com/MT/en/sds/aldrich/278386?userType=anonymous
5	2-Ethyl-1,3-hexanediol	0.0119	42	364	811	https://www.fishersci.com/store/msds?partNumber=AC118510010&productDescription=2-ETHYL-1+3-HEXANEDIOL+1LT&vendorId=VN00032119&countryCode=US&language=en
5	2-Ethylhexanoic acid	0.0153	1.4	70	85.4	https://www.merckmillipore.com/INTL/en/product/2-Ethylhexanoic-acid,MDA_CHEM-800758?ReferrerURL=https%3A%2F%2Fwww.ecosia.org%2F
5	2-Methylnaphthalene	0.0068	0.0001	1.45	1.5	https://www.sigmaaldrich.com/MT/en/sds/aldrich/m57006?userType=undefined / https://www.fishersci.com/store/msds?partNumber=AAL0245936&productDescription=2-METHYLNAPHTHALENE+97%25+500G&vendorId=VN00024248&countryCode=US&language=en
5	6PPD-quinone	0.0768	0.000038	0.028	0.23	https://www.hpc-standards.com/msds/687855_6PPDquinone_MSDS_EN_HPC-Standards.pdf
7	Acesulfame K	0.0122	270	1800	1000	https://www.sigmaaldrich.com/MT/en/sds/sial/04054?userType=undefined
5	Acetophenone	0.0086	6.3	162	528	https://www.sigmaaldrich.com/MT/en/sds/aldrich/w200910?userType=undefined
6	Amoxicillin	0.0376	4	184.36	15.35	https://iopscience.iop.org/article/10.1088/1755-1315/1414/1/012034/pdf
6	Aniline	4.5428	35	10.6	0.16	https://op.europa.eu/en/publication-detail/-/publication/8b34c190-c681-11e6-a6db-01aa75ed71a1#:~:text=Aniline%20is%20moderately%20soluble%20in,(25%20C2%B0C)%2C%20the
7	Arsenic	0.0209	0.0106	28.68	0.85	https://www.sigmaaldrich.com/MT/en/sds/sial/04054?userType=undefined
6	Atenolol	0.0079	35	1800	313	https://www.astrazeneca.com/content/dam/az/PDF/Sustainability/era/Atenolol.pdf
5	Avermectin B1a	0.6407	0.000002	0.0087	0.00056	https://assets.lgcstandards.com/sys-master%2Fpdfs%2Fh3a%2Fhe8%2F10657429815326%2FSDS_DRE-CA10001100_ST-WB-MSDS-5953924-1-1-1-PDF
5	Avermectin B1b	1.9218	0.0000078	0.0096	0.00022	https://www.endmemo.com/concentration_solution/gram_literpartperbillion.html
5	Azobenzene	0.0063	0.0001	0.5	5	https://www.sigmaaldrich.com/MT/en/sds/sial/424633?userType=undefined / https://www.fishersci.com/store/msds?partNumber=AAA1042514&productDescription=AZOBENZENE+25G&vendorId=VN00024248&countryCode=US&language=en
5	Benzenesulfonanilide	0.0000	0.0001	1000	48	https://www.researchgate.net/profile/Da-Ji-Huang/publication/265731249_Toxicity_of_the_Veterinary_Sulfonamide_Antibiotic_Sulfamonomethoxine_to_Five_Aquatic_Organisms/links/5d9403b6299bf10cff1f62de/Toxicity-of-the-Veterinary-Sulfonamide-Antibiotic-Sulfamonomethoxine-to-Five-Aquatic-Organisms.pdf
5	Benzenesulfonamide, N-butyl	0.0005	0.00043	36.7	56	https://echa.europa.eu/registration-dossier/-/registered-dossier/13402/6/2/2
8	Benzophenone	0.0381	0.14	14.2	6.78	https://www.health.state.mn.us/communities/environment/risk/docs/guidance/gw/benzopheninfo.pdf
7	Benzotriazole	0.1092	19	180	8.85	https://www.sigmaaldrich.com/MT/en/sds/sial/b11400?userType=undefined
5	Beta-estradiol	0.0184	0.0015	0.46	9.58	https://www.sigmaaldrich.com/MT/en/sds/SIGMA/E8875?userType=undefined
6	Bisphenol A	0.0788	0.298	4.7	10.2	https://www.sigmaaldrich.com/MT/en/sds/aldrich/239658?srltid=AfmBOorbDTfdU8aD3n1Ea9dRTTYD7yAuD0oUkJqyD8P6owFVPU3Yv6b7
6	Bis(2-ethylhexyl) adipate	0.0005	0.0001	0.78	500	https://www.sigmaaldrich.com/MT/en/sds/aldrich/525197?userType=anonymous

5	Bromuconazole	0.4227	40.85	10.44	21.9	https://cdn.nufarm.com/wp-content/uploads/sites/26/2020/04/30173759/SDS-Soleil-UK-IE-v3.0-F-191007.pdf
5	Butyl methoxydibenzoyl-methane	0.0001	0.0001	100	100	https://www.sigmaaldrich.com/MT/en/sds/sial/16633?userType=undefined / https://www.atamanchemicals.com/butyl-methoxydibenzoylmethane_u32120/
6	Carbamazepine	0.0024	0.0001	43	0.414	https://www.fishersci.com/store/msds?partNumber=AC344360050&productDescription=CARBAMAZEPINE%2C+98%25+5GR&vendorId=VN00032119&countryCode=US&language=en
5	Chloroxlenol	0.1856	0.3	1.3	6.7	https://www.parchem.com/siteimages/attachment/ghs%20chloroxlenol%20msds.pdf / https://www.spectrumchemical.com/media/sds/CH136_AGHS.pdf?srltid=AfmBOoooAEm2INKjm-f5lWIO4l-zpAgJof-x2TAMzyCbbBhb57D_zT3h
5	Climbazole	0.0290	0.058	5.5	12.5	https://www.echemi.com/sds/climbazole-temppid160705010179.html
5	Clindamycin	0.0107	50	435	1000	https://www.sigmaaldrich.com/MT/pt/sds/sigma/c5269?userType=undefined /
5	Cyazofamid	0.0317	0.000107	0.56	0.19	https://assets.lgcstandards.com/sys-master%2Fpdfs%2Fh2b%2Fh42%2F10783710642206%2FSDS_DRE-C11816000_ST-WB-MSDS-6498138-1-1-1.PDF
6	Diclofenac	0.6475	50	9.8	12.17	file:///C:/Users/acl/Downloads/Assessment of diclofenac LC50 refer.pdf
5	Dicyclohexyl phthalate	0.0159	0.00101	2	2	https://www.sigmaaldrich.com/MT/en/sds/aldrich/306150?userType=undefined
6	Diethyl phthalate	0.0294	0.932	12	90	https://www.sigmaaldrich.com/MT/en/sds/aldrich/w512206?userType=undefined
5	Difenoconazole	3.8286	0.015	0.001329	0.77	https://www.sigmaaldrich.com/MT/en/sds/sial/36531?userType=undefined
5	Dimethyl phthalate	0.1050	4	11	33	https://www.sigmaaldrich.com/MT/en/sds/SIAL/41320?userType=undefined
5	di-n-butyl phthalate	0.3010	0.13	0.48	2.99	https://chemicalstore.com/MSDS/SDS_DBP1.pdf / https://www.fishersci.co.uk/chemicalProductData_uk/wercs?itemCode=10101570&lang=EN
5	Diphenyl sulfone	0.0040	0.014	29	30	https://store.sangon.com/productImage/SDS/A601382/A601382_EN_S.pdf
5	d-Limonene	0.0196	0.0001	0.72	0.36	https://www.parchem.com/siteimages/attachment/ghs%20d-limonene%20msds.pdf
5	Epoxiconazole	0.0161	0.00705	3.14	8.69	https://www.echemi.com/sds/1-2s-3s-3-2-chlorophenyl-2-4-fluorophenylloxiran-2-ylmethyl-1-2-4-triazole-pd180521105550.html
6	Ethylbenzene	0.1627	0.2	4.2	1.8	https://www.sigmaaldrich.com/MT/en/sds/sial/296848?userType=undefined
5	EthylenDiamino-Tetracetyc Acid (EDTA)	0.0040	0.4	41	625	https://www.sigmaaldrich.com/MT/de/sds/aldrich/431788?userType=undefined
5	Ettoxazole	0.0593	0.00007	2.8	0.0071	https://assets.lgcstandards.com/sys-master%2Fpdfs%2Fh29%2Fh88%2F10471497957406%2FSDS_TRC-E936600-100MG_ST-WB-MSDS-4393245-1-1-1.PDF /
5	Fenpiclonil	0.0679	0.0048	0.8	1.3	http://cdn.chemservice.com/product/msdsnew/External/English/N-14356%20English%20SDS%20US.pdf
5	Fipronil	0.4958	0.00397	0.085	0.19	https://www.genfarm.com.au/sites/genfarm/files/2021-07/documents/SDS_GNF%20FIPRONIL%20200%20INSECTICIDE.pdf / https://www.sigmaaldrich.com/MT/de/sds/SIAL/46451?userType=undefined
5	Fluoxetine	0.6173	0.05	0.16	0.82	https://www.merckmillipore.com/INTL/en/product/msds/EMD_BIO-343290 / https://www.sigmaaldrich.com/MT/en/sds/sigma/f132?userType=anonymous
5	Flurenol-methylester	0.0001	0.0001	318	86.7	https://www.sigmaaldrich.com/MT/en/sds/sial/31520?userType=anonymous
7	Glyphosate	1.7642	10.1	1.1	2.95	https://www.sigmaaldrich.com/MT/fr/sds/sial/45521?userType=undefined
5	Guanylurea	0.0050	91.6	1000	3,600	https://assets.lgcstandards.com/sys-master%2Fpdfs%2Fh5b%2Fh20%2F10649666781214%2FSDS_DRE-A14057250AL-100_ST-WB-MSDS-5896015-1-1-1.PDF
5	1,6-Hexanediol diacrylate	0.5923	0.36	0.38	2.7	https://www.sigmaaldrich.cn/MT/en/sds/aldrich/246816?userType=undefined
5	Imidacloprid	0.1844	610	211	85	https://www.sigmaaldrich.com/MT/ko/sds/sial/68694?userType=undefined
5	Indane	0.3535	6	14	3.43	https://www.chemicalbook.com/msds/indan.htm
4	Isopropylbenzene	0.0079	0.0001	2.7	0.6	https://www.fishersci.com/store/msds?partNumber=AC329735000&countryCode=US&language=en
5	Itraconazole	0.0003	0.0001	33	33.4	https://assets.lgcstandards.com/sys-master%2Fpdfs%2Fhc2%2Fh22%2F10148048371742%2FSDS_EPY0001100_ST-WB-MSDS-2465747-1-1-1.PDF
5	Ketoconazole	0.0000	0.0001	350	468	https://academic.oup.com/etc/article/26/6/1214/7764104
5	Mefentrifluconazole	0.0399	0.0008	0.532	0.944	https://assets.lgcstandards.com/sys-master%2Fpdfs%2Fh51%2Fhd4%2F10743511515166%2FSDS_DRE-C14860600_ST-WB-MSDS-6384585-1-1-1.PDF

5	Metformin	0.0525	352	982	130	https://www.sigmaaldrich.com/MT/de/sds/SIAL/PHR1084?userType=undefined
7	Methylbenzotriazole	0.0377	6	43	98	https://d1wqtxts1xzle7.cloudfront.net/47357511/etc.562019060120160719-1269-1d65zj6-libre.pdf?1468953171=&response-content-disposition=inline%3B+filename%3DCOMPARATIVE_MEASURES_OF_THE_TOXICITY_OF.pdf&Expires=1739873104&Signature=CT5Tfy6GnAdlgoj3JtvXOSIFnESzHJfpX2MA~y8lFwAbzfk~nvIO5MFnSZEer49CyYine6LCHHKZhtm6GNA26cdWXbogDtwcjlYUFnH6hiZg08kO1Tva3C8vEiO7hGYHffxoWY2dM-Gr4Kt9cfc9a0xpRweUpHwwZJb~J5EVbfJcapHeEosQFR~LrDQ-pB4kkeVTAEJbEn1XZzb5Wr0sZUmwsyVUNX1PHyFAGx6zwtmGfKz-36N~wgWXm7l1QZCghsTDrrwfvH~gY23lm7vZ3qvJkLpADfzbf~Dy4BM1iahOI0Xx8W381VhCgBBRC9WGligMhBCT5lgZ-yStuhqPuw__&Key-Pair-Id=APKAJLOHF5GGSLRBV4ZA
5	N,N-Diethyl-m-toluamide	0.0001	0.0001	110	75	https://www.sigmaaldrich.com/MT/en/sds/sial/36542?userType=undefined / https://www.fishersci.com/store/msds?partNumber=AC114575000&productDescription=N+N-DIETHYL-M-TOLUAMIDE+500GR&vendorId=VN00032119&countryCode=US&language=en
5	N-1,3-Dimethylbutyl-N'-phenyl-p-phenylenediamine (6PPD)	0.2786	0.0005	0.028	0.23	https://www.sigmaaldrich.com/MT/en/sds/aldrich/cds013697?userType=anonymous / https://www.nocil.com/wp-content/uploads/2023/09/TDS-Piiflex-13.pdf
5	n-Propylbenzene	2.7474	23.4	1.55	2	https://www.chemicalbook.com/msds/n-propylbenzene.pdf
5	Neodecanoic acid-ethenyl ester	4.8387	5.9	0.84	0.3	https://www.coastalwiki.org/wiki/Neodecanoic_acid,_ethenyl_ester
5	Octisalate (2-ethylhexyl salicylate)	0.0003	0.00007	82	10	https://www.sigmaaldrich.com/MT/en/sds/aldrich/437379?userType=anonymous
7	Octocrylene	0.0003	0.00004	100	3.6	https://www.parchem.com/siteimages/attachment/ghs%20octocrylene%20msds.pdf
5	Ofloxacin	0.0011	0.004	1000	3.13	https://www.sigmaaldrich.com/MT/en/sds/sial/phr1168?userType=anonymous
5	Oxacyclohexadecan-2-one	0.0268	0.0001	0.11	1.27	https://www.vigon.com/product/exaltolide-total/?doc=MSDS/502775_vigon_sds_us_english.pdf&name=ExaltolideTotalSDS
5	Oxytetracycline	0.0001	0.0014	663.8	102	https://www.sigmaaldrich.com/MT/en/sds/SIAL/46598?userType=undefined
5	Phenanthrene	0.0094	0.0001	3.2	0.35	https://www.fishersci.com/store/msds?partNumber=AC130090050&productDescription=PHENANTHRENE+97%2B%25+5G&vendorId=VN00032119&countryCode=US&language=en
5	Phenol	1.7758	87	8.9	3.1	https://www.sigmaaldrich.com/MT/en/sds/sial/p5566?userType=undefined
5	Propiconazole	0.0644	0.11	2.6	10.2	https://www.sigmaaldrich.com/MT/en/sds/sial/45642?userType=undefined
5	Propranolol	0.1785	0.0617	1.21	1.6	https://assets.lgstandards.com/sys-master%2Fpdfs%2F1c%2Fhcf%2F10571749752862%2FSDS_LPM-PPN-1209-HC-50_ST-WB-MSDS-5237264-1-1-1.PDF
4	Propylparaben	0.0004	0.0001	10	50	https://www.parchem.com/siteimages/attachment/ghs%20propyl%20paraben%20msds.pdf
5	Styrene	0.0825	0.32	10	4.7	https://www.sigmaaldrich.com/MT/en/sds/sial/s4972?userType=undefined
5	Squalane	0.0001	0.0001	100	100	https://www.selleckchem.com/datasheet/squalane-S540700-DataSheet.html
7	Sulfamethoxazole	0.0033	0.281	536	48	https://www.merck.com/docs/product/safety-data-sheets/ah-sds/Sulfamethoxazole%20and%20Trimethoprim%20Formulation_AH_IN_6N.pdf
5	Sulfolane	0.0343	100	100	852	https://www.merckmillipore.com/INTL/en/product/msds/MDA_CHEM-807993
5	Tetracycline	0.0018	0.231	220	340	https://www.sigmaaldrich.com/MT/en/sds/sigma/t7660?userType=undefined . https://www.merck.com/docs/product/safety-data-sheets/ah-sds/Tetracycline%20Hydrochloride_AH_CA_EN.pdf
4	Toluene	0.1670	0.58	5.5	3.78	https://www.sigmaaldrich.com/MT/en/sds/sial/244511?userType=undefined
5	Tributyl acetylcitrate	0.0109	0.00449	38	1	https://www.sigmaaldrich.com/MT/en/sds/sial/y0001055?userType=anonymous
5	Tributyl phosphate	0.8607	6	4.5	1.8	https://www.sigmaaldrich.com/MT/en/sds/aldrich/240494?userType=anonymous
6	Triisobutylphosphate	0.0323	0.264	23	11	https://actylis.com/-/msds/GRPP104239_1333300_American_English.PDF?file=1333300+(American+English).PDF
5	Tris-(1,3-dichloroisopropyl) phosphate	0.0039	0.007	3.6	131	http://cdn.chemservice.com/product/msdsnew/External/English/N-18003%20English%20SDS%20US.pdf
5	Triticonazole	0.0190	0.0093	5.57	4.61	https://labelsds.com/images/user_uploads/Trinity%20TR%20SDS%2011-7-22.pdf / https://pubchem.ncbi.nlm.nih.gov/compound/Triticonazole#section=Odor

¹ Surface waters in this context refer to Inland Surface, Stormwater, Transitional, New waters and Coastal waters

² Score calculated as $Risk\ Quotient = \sqrt{(solubility \times (1 \div (LC_{fish} \times LC_{daphnia})))}$

³ Compounds classed as insoluble were given a token solubility of 0.0001mg/L

Table 17 Toxicity score of short-listed compounds (Groundwaters)

Prior- ity list score	Compound	Risk quotient ¹	Solubility ² (g/l)	LC50 fish (mg/L)	LC50 daphnia (mg/L)	Reference
4	Bis(2-ethylhexyl) adipate	67.00594	5.5	0.035	0.035	https://pubmed.ncbi.nlm.nih.gov/18483781/
5	Tetrahydrofuran	11.52582	1000	2.16	3.485	https://www.merckmillipore.com/INTL/en/product/msds/MDA_CHEM-108110?Origin=PDP https://en.wikipedia.org/wiki/Tetrahydrofuran
4	Aniline	4.54277	35	10.6	0.16	https://op.europa.eu/en/publication-detail/-/publication/8b34c190-c681-11e6-a6db-01aa75ed71a1#:~:text=Aniline%20is%20moderately%20soluble%20in,(25%20C2%B0C)%2C%20the
4	Acetone	4.27773	1000	6.21	8.8	https://www.sigmaaldrich.com/MT/en/sds/sigald/179124?userType=undefined
4	Formaldehyde	3.20833	400	6.7	5.8	https://www.sigmaaldrich.com/MT/en/sds/sigma/f8775?userType=undefined
5	1,2,4-Trichlorobenzene	3.10530	37.8	2.8	1.4	https://www.sigmaaldrich.com/MT/en/sds/sigald/256412?userType=anonymous
5	n-Propylbenzene	2.74743	23.4	1.55	2	https://www.chemicalbook.com/msds/n-propylbenzene.pdf
5	Phenol	1.77576	87	8.9	3.1	https://www.sigmaaldrich.com/MT/en/sds/sial/p5566?userType=undefined
4	4-chloro-3-methylphenol	1.38015	4	0.917	2.29	https://www.sigmaaldrich.com/MT/en/sds/aldrich/24940?userType=anonymous
4	DEHP	0.89568	0.086	0.67	0.16	https://www.sigmaaldrich.com/MT/en/sds/sial/36735?userType=undefined
5	Tributyl phosphate (4)	0.86066	6	4.5	1.8	https://www.sigmaaldrich.com/MT/en/sds/aldrich/240494?userType=anonymous
4	p-Cresol (4-methylphenol)	0.79661	21.5	4.4	7.7	https://www.sigmaaldrich.com/MT/en/sds/sigald/c85751?userType=anonymous
4	Diclofenac	0.64748	50	9.8	12.17	file:///C:/Users/acl/Downloads/Assessment_of_diclofenac_LC50_refer.pdf
5	o-Toluidine	0.62662	16.6	81.3	0.52	https://www.carlroth.com/medias/SDB-4788-IE-EN.pdf?
5	Crotamiton	0.43138	0.353	0.891	2.129	https://pubchem.ncbi.nlm.nih.gov/compound/Crotamiton#section=Boiling-Point
5	1,2-Dichlorobenzene	0.42342	0.1558	1.58	0.55	https://www.sigmaaldrich.com/MT/en/sds/sial/240664?srltid=AfmB0oqDrCww-YlyCgcHk4jYoIRVLh4MyVkuUifZcumRBdb8y7WKlxqbK
5	Chlorobenzene	0.41587	0.5	4.9	0.59	https://en.wikipedia.org/wiki/Chlorobenzene
4	o-Cresol (2-methylphenol)	0.39778	25	10	15.8	https://www.cdhfinechemical.com/images/product/msds/19_454117043_o-Cresol-CASNO-95-48-7-MSDS.pdf
4	Coumarin	0.28401	1.9	2.94	8.012	https://www.sigmaaldrich.com/MT/en/sds/sial/01260595?userType=undefined
4	m-Cresol (3-methylphenol)	0.17326	22.7	7.6	99.5	https://www.sigmaaldrich.com/MT/en/sds/aldrich/w353000?userType=undefined
6	Toluene	0.16703	0.58	5.5	3.78	https://www.sigmaaldrich.com/MT/en/sds/sial/244511?userType=undefined
5	Tetraglyme	0.16366	1	5	7.467	https://www.merckmillipore.com/INTL/en/product/msds/MDA_CHEM-820959
5	Ethylbenzene	0.16265	0.2	4.2	1.8	https://www.sigmaaldrich.com/MT/en/sds/sial/296848?userType=undefined

5	total Xylenes	0.13693	0.156	2.6	3.2	https://www.carlroth.com/medias/SDB-2662-GB-EN.pdf?context=bWFzdGVyfHNIY3VyaXR5RGF0YXNoZWV0c3wyOTI4ODN8YXBwbGljYXRpb24vcGRmfGFZ3lMMmhoWmk4NU1UZ3lPVGm1TmptMk5ETXdMMU5FUWw4eU5qWXIYMGRDWDWBT0xuQmtaZ3wwYWFjOGJmZDZjYWQ3ZGM0MDc0MzBkYTZjYwNTcyNmFhMjYyOWRkNDUxMDYyMDg5OTExZGQ0NWYxOTk4Nzkx
4	Paracetamol	0.12662	19	100	11.85	https://www.caelo.de
6	Benzotriazole	0.10921	19	180	8.85	https://www.sigmaaldrich.com/MT/en/sds/sial/b11400?userType=undefined
5	Styrene	0.08251	0.32	10	4.7	https://www.sigmaaldrich.com/MT/en/sds/sial/s4972?userType=undefined
5	1,2,3-Trichlorobenzene	0.07512	0.018	2.2	1.45	https://www.sigmaaldrich.cn/MT/en/sds/aldrich/t54402?userType=undefined
4	Ethylparaben	0.06272	0.885	15	15	https://www.sigmaaldrich.cn/MT/en/sds/aldrich/111988?userType=undefined
4	Trichloromethane	0.06086	8.7	15.4	152.5	https://www.carlroth.com/medias/SDB-1YK1-IE-EN.pdf?context=bWFzdGVyfHNIY3VyaXR5RGF0YXNoZWV0c3wzNjQ5MDd8YXBwbGljYXRpb24vcGRmfGFHRXpMMmhpWmk4NU1UZ3lOakeOTmptRME1USTJMMU5FUWw4eFVc3hYMgXGWDBWT0xuQmtaZ3xlZDEwOGY0ODA2ZDg3NTFmZjZkNWU5NmRmZDZmNGY4ZTk0ODk2NjZmMDkxMGJlZjM4NGY2MjFiNmRiYTl3YTU0
5	1,2-dichloropropane	0.05858	1.297	140	2.7	https://www.sigmaaldrich.com/MT/en/sds/aldrich/d72182?userType=undefined
5	Dimethyl phthalate	0.05575	4	39	33	https://www.fishersci.se/chemicalProductData_uk/wercs?itemCode=11418213&lang=EN
5	Methylparaben	0.05455	2	60	11.2	https://redox.com/wp-content/sds/2530.pdf https://www.parchem.com/siteimages/attachment/ghs%20methyl%20paraben%20msds.pdf https://www.agilent.com/cs/library/msds/FLPK-002F_NAEnglish.pdf
5	1,1,2-Trichloroethane	0.05115	4.5	40	43	https://www.sigmaaldrich.com/MT/en/sds/aldrich/466212?userType=undefined
4	Xylenes	0.04164	0.16	2.6	35.5	https://www.merckmillipore.com/INTL/en/product/msds/MDA_CHEM-108633
6	Benzophenone	0.03813	0.14	14.2	6.78	https://www.health.state.mn.us/communities/environment/risk/docs/guidance/gw/benzopheninfo.pdf
6	Methylbenzotriazole	0.03773	6	43	98	https://d1wqtxts1xzle7.cloudfront.net/47357511/etc.562019060120160719-1269-1d65zj6-libre.pdf?1468953171=&response-content-disposition=inline%3B+filename%3D
4	Amoxicillin	0.03760	4	184.36	15.35	https://iopscience.iop.org/article/10.1088/1755-1315/1414/1/012034/pdf
5	Tetrachloromethane / Carbon tetrachloride	0.03154	0.8461	24.3	35	https://www.sigmaaldrich.com/MT/en/sds/ALDRICH/571016?userType=undefined
5	Tribromomethane	0.03061	1.25	29	46	https://www.sigmaaldrich.com/MT/en/sds/aldrich/241032?userType=undefined
4	Diethyl phthalate	0.02938	0.932	12	90	https://www.sigmaaldrich.com/MT/en/sds/aldrich/w512206?userType=undefined
5	Chloroethane	0.02908	5.74	117	58	https://www.sigmaaldrich.com/MT/pt/sds/aldrich/295310?userType=undefined
5	cis-1,2-Dichloroethene	0.02271	3.5	117	58	https://www.siad.com/safety/material-safety-data-sheet?
5	1,1,1-Trichloroethane	0.02265	1.25	42.3	57.6	https://echa.europa.eu/registration-dossier/-/registered-dossier/12667/6/2/4
5	tert-butyl methyl ether; methoxy-2-methylpropane	0.01978	42	574	187	https://www.sigmaaldrich.com/MT/en/sds/mm/1.01995?userType=anonymous
5	d-Limonene (4)	0.01964	0.0001	0.72	0.36	https://www.parchem.com/siteimages/attachment/ghs%20d-limonene%20msds.pdf
5	Clopidol	0.01736	0.01	4	8.3	https://pubchem.ncbi.nlm.nih.gov/compound/18087#section=Melting-Point
5	Erythromycin	0.01598	2	349	22.45	https://www.fishersci.com/store/msds?partNumber=BP92025&productDescription=ERYTHROMYCIN+25G&vendorId=VN00033897&countryCode=US&language=en
5	2-Ethylhexanoic acid	0.01530	1.4	70	85.4	https://www.merckmillipore.com/INTL/en/product/2-Ethylhexanoic-acid,MDA_CHEM-800758?ReferrerURL=https%3A%2F%2Fwww.ecosia.org%2F
5	Diisopropylether	0.01336	3.11	91.7	190	https://www.sigmaaldrich.com/MT/en/sds/sial/296856?userType=undefined

6	Acesulfame K	0.01225	270	1800	1000	https://www.sigmaaldrich.com/MT/en/sds/sial/04054?userType=undefined
	EDTA	0.01141	0.5	34	113	https://www.fishersci.com/store/msds?partNumber=BP118500&productDescription=EDTA+%28FREE+ACID%29+500G&vendorId=VN00033897&countryCode=US&language=en
5	Tributyl acetylcitrate	0.01087	0.00449	38	1	https://www.sigmaaldrich.com/MT/en/sds/sial/y0001055?userType=anonymous
5	2-Ethoxy-2-methylpropane	0.01058	12	974	110	http://cdn.vitol.com/pdfs/006c0f69f20a84d617230fab62bd3c5a/9a2c6f2ae8509e097ef61fd52c90ab6d/v4020a_ethyl-tert-butyl-ether_etbe-2-ethoxy-2-methylpropane.pdf
4	Atenolol	0.00788	35	1800	313	https://www.astrazeneca.com/content/dam/az/PDF/Sustainability/era/Atenolol.pdf
7	Isopropylbenzene	0.00786	0.0001	2.7	0.6	https://www.fishersci.com/store/msds?partNumber=AC329735000&countryCode=US&language=en
5	Primidone	0.00693	0.48	100	100	https://www.pharmacopoeia.com/content/file/products/healthandsafety/CAT-293_GB.pdf
5	Nitrilotriacetic Acid (NTA)	0.00448	1.28	114	560	https://www.sigmaaldrich.com/MT/en/sds/sial/n9877?userType=anonymous
5	Diethylene glycol dimethyl ether	0.00446	1000	8569	5868	https://www.fishersci.co.uk/chemicalProductData_uk/wercs?itemCode=10020110&lang=EN
5	Trifluoroacetic Acid	0.00317	10	999	999	https://www.sigmaaldrich.com/MT/en/sds/sigma/t1647?userType=anonymous
5	Amidotrizoic Acid	0.00316	0.0089	8.9	100	https://core.ac.uk/download/pdf/58774201.pdf
5	Diphenyl sulfone (3)	0.00216	0.014	100	30	https://www.fishersci.com/store/msds?partNumber=AAL0823230&productDescription=DIPHENYL+SULFONE+250G&vendorId=VN00024248&countryCode=US&language=en
5	1,1-Dichloroethane	0.00106	5.06	29000	155	https://www.agilent.com/cs/library/msds/RHH-012_NAEnglish.pdf
5	Tert-butanol	0.00106	1	961	933	https://www.carlroth.com/medias/SDB-AE16-MT-EN.pdf?
5	1,1-Dichloroethene	0.00055	0.0001	29	11.6	https://www.agilent.com/cs/library/msds/HC-170-1_NAEnglish.pdf
5	Octocrylene	0.00033	0.00004	100	3.6	https://www.parchem.com/siteimages/attachment/ghs%20octocrylene%20msds.pdf
5	1,4-Dioxane	0.00022	1	4269	4700	https://www.sigmaaldrich.com/MT/en/sds/sial/296309?userType=undefined
5	N,N-Diethyl-m-tolamide	0.00011	0.0001	110	75	https://www.sigmaaldrich.com/MT/en/sds/sial/36542?userType=undefined / https://www.fishersci.com/store/msds?partNumber=AC114575000&productDescription=N+N-DIETHYL-M-TOLUAMIDE+500GR&vendorId=VN00032119&countryCode=US&language=en
4	Trimethoprim	0.00009	0.0001	100	123	https://www.fishersci.com/store/msds?partNumber=AC455120050&productDescription=TRIMETHOPRIM%2C+98%25+5GR&vendorId=VN00032119&countryCode=US&language=en
5	trans-1,2-Dichloroethene	0.00005	0.0001	120	270	https://www.fishersci.nl/store/msds?partNumber=10481011&productDescription%3D25GR+trans-1%2C2-Dichloroethylene%2C+99+%25%2C+stabilized&countryCode=NL&language=en
5	Benzenesulfonanilide (3)	0.00005	0.0001	1000	48	http://cdn.chemservice.com/product/msdsnew/External/English/S-13594M1%20English%20SDS%20US.pdf https://www.researchgate.net/profile/Da-Ji-Huang/publication/265731249_Toxicity_of_the_Veterinary_Sulfonamide_Antibiotic_Sulfamonomethoxine_to_Five_Aquatic_Organisms/links/5d9403b6299bf10cff1f62de/Toxicity-of-the-Veterinary-Sulfonamide-Antibiotic-Sulfamonomethoxine-to-Five-Aquatic-Organisms.pdf
5	Clarithromycin	0.00004	0.00033	100	2000	https://www.sigmaaldrich.com/MT/en/sds/sigma/c9742?srltid=AfmBOoqdd6WTD0_j7RWAdwZhL-lvDF0tlQzfX44SaOubdhluQjiYl6Fu
4	4,4'-Methylenebis(phenyl isocyanate) (1)	0.00001	0.00003	1000	1000	https://www.fishersci.com/store/msds?partNumber=AAL1574036&productDescription=44-METHYLENEBIS+PHENYL+ISO+500G&vendorId=VN00024248&countryCode=US&language=en

¹ Score calculated as $Risk\ quotient = \sqrt{(solubility \times (1 \div (LC_{fish} \times LC_{daphnia})))}$

1 Compounds classed as insoluble were given a token solubility of 0.0001mg/L