PRIORITIZATION OF EMERGING CONTAMINANTS FOR A NORDIC SCREENING STUDY

Scientific Report from DCE – Danish Centre for Environment and Energy No. 446 2021

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Data sheet

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Abstract: The aims of this report are 1) to identify knowledge gaps and monitoring needs for new emerging contaminants, expected to be present in the (aquatic) environment, based on lists of possibly hazardous chemical substances and 2) suggest a pan-Nordic screening study for prioritized substances. The report shall support the Joint Nordic Screening group in evaluating and prioritizing chemicals in national aquatic environmental monitoring programs.

1872 compounds identified from international lists and databases have been filtered through five filters based on PBT-profile, human and environmental profile, exposure, total use and previous environmental screening. The result of the filtering was a list of 16 chemical proposed candidates for screening studies. The report builds on a report by Woldegiorgis et al. (2019). The same method as in Woldegiogis et al. (2019) has been used, although with slight revisions

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Summary

This report was commissioned by the Nordic Council of Minister (NMR) and has been submitted to the Joint Screening Group under NMR. The report shall support the Joint Nordic Screening group in evaluating and prioritizing chemicals in national aquatic environmental monitoring programmes. The aims of the report are 1) to identify knowledge gaps and monitoring needs for new emerging substances, expected to be present in the (aquatic) environment, based on lists of possibly hazardous chemical substances. 2) Suggest a pan-Nordic screening study for prioritized substances.

This report builds on a report by Woldegiorgis et al. (2019). We applied the same methods with slight revisions to accommodate a pan-Nordic assessment (use, exposure, monitoring). We updated the analysis to include data from 2018-2020. The prioritization process comprises 5 filtering steps. We started with 1872 compounds for filtering. 194 passed the first filter and 23 passed the 4th filter, and finally 16 passed the last filter on monitoring. The resulting screening lists need to be analysed with expert-judgement and supplemented with problematic compounds that did not pass the 3-5 filters.

Comparing the list of 16 proposed chemical candidates to the 13 proposed chemical candidates for screening in Table 18 in Woldegiorgis et al. (2019), we find that 10 of these are also prioritized in the present study. Two chemicals, i.e. CAS 2425-85-6 Pigment Red 3 and CAS 2814-77-9 Pigment Red 4 are the only prioritized chemicals not assessed before, as they are new additions in the CoRAP list.

			Total points						
CAS Number	EC Number	Name	PBT	Hazard (not weighted Hazard lists)	Hazard (weighted Hazard lists)	Exposure	Quantity	Environmental Monitoring	Total sum
26471-62-5	247-722-4	m-tolylidene diisocyanate	0.7	6	3	7	6	7	23
2451-62-9	219-514-3	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	0.7	5.4	5.4	5	5	7	22.4
96-69-5	202-525-2	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	0.7	4.6	2.3	6	6	7	21.3
101-68-8	202-966-0	4,4’-Methylenediphenyl diisocyanate	0.7	5	5	7	6	2	20
75980-60-8	278-355-8	Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	0.7	3.5	1.75	6	5	7	19.75
98-29-3	202-653-9	4-tert-butylpyrocatechol	0.7	3.2	1.6	6	5	7	19.6
628-96-6	211-063-0	Ethylene dinitrate	0.7	3	1.5	5	6	7	19.5
115-27-5	204-077-3	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	0.7	4.8	2.4	5	5	7	19.4
2814-77-9	220-562-2	Pigment Red 4	0.7	4.5	2.25	4	5	7	18.25
110-88-3	203-812-5	1,3,5-trioxane	0.7	3.9	1.95	5	3.5	7	17.45
693-21-0	211-745-8	Oxydiethylene dinitrate	0.7	4.3	2.15	4	3.5	7	16.65
2425-85-6	219-372-2	Pigment Red 3	0.7	4.5	2.25	6	5	3	16.25
127-18-4	204-825-9	Perchloroethylene; tetrachloroethylene	0.7	5.9	2.95	6	5	2	15.95
81-15-2	201-329-4	Musk Xylene	1	4	4	5	3.5	2	14.5
79-94-7	201-236-9	Tetrabromobisphenol A (TBBPA)	0.7	3.6	1.8	5	5	2	13.8
4979-32-2	225-625-8	N,N-dicyclohexylbenzothiazole-2-sulphenamide	0.7	4.1	2.05	4	3.5	2	11.55

The analysis provides an objective, semi-quantitative risk based prioritization screening of compounds for consideration in a monitoring context in the Nordic region. The method can be adjusted and further developed, e.g. scores and cut-offs can be adjusted and other properties can be added e.g. mobility. The database analysis could moreover be further developed by including databases outside the EU system e.g. via the OECD e-chem portal and the US EPA ToxCast and chem-dashboard. In the not too distant future the analysis could be expanded in a machine-learning / artificial intelligence (AI) environment.

The Joint Nordic Screening group has had a presentation of the draft findings in Dec 2020 and has also received a draft of the report in late Dec 2020.

Sammenfatning

Denne rapport blev bestilt af Nordisk Ministerråd (NMR) og er blevet forelagt den fælles nordiske screeningsgruppe under NMR. Rapporten skal støtte screeningsgruppen i evaluering og prioritering af kemikalier i nationale overvågningsprogrammer for vandmiljø i Norden. Formålet med rapporten er 1) at identificere viden huller og overvågningsbehov for nye stoffer, der forventes at være til stede i (vand)miljøet baseret på lister over muligvis farlige kemiske stoffer. 2) Foreslå en pan-nordisk screeningundersøgelse for prioriterede stoffer.

Rapporten bygger på rapporten fra Woldegiorgis et al. (2019). Vi anvendte de samme metoder med lette revisioner af analysefiltrene (brug, eksponering, overvågning) for at gennemføre en pan-nordisk vurdering. Vi opdaterede analysen til at inkludere data fra 2018-2020. Prioriteringsprocessen omfattede 5 filtreringstrin. Vi startede med 1872 stoffer. 194 passerede det første filter og 23 passerede det 4. filter, og til sidst passerede 16 stoffer det sidste filter (overvågning). De resulterende screeningslister bør underkastes ekspertvurdering og suppleres med problematiske forbindelser, der ikke passerede filtre 3-5. Hvis man sammenligner listen med de 16 prioriterede stoffer med de 13 prioriterede stoffer i Woldegiorgis et al. (2019) finder vi, at 10 af disse også prioriteres i denne undersøgelse. To kemikalier, CAS 2425-85-6 Pigment Red 3 og CAS 2814-77-9 Pigment Red 4 er de eneste prioriterede kemikalier, der ikke er vurderet før, da de er nye tilføjelser på CoRAP-listen.

			Total points						
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75980-60-8	278-355-8	Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	0.7	3.5	1.75	6	5	7	19.75
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Analysen giver en objektiv, semikvantitativ risikobaseret prioriteringsscreening af kemikalier til overvejelse i en overvågningssammenhæng i Norden. Metoden kan justeres og videreudvikles, f.eks. kan score og cut-offs justeres, og andre egenskaber kan tilføjes f.eks. mobilitet. Desuden vil databaseanalysen kunne videreudvikles ved at inkludere databaser uden for EU-systemet, f.eks. via OECD-e-chem-portalen og US EPA ToxCast og chem-dashboard. I en ikke alt for fjern fremtid kunne analysen udvides i et maskinlæring / AI-miljø.

Screeningsgruppen har fået en præsentation af udkastet til konklusioner i december 2020 og har også modtaget et udkast til rapporten i slutningen af december 2020.

1 Introduction

The number of chemicals with an identification in the CAS system has increased with more than 75 million structures over the past decade adding up to more than 100 million structures available today. Globally, approximately 500 million tons of chemicals are produced every year – or in rough terms, 1 kg chemicals per global inhabitant per year. Apart from enabling our modern life, chemicals can also be a burden for humans and the environment. The World Health Organization (WHO) of the United Nations estimated in 2016 that 12.6 million people had died in 2012, as a result of living or working in an unhealthy chemical environment – nearly 1 in 4 of total global deaths (WHO, 2012). Meanwhile, we are currently in an accelerated 6th mass extinction in the global environment to which several stressors contribute - one of them being chemicals.

Prioritization schemes have been developed by regulatory agencies across the world in recent years, largely to identify candidate substances for risk assessment or further investigation. The chemical legislation in the Nordic countries is harmonized with the rest of the European Union (EU); hence, REACH legislation and the European Green Deal are central to our management of chemicals. The European Green Deal sets a political ambition of a zero pollution and toxic free environment in the coming years, as presented in EU's Chemical Strategy for Sustainability. This ambition necessitates a prioritization of chemical compounds of concern that need to be managed. A risk-based analysis of the potential environmental exposures to chemicals is thus needed to sustainably prioritize chemicals and identify monitoring needs as a measure to control the sustainable use of chemicals in our societies.

The Swedish EPA commissioned a project to identify gaps and propose chemical candidates for future screening and received a report and database by Woldegiorgis et al. 2019 from WSP Environmental in April 2019. The study by Woldegiorgis et al. (2019) provided a methodology for the prioritization of chemicals in Sweden up until 2018 resulting in a list of 13 chemicals prioritized for screening at that time. The present report builds on the study by Woldegiorgis et al. (2019) and provides an update, which includes additional chemicals and encompasses all Nordic countries. Prior to the work each member country and representative of the screening group was asked to submit access to their national monitoring databases. The database for the prioritized chemicals, updated from Woldegiorgis et al. (2019), is provided as Appendix 1 (http://dce2.au.dk/pub/SR446_App1.xlsx) as a separate electronic Excel database.

1.1 Objectives

Building on the study by Woldegiorgis et al. (2019), the present study had the following objectives:

- Identification of knowledge gaps and monitoring needs for new emerging substances, expected to be present in the (aquatic) environment in the Nordic countries, based on lists of possibly hazardous chemical substances; and
- Provide suggestions regarding pan-Nordic screening studies for the prioritized substances.

2 Methods

We applied the same approaches and scoring system as outlined by Woldegiorgis et al. (2019) to the extent possible and meaningful for the broader scope of this update. Some modifications were introduced, to account for the pan-Nordic approach, as further detailed below. We used the previous list (including data from Sweden until 2018) as a starting point and extended it in time and geographical coverage. The first element in the analysis is based on a review of the substances on the following lists and databases:

- REACH Article 59 candidate list;
- REACH Annex XIV Authorisation list;
- REACH Annex XVII Restriction list;
- Community Rolling Action Plan (CoRAP) list of the European Chemical Agency (ECHA);
- SIN list (https://chemsec.org/buisness-tool/sin-list);
- List of possible endocrine disrupting compounds (https://edlists.org).

The original substance list was thus extended with new compounds in any of these six lists and databases above.

In the scoring system, we moved from a focus on Sweden to an approach covering all Nordic countries. This resulted in differences in the evaluation of use, exposure and monitoring, which we will describe in detail below. However, we applied the same five filters and generally used the same scoring cut-off values as Woldegiorgis et al. (2019), with some adjustments for the exposure and monitoring filters, as detailed below. The original scoring and cut-offs can be seen in chapters 5 and 7 of the report by Woldegiorgis et al. (2019). In accordance with Woldegiorgis et al. (2019) UVCBs (Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials); metals and intermediates were not included in the prioritization.

Filter 1: PBT Screening:

We reviewed the lists of chemicals for the first filtering criteria based on their physical-chemical properties indicating persistence (P) and bioaccumulation (B) and with regard to their toxicity (T) expressed via their presence in the above mentioned lists. The same approach, scoring and cut-off as previously applied by Woldegiorgis et al. (2019) were used. If a compound scored ≥ 0.7 the substance progressed to the next filter.

The scoring can be seen in the two tables below:

Table 1a and 1b Identification and scoring of substances considered to be PBT and vPvB (from Woldegiorgis et al., 2019).

Search term	Colum	List	Scoring
"PBT"	"Intrinsic property referred to in article 57"	Reach article 59	1
"Suspected PBT"	"initial grounds for concern"	CoRAP-list	0.7
"Concluded to be PBT"	"Reasons for inclusions on the SIN list"	SIN-list	1
"PBT"	"initial grounds for concern"	CoRAP-list	1
"PBT cand"	"Hazard class and category codes"	SIN-list	0.5
"PBT"	"Hazard class and category codes"	SIN-list	1

Search term	Colum	List	Scoring
"vPvB"	"Intrinsic property referred to in article 57"	Reach article 59	1
"Suspected PBT/vPvB"	"initial grounds for concern"	CoRAP-list	0.7
"vPvB"	"initial grounds for concern"	CoRAP-list	1
"Concluded to be a vPvB"	"initial grounds for concern"	CoRAP-list	1
"Identified as vPvB"	"Reasons for inclusions on the SIN list"	SIN-list	1
"Concluded to be vPvB"	"Reasons for inclusions on the SIN list"	SIN-list	1
"Concluded to be both PBT and vPvB"	"initial grounds for concern"	CoRAP-list	1
"Concluded to be both PBT and vPvB"	"Reasons for inclusions on the SIN list"	SIN-list	1

Filter 2: Σ Human and environmental hazard:

The second filter reviewed the compounds with regards to total hazard. Total hazard pertains to 27 different properties such as potential for endocrine disruption or carcinogenicity, mutagenicity and reproductive toxicity (CMR), or if the compound has certain hazard sentences such as H410 etc. The total hazard points are calculated as the sum of scores from the tables below, and the cut-off score for this filter is set to ≥ 3 in accordance with Woldegiorgis et al. (2019).

Table 2a-2f Identification and scoring of carcinogenic, mutagenic, reprotoxic, carcinogenic; mutagenic, reprotoxic (CMR), endocrine disrupting substances, and substances of other hazard based concern.

Search term	Colum	List	Scoring
H350-H351	All relevant	All	1
"carcinogenic"	"Intrinsic property referred to in article 57"	Reach article 59	1
"suspected carcinogenic"	"initial grounds for concern"	CoRAP-list	0.7

Search term	Colum	List	Scoring
H340-H341	All relevant	All	1
"Mutagenic"	"Intrinsic property referred to in article 57"	Reach article 59	1
"Suspected mutagenic"	"initial grounds for concern"	CoRAP-list	0.7

Search term	Colum	List	Scoring
H360-H361	All relevant	All	1
"Reproduction"	"Intrinsic property referred to in article 57"	Reach article 59	1
"Suspected reprotoxic"	"initial grounds for concern"	CoRAP-list	0.7
"Reprotoxic"	"initial grounds for concern"	CoRAP-list	1
"Reprotoxic"	"Reasons for inclusions on the SIN list"	SIN-list	1

Search term	Colum	List	Scoring
"CMR"	"Reasons for inclusions on the SIN list"	SIN-list	3
"Suspected CMR"	"initial grounds for concern"	CoRAP-list	2.1
"CMR"	"initial grounds for concern"	CoRAP-list	3

Search term	Colum	List	Scoring
Cat 1	Category	EDC	1
Cat 2	Category	EDC	0.5
Cat 3	Category	EDC	0.3
"Concluded to be endocrine"	Reasons for inclusion on the SIN List	SIN-List	1
"Categorised as endocrine"	Reasons for inclusion on the SIN List	SIN-List	1
"Endocrine disrupting"	Intrinsic property(ies) referred to in Article 57	REACH article 59	1
“Endocrine disrupting”	Reasons for inclusion on the SIN List	SIN-List	1
"Suspected endocrine"	Initial grounds for concern	CoRAP-list	0.5
"Potential endocrine"	Initial grounds for concern	CoRAP-list	0.5
“Suspected sensitiser”	“initial grounds for concern”	CoRAP-list	0.4
“Sensitiser”	“initial grounds for concern”	CoRAP-list	0.6
“Other hazard based concern”	“initial grounds for concern”	CoRAP-list	0.4

The total hazard points of a compound are then weighted in accordance to the list of their origin. The regulatory lists containing compounds with harmonized classification were given weight 1. The weighting correspond to Woldegiorgis et al. (2019) with the addition of the EDC list (Endocrine Disrupting Chemicals), which has been given the weight 0.3, which is similar to the SIN list.

Table 3. Weighting applied to each of the lists of compounds used

List	Weight
REACH Appendix XVII	1
REACH Appendix XIV	1
REACH Article 59	1
CoRAP list	0.5
SIN list	0.3
EDC list	0.3

Filter 3: Total Exposure:

The total exposure estimation has been modified compared to the Woldegiorgis et al. (2019) method since we assessed the exposure across all Nordic

countries. We used the exposure estimation tool under the Substances in Preparations in the Nordic Countries (SPIN) database (http://www.spin2000.net/spinmyphp/) for the compounds that had passed the first two filters. Here four exposure index tools are presented that are included in the scoring approach.

- Quantity Index: This is based on the amount of annually consumed substance. Max index value: 5.
- Use Index: A general emission/exposure estimation for different human and environmental target groups. The primary recipients/target groups are: Surface water, Air, Soil, Waste water, Consumer, and Occupational. Max index value: 5 for each recipient/target group.
- Range of Use index: Indicates the broadness of the use of a substance in a Nordic country. Max index value: 5.
- Article Index: Gives indications if a substance may end up as a part of an article. Max index value: 3.

We viewed the Nordic countries as one entity and aggregated the scores in a max exposure value = max (Quantity + maximum Use Index + Range of Use + Article Index), where maximum Use Index is the maximum index value for any of the recipients/target groups. Below is an example of the Exposure indices for benzo[a]pyren (BaP).

Table 4. Benzo[a]pyren exposure index values from SPIN.

Substance

Cas no: 50-32-8 **Name:** BENZO[a]PYREN

EC no: 200-028-5

EXPOSURE

Country	Latest Year	Quantity (max: 5)	Use Index (UI, max: 5)						Range of Use (RoU, max: 5)	Article Index (AI, max: 3)
			Surface water	Air	Soil	Waste water	Consumer	Occu-pational		
DK	2018	1	2	2	3	3	3	4	2	3
NO	2018		3	3	3	4	5	4	2	3
SE	2018	4	2	3	3	2	5	4	2	3

We calculated the max exposure value from the indices of the country with the highest Quantity, for any year in the period 2013-2018. For the BaP example, in Table 4, it can be seen that Sweden has the highest Quantity (4) and therefore the country we used to serve as a conservative surrogate for the whole Nordic region. The resulting max exposure value is thus = 4+5+2+3 = 14 p, i.e. Quantity (4) + maximum Use Index (5) + Range of Use (2) + Article Index (3). Max exposure values can range from 4 to 18, and these were in turn attributed scores from 1 to 7, see Table 2. If no information is available, a penalty score of 3.5 scoring points is used. We have adapted the Woldegiorgis et al. (2019) scoring method to the pan-Nordic approach by using ≥ 4 scoring points as the cut off value instead of > 4, as used by Woldegioris et al. (2019), reflecting a max exposure value of 10 or more. Only the compounds that passed the first two filters were scored in this filter.

Table 5. Exposure scoring based on calculated exposure index values from SPIN.

Exposure	Score
4 - 6	1
6 - 8	2
8 - 10	3
10 - 12	4
12 - 14	5
14 - 16	6
16 - 18	7
Penalty	3,5

Filter 4: Total use

This element consists of data collection on the total use volumes of the identified compounds, taken from the SPIN database. Data from the national product registers of Norway, Sweden, Denmark and Finland are included in SPIN. There are no product register data from Iceland, Faroe Islands, Greenland. The tonnage (Tonnes in Table 7 below) represents the total registered volume of the substance in the particular year in the reporting country. The volume is calculated as production volume + imported volume – exported volume. If the value is "0.0" it means that the volume is below the limit of accuracy, which is 100 kg. Data are reported to SPIN on a yearly basis. The data reflect the status of the substance in that particular year in the reporting country. We applied the same scoring and cut-off methods as described by Woldegiorgis et al. (2019) where the filtering criteria was set for a Total use score ≥ 3. .

Table 6. Scoring of used quantities.

Quantities	Score
0 - 0.000002	1
0.000002 - 0.0002	2
0.0002 - 0.02	3
0.02 - 2	4
2 - 200	5
200 - 20 000	6
20 000 - +∞	7
Intermediate use only	-40
Penalty	3,5

We reviewed the five most recent years (2013-2018) tonnage data across the reporting countries and used the highest value reported as a conservative estimate for the pan-Nordic region. If there are only 0 (confidential) or blank (-) (no info), then the default scoring = 3.5 p was used, in agreement with Woldegiorgis et al. (2019). Below is the example of BaP:

As an example, in the case of BaP the total used value used was 2946.5 tonnes (Denmark 2016) for the scoring.

Table 7. Total BaP use data from SPIN.

Cas no: 50-32-8 **Name:** BENZO[a]PYREN
EC no: 200-028-5

Total Use

Country	Year	#prep	Tonnes
SE	2018	8	515.4
NO	2018	9	355.5
FI	2018	0	
DK	2018	11	0.0
SE	2017	8	689.0
NO	2017	9	374.5
FI	2017	0	
DK	2017	13	0.0
DK	2016	12	2,946.5
SE	2016	8	748.0
NO	2016	9	189.3
FI	2016	0	
DK	2015	19	2,946.0
SE	2015	9	513.0
NO	2015	13	292.0
FI	2015	0	
DK	2014	19	2,399.9
NO	2014	11	626.8
SE	2014	5	2.0
FI	2014	0	
DK	2013	18	2,399.0
NO	2013	9	1,069.0

Filter 5: Environmental monitoring

We reviewed the available national monitoring databases for the list of compounds that had passed Filter 4, i.e. databases provided from Norway, Sweden and Denmark and information from Finland. Again, we treated the whole Nordic area as one entity, for example in a review of how often the compound had been tested. Regarding the criterion whether or not a compound had been tested in the last ten years, the period since 2010 was reviewed, with 2010 included. “Two locations” were regarded as two different sampling stations. The term “tested” was interpreted as “the compound was sought”, i.e. included in the monitoring programme, irrespective of its detection or concentration. The search included occasional data from air monitoring, but the majority originated from the aquatic environment.

Table 8. Summary of databases searched for compounds identified after Filter 4.

Country	Databases	Approach
Norway	Norwegian emerging contaminant data https://vann-miljo.miljodirektoratet.no/	Search by CAS number
Sweden	Swedish screening database https://dvsb.ivl.se/dvss/DataSelect.aspx Biota https://dvsb.ivl.se/ Pollutants in sediment https://dvsb.ivl.se/dvss/DataSelect.aspx	Screening database: Search by CAS number; biota database: Search within PFAS, brominated flame retardants and PAHs; sediment database: Database download, search by compound name
Denmark	Danish environmental monitoring database (Overfladevandsdatabase) https://odaforalle.au.dk/login.aspx	Downloads of databases for contaminants in sea, lakes and rivers; search by Standat code in sediment database (sea), otherwise by compound name
Finland	E-mail information regarding monitoring parameters	Included in overall data compilation

We applied the same scoring methods as Woldegiorgis et al. (2019), but a different cut-off value of ≥ 2 instead of ≥ 3.

Table 9. Scoring of compounds which have previously been screened.

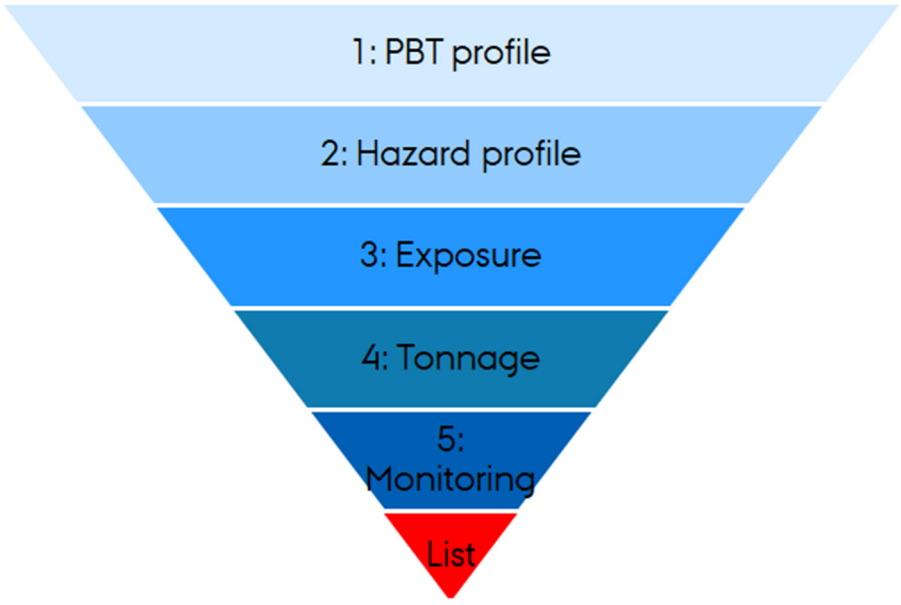
Description	Scoring	Comment
The last date was less than 10 years ago	1	If "*yes*", then 0p.
The compound has been tested at less than 2 locations	1	If "*no*", then 0p.
The compound has been tested during less than one year	1	If "*no*", then 0p.
The compound has been tested in less than 2 recipients/matrices	1	If "*no*", then 0p.
The compound has been tested over 300 times	1	If "*no*", then 0p.If "*yes*" then 1p
The compound has been tested between 50 and 300 times	2	If "*no*", then 0p If "*yes*", then 2p.
The compound has been tested less than 50 times	3	If "*no*", then 0p. If "*yes*", then 3p.
Aggregated Maximum	7	

In Woldegiorgis et al. (2019), the criterion "The compound has been tested less than 50 times" resulted in a score of 3 and effectuated that the compound passed this filter, based on the consideration that few existing measurements (in combination with the other filters) may warrant more study. Due to the extended geographical scope and the search in multiple database, a compound was, if included in a monitoring programme, usually tested more than 50 times. This meant that even a less studied compound usually fell into the

category of 50-300 tests rather in the category < 50 tests. The criterion “The compound has been tested between 50 and 300 times” resulted in a score of 2. For this reason, a score of 2 was used as a cut-off value. For compounds not included in the databases, a score of 1.4 was used for each of the categories, resulting in a total score of 7. This approach was unchanged compared to Woldegiorgis et al. (2019). For BaP, the example used above, the database review resulted in only one score ≠ 0, for the criterion “The compound has been tested over 300 times”. The affirmative answer resulted in a score of 1, which also was the total score for BaP in this filter. For this reason, BaP would not pass this filter as a compound prioritized for future monitoring.

In summary, the structure of the filters look like the figure 1 below:

Figure 1. Screening Filters.



For the compounds without data in the monitoring databases, an additional literature search was conducted in Web of Science. This was not intended for inclusion in the scoring system, but for additional information of relevance, for example from monitoring programs outside the Nordic countries. The compound names were combined with each of the search terms ”environment”, ”screening” and ”monitoring”. As multiple names exist for each compounds, the search was repeated for common alternative compound names, as detailed in Annex 1.

3 Results

We built upon the list by Woldegiorgis et al. (2019) and updated this from 2018 to 2020. Table 10 summarizes the number of compounds reviewed in the former and the new study, the latter only given by additional compounds. A total of 172 new compounds were identified and added to the existing list of 1700 compounds bringing the total review compounds to 1872.

Table 10. Summary of compound numbers included in this study and the study by Woldegiorgis et al. (2019).

List	Existing compounds (2018)	New compounds (2018-2022)	Total
SIN list	684	77	761
REACH XVII	125	0	125
REACH art 59	155	39	194
REACH XIV	36	19	55
CoRAP	278	29	307
EDC list	422	8	430
TOTAL	1700	172	1872

Some of the 1872 compounds were not included in the ranking exercise because they were either metals, UVCBs, or intermediates, in accordance with Woldegiorgis et al. (2019). This brought the total number of reviewed chemicals down from 1872 to 1529.

Filter 1: PBT Screening

The first filter reduced the 1529 total compounds to 194 compounds in total that scored 0.7 or higher. These 194 progressed to the next filter.

Filter 2: Σ Human and environmental hazard:

Among the 194 compounds from the first filter, 51 compounds scored 3 or higher for the total hazard without weighted hazard lists, and thus also passed the second filter with regards to total human and environmental hazard. These 51 compounds out of the total 1529 old and new compounds are therefore identified as potentially problematic and progressed to the exposure and monitoring analysis in filters 3-5 below. As mentioned under the methods section above we only reviewed the exposure potential for these 51 prioritized potentially problematic candidate compounds in the subsequent filters below.

Filter 3: Total Exposure:

Out of the 51 compounds which passed both two previous filters 23 compounds passed the cut-off ≥ 4 for the total exposure filter and progressed to the next total use filter.

Filter 4: Total use:

All of the 23 compounds from filter 3 also passed the fourth filter with a cut-off value of ≥ 3. Hence, a total of 23 compounds progressed to the final filter on monitoring efforts. See the total scored list after the first four filters in Table 11 below.

Table 11. Name, CAS and EC-number and scoring points for the first 4 filter levels of 23 proposed chemical candidates for screening. PBT score is not included in the "Total points 4 filters", it is used as the first filter, and for calculating "Total points Hazard". "Total points 4 filters" uses the "Total points Hazard" with weighted hazard lists

CASNumber	EC Number	Name	PBT	Total points Hazard (not weighed Hazard lists)	Total points Hazard (weighed Hazard lists)	Total points Exposure	Total points Quantity	Total points 4 filters (weighed hazard lists)
50-32-8	200-028-5	Benzo[def]chrysene	1	7	7	6	6	19
101-68-8	202-966-0	4,4'-Methylenediphenyl diisocyanate	0.7	5	5	7	6	18
556-67-2	209-136-7	Octamethylcyclotetrasiloxane	1	5	5	7	5	17
26471-62-5	247-722-4	m-tolylidene diisocyanate	0.7	6	3	7	6	16
2451-62-9	219-514-3	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	0.7	5.4	5.4	5	5	15.4
84852-15-3	284-325-5	4-nonylphenol, branched	0.7	3.4	1.7	7	6	14.7
218-01-9	205-923-4	Chrysene	1	6	6	5	3.5	14.5
96-69-5	202-525-2	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	0.7	4.6	2.3	6	6	14.3
127-18-4	204-825-9	Perchloroethylene; tetrachloroethylene	0.7	5.9	2.95	6	5	13.95
2425-85-6	219-372-2	Pigment Red 3	0.7	4.5	2.25	6	5	13.25
118-82-1	204-279-1	2,2′,6,6′-Tetra-tert-butyl-4,4′- methylene-diphenol	0.7	4.4	2.2	6	5	13.2
75980-60-8	278-355-8	Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	0.7	3.5	1.75	6	5	12.75
98-29-3	202-653-9	4-tert-butylpyrocatechol	0.7	3.2	1.6	6	5	12.6
628-96-6	211-063-0	Ethylene dinitrate	0.7	3	1.5	5	6	12.5
81-15-2	201-329-4	Musk Xylene	1	4	4	5	3.5	12.5
115-27-5	204-077-3	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	0.7	4.8	2.4	5	5	12.4
79-94-7	201-236-9	Tetrabromobisphenol A (TBBPA)	0.7	3.6	1.8	5	5	11.8
2814-77-9	220-562-2	Pigment Red 4	0.7	4.5	2.25	4	5	11.25
3380-34-5	222-182-2	Triclosan	0.7	3.4	1.7	5	4	10.7
191-24-2	205-883-8	Benzo[ghi]perylene	1	3	3	4	3.5	10.5
110-88-3	203-812-5	1,3,5-trioxane	0.7	3.9	1.95	5	3.5	10.45
693-21-0	211-745-8	Oxydiethylene dinitrate	0.7	4.3	2.15	4	3.5	9.65
4979-32-2	225-625-8	N,N-dicyclohexylbenzothiazole-2-sulphenamide	0.7	4.1	2.05	4	3.5	9.55

Filter 5: Environmental monitoring:

Of the 23 compounds that had passed Filter 4, ten compounds could not be found in the databases, leading to a score of 7. The other compounds scored between 1 and 3 (Figure 2).

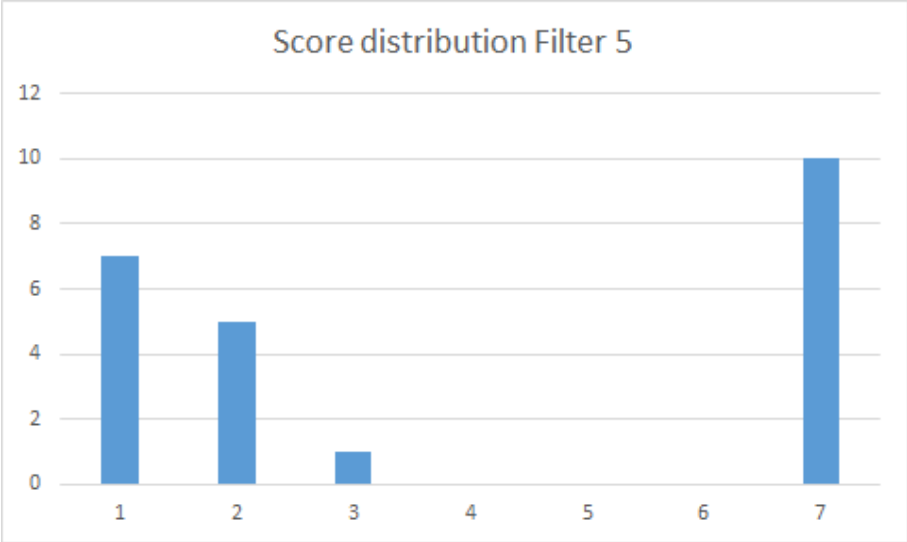


Figure 2. Chemicals score distribution in filter 5 monitoring.

The database search was challenged by the fact that it proceeded by compound name in some cases (Table 8), introducing risks of ambiguity and potentially false negatives. The compounds passing through this filter are those with a score ≥ 2, *i.e.* 16 of the original 23 substances. A score of only 1 reflected the situation that the compound had been widely included in the monitoring programs. Table 12 summarises the compounds that have passed Filter 5.

Table 12. Substances with score ≥ 2 after Filter 5 (Environmental monitoring). Compounds in bold were not prioritized by Woldegiorgis et al. (2019).

CAS number	Compound name	Score
26471-62-5	m-tolylidene diisocyanate	7
96-69-5	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	7
628-96-6	Ethylene dinitrate	7
2451-62-9	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	7
115-27-5	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	7
2814-77-9	Pigment Red 4	7
75980-60-8	Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	7
98-29-3	4-tert-butylpyrocatechol	7
693-21-0	Oxydiethylene dinitrate	7
110-88-3	1,3,5-trioxane	7
2425-85-6	Pigment Red 3	3
101-68-8	4,4'-Methylenediphenyl diisocyanate	2
127-18-4	Perchloroethylene; tetrachloroethylene	2
79-94-7	Tetrabromobisphenol A (TBBPA)	2
81-15-2	Musk Xylene	2
4979-32-2	N,N-dicyclohexylbenzothiazole-2-sulphenamide	2

The 10 compounds for which no data were available from the monitoring programs were included in a Web of Science environmental monitoring search[1], as described in section 3, using the compound names stated in Annex 1. However, there is a risk of incomplete searches by substance names, and searches by CAS numbers would be more unambiguous. Very few articles were identified with a direct relevance for environmental monitoring of these compounds. The only 2 compounds for which some monitoring experience was documented were the explosives ethylene dinitrate (CAS number 628-96-6) and oxidiethyl dinitrate (CAs number 693-21-0). Details of the literature search results are summarized in Annex 1.

In Table 13 the names, CAS and EC-numbers and total scoring points of proposed chemical candidates for screening, after the five filters, are shown. Compared to the 13 proposed chemical candidates for screening in Table 18 in Woldegiorgis et al. (2019), 10 of these are also in Table 13. Three of the chemicals, i.e. CAS no. 25155-23-1, 68855-45-8 and 118-82-1, in Table 18 in Woldegiorgis et al. (2019) are omitted for further prioritization here, as the first two are classified as UVCBs, part of mixtures or intermediates and the latter does not pass the monitoring filter. Six compounds are included in Table 13, i.e. the updated prioritization, which had not been included in the prioritization by Woldegiorgis et al. (2019), for the following reasons: CAS 79-94-7 and 4979-32-2 did not pass the monitoring filter in Woldegiorgis et al. (2019), CAS 127-18-4 and 81-15-2 did not pass the exposure, quantity and monitoring filters in Woldegiorgis et al. (2019), and CAS 2425-85-6 and 2814-77-9 are new additions in the CoRAP list.

Table 13. Name, CAS and EC-number and total scoring points of 16 proposed chemical candidates for screening.

CAS Number	EC Number	Name	PBT	Total points Hazard (not weighted Hazard lists)	Total points Hazard (weighted Hazard lists)	Total points Exposure	Total points Quantity	Total points Environmental Monitoring	Final points - total sum
26471-62-5	247-722-4	m-tolylidene diisocyanate	0.7	6	3	7	6	7	23
2451-62-9	219-514-3	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	0.7	5.4	5.4	5	5	7	22.4
96-69-5	202-525-2	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	0.7	4.6	2.3	6	6	7	21.3
101-68-8	202-966-0	4,4'-Methylenediphenyl diisocyanate	0.7	5	5	7	6	2	20
75980-60-8	278-355-8	Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	0.7	3.5	1.75	6	5	7	19.75
98-29-3	202-653-9	4-tert-butylpyrocatechol	0.7	3.2	1.6	6	5	7	19.6
628-96-6	211-063-0	Ethylene dinitrate	0.7	3	1.5	5	6	7	19.5
115-27-5	204-077-3	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	0.7	4.8	2.4	5	5	7	19.4
2814-77-9	220-562-2	Pigment Red 4	0.7	4.5	2.25	4	5	7	18.25
110-88-3	203-812-5	1,3,5-trioxane	0.7	3.9	1.95	5	3.5	7	17.45
693-21-0	211-745-8	Oxydiethylene dinitrate	0.7	4.3	2.15	4	3.5	7	16.65
2425-85-6	219-372-2	Pigment Red 3	0.7	4.5	2.25	6	5	3	16.25
127-18-4	204-825-9	Perchloroethylene; tetrachloroethylene	0.7	5.9	2.95	6	5	2	15.95
81-15-2	201-329-4	Musk Xylene	1	4	4	5	3.5	2	14.5
79-94-7	201-236-9	Tetrabromobisphenol A (TBBPA)	0.7	3.6	1.8	5	5	2	13.8
4979-32-2	225-625-8	N,N-dicyclohexylbenzothiazole-2-sulphenamide	0.7	4.1	2.05	4	3.5	2	11.55

Table 14 below, summarizes the physical-chemical properties of the prioritized compounds and includes suggestions for matrices to monitor and instrumental analysis. These suggestions are based on the physical-chemical properties and occasional references and does not include an in depth-literature search. The national databases include analytical methods in some, but not all cases. Table 15 illustrates where there were data gaps in the current prioritization, which triggered the attribution of a penalty score. Most data gaps were identified for the monitoring filter, with the caveats of potential false negatives as discussed above.

Table 14. Physical/Chemical properties, analytical methods and suggested matrixes to consider for the prioritized chemical candidates (Woldegeorgis et al., 2019 and US EPA CompTox Chemicals Dashboard, and SPIN max. exposure index)

CAS Number	EC Number	Name	Water Solubility (mg/L)	Log Kow	BCF (L/kg)	Log Koc	Exposure Index	Typical instrumental method	Matrix
26471-62-5	247-722-4	m-tolylidene diisocyanate	124	3.43	180	na	Wastewater	LC [a)]-MS or GC [a)]-MS	Slugde/water/Sediment
2451-62-9	219-514-3	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	9000	-0.8	na	1.5-1.7	Occupational	LC-MS	Water
6-69-5	202-525-2	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	0	5.24	6.5	5.61	Occupational	GC-MS	Slugde/Sediment/biota
101-68-8	202-966-0	4,4'-Methylenediphenyl diisocyanate	6.8	4.51	200	na	Wastewater	LC-MS or GC-MS	Slugde/Sediment/biota
75980-60-8	278-355-8	Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	3.1-11	3.1-3.9	39	2.9	Occupational	LC-MS	Water
98-29-3	202-653-9	4-tert-butylpyrocatechol	4200	1.98	6.6	1.37	Occupational	LC-MS	Water
628-96-6	211-063-0	Ethylene dinitrate	5200	1.16	na	na	Occupational	LC-MS [b)]	Water
115-27-5	204-077-3	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	3.5-500	-1.59	na	0.76 (soil)	Occupational	LC-MS	Slugde/water/biota
2814-77-9	220-562-2	Pigment Red 4	0.000013	4.85	1002	601 (soil)	Wastewater	GC-MS	Slugde/Sediment/biota
110-88-3	203-812-5	1,3,5-trioxane	172000	-0.5	0.8	-0.416	Occupational	LC-MS	Water
693-21-0	211-745-8	Oxydiethylene dinitrate	3900	0.98	na	2.1	Occupational	LC-MS	Water
2425-85-6	219-372-2	Pigment Red 3	2.33	4.62	46.7	868 (soil)	Occupational	GC-MS	Slugde/Sediment/biota
127-18-4	204-825-9	Perchloroethylene; tetrachloroethylene	3.4	0.0018	134	251	Occupational	GC-MS	Water
81-15-2	201-329-4	Musk Xylene	0.0008	4.06	4070	8760 (soil)	Consum	GC-MS	Slugde/Sediment/biota
79-94-7	201-236-9	Tetrabromobisphenol A (TBBPA)	1.74	6.99	269	12580 (soil)	Occupational	LC-MS	Slugde/Sediment/biota
4979-32-2	225-625-8	N,N-dicyclohexylbenzothiazole-2-sulphenamide	0.0000016	4.8	211	1490	Occupational	LC-MS	Slugde/Sediment/biota

[a)] The description of “LC-MS” or “GC-MS” includes tandem mass spectrometry approaches, which are increasingly used instead of single quadrupole approaches in monitoring laboratories. Typical LC-MS approaches can also use GC-MS techniques instead, often including a derivatization step. [b)] Direct MS analysis after thermal desorption used by McEneff et al. (2018), see Annex 1. It can probably also be applied to oxydiethylene dinitrate (CAS 693-21-0).

Table 15. Data gaps for the 16 chemical candidates proposed for screening. X indicates penalty scores and knowledge gaps.

CAS Number	EC Number	Name	Hazard (not weighted Hazard lists)	Exposure	Quantity	Environmental Monitoring
26471-62-5	247-722-4	m-tolylidene diisocyanate				X
2451-62-9	219-514-3	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione				X
96-69-5	202-525-2	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol				X
101-68-8	202-966-0	4,4'-Methylenediphenyl diisocyanate				
75980-60-8	278-355-8	Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	X			X
98-29-3	202-653-9	4-tert-butylpyrocatechol				X
628-96-6	211-063-0	Ethylene dinitrate				X
115-27-5	204-077-3	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride				X
2814-77-9	220-562-2	Pigment Red 4				X
110-88-3	203-812-5	1,3,5-trioxane			X	X
693-21-0	211-745-8	Oxydiethylene dinitrate			X	X
2425-85-6	219-372-2	Pigment Red 3				
127-18-4	204-825-9	Perchloroethylene; tetrachloroethylene				
81-15-2	201-329-4	Musk Xylene			X	
79-94-7	201-236-9	Tetrabromobisphenol A (TBBPA)				
4979-32-2	225-625-8	N,N-dicyclohexylbenzothiazole-2-sulphenamide			X	

4 Conclusions

This project has strived for an objective approach to a prioritization of chemicals, applying a transparent and clearly defined scoring system. However, as also pointed out by Woldegiorgis et al. (2019), the current approach relies on an a priori interest in the compounds included in the current prioritisation, based on a suspected or identified environmental or health concern. This preselection influences the final compound selection, and it is important to note that the current prioritisation has taken place within the frame of the lists and databases described in the method section. Other prioritisation processes may be based on other input material, thus potentially reaching different conclusions. For example, the study by Muir et al. (2019) identifying potential Arctic pollutants was based on databases of all chemicals in commerce in Europe and North America.

The current prioritization is, rightfully, strongly based on a PBT and hazard characterisation of the selected chemicals, as described under Filter 1. This approach could be expanded to also include persistent, mobile and toxic (PMT) compounds. While the P and T criteria are identical with the PBT assessment, potential PMT compounds do not necessarily bioaccumulate, but are characterised by mobility, for example through soils and in aquifers. It might be useful to extend further risk assessments to this criterion, in order to ensure a comprehensive approach. It particularly concerns perfluorinated alkylated substances (PFAS), but is not limited to them.

PFAS compounds were introduced via wild cards by Woldegiorgis et al. (2019), as they did not emerge during the prioritization approach. This was confirmed in the current study. While we did not explicitly propose wild cards, we confirm the relevance of this compound group. Other substances receiving attention in the scientific literature include, but are not limited to chlorinated paraffins, current-use pesticides, flame retardants and UV filters.

The current basis with a strong focus on REACH regulations also implies that chemicals managed under other programs are not considered to the same extent, for example pesticides, pharmaceuticals and personal care products. These groups may also include chemicals of concern for which monitoring data could be of interest for risk assessment purposes.

As mentioned above, the cases of lack of data have been taken into account in the current prioritization through the attribution of penalty scores for each of the five assessment filters. Penalty scores indicate that there is missing information or data and thus missing knowledge that is necessary in the proposed methodology. In Table 15 it is seen that the monitoring filter has ten chemicals with penalty scores, four chemicals have penalty scores for missing information on exposure, and one chemical has a penalty score for the hazard filter. The missing information in the monitoring filter has to be interpreted with caution, as there is a risk of false negatives, as mentioned above. However, potential false negatives do not exclude, but include a compound due to the penalty system. As such, the penalty system supports the conservative approach generally applied in this prioritization scheme.

The search of environmental data based on the Nordic monitoring programs carries the risk of being non-exhaustive, for example due to unambiguous search criteria or time gaps in measurements and updates of databases. If a compound has been measured but classified as “not included” in this prioritization, this could lead to false positives. However, considering the conservative approach generally chosen for this prioritization, this seems acceptable. In the scoring system applied here, which includes all compounds above a certain score instead of a defined number of ranked compounds, potential false positives do not exclude other compounds. The analysis of the monitoring of the prioritized compounds is more subjective than intrinsic properties to the compounds or the use data due to the inherent cost related to monitoring making this the less objective and general than the other filters. This does not mean it is less important than the previous ones but it would be possible to stop the more objective filtering of the compounds after the fourth filter and then assess the 23 compounds in Table 6 based on expert judgement. It is, of course, also possible to stop the filtering of the compounds after the fourth filter and then assess the 23 compounds in Table 6 based on expert judgement.

The level of build-in conservatism can be adjusted according to regulatory needs, which can be implemented by changing the scoring system and cut-off values to include more compounds – this is a risk management, and not a technical, challenge but an option to bear in mind. Moreover, after assessing the list it is possible to add problematic compounds based on expert judgement that were not prioritized, as was done in the wild card approach by Woldegiorgis et al. (2019), adding relevant PFAS compounds which did not emerge as prioritized compounds from this approach. UVCBs and some intermediates could also be considered included in the prioritization as well as organometals. The methodology would in time lead itself to a more automated machine-learning / AI environment combining more databases and models.

New analytical techniques include suspect screening and non-target screening approaches based on high resolution mass spectrometry, algorithms for peak identification and comparison with spectra databases. These techniques enable detections of suspected and unknown compounds in a sample. However, the identification of completely unknowns is complex and might only allow tentative compound suggestions. Knowing the molecular mass of a compound and its potential mass spectra, as in the case of suspect screening, obviously increases the chances of compound identification. Other obstacles in these emerging techniques can be a reduced instrumental sensitivity compared with conventional targeted analyses, which are optimised for specific compounds, in combination with matrix interferences, due to reduced sample purification. Thus, while these are promising techniques, which have an important complementary function to target screening analyses, there are limitations that need further developments prior to more routine use. The priority list generated in this project could be a starting point for a suspect screening, bearing in mind that suitable extraction methods with the right degree of selectivity and optimized method detection limits might be needed.

Compound properties such as partition coefficients (i.e. Kow and Koc values) can be used to characterise the sorption of the compounds. Equilibrium partitioning modelling (Di Toro et al, 1991) has been used to convert measurements in one environmental compartment to another, needing knowledge of sorption kinetics and related partition coefficients. This is a wide research field, also involving the use of passive samplers as reference phases, with

potential applications in monitoring programs in the future (Booji et al., 2016). Besides the question of matrix, it is important to specify whether point sources (e.g. waste water treatment plants) or diffuse sources are being addressed. Sampling frequencies are related to the variability of the system, however, practical considerations such as logistics and costs will play a role as well. It is common practice to perform a first screening exercise, possibly involving the new screening techniques as described above and opportunistic sampling. In many of the cases discussed here, developments of analytical method for quantification purposes will have to be considered, also affecting factors like sample size needed to reach certain limits of detection / quantification or potential limitations in sample preparation and efficiency.

All research based consultancy at DCE / AU is covered by a quality management system, which is built according to the principles in the ISO-9001 standard for Requirements for quality management systems. The quality management system is based on the Quality Assurance of the research-based government consultancy at Aarhus University. According to AU's guidelines, the report must be reviewed by internal peer assessment by an assessor with relevant academic competencies.

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Annex 1

Summary of the literature search in Web of Science. As the search was conducted on compound names, there is a risk of studies being overlooked

CAS number	Name used in this study	Alternative names for the same CAS number used in the search	Summary of search results	References and other comments
26471-62-5	m-tolylidene diisocyanate	Toluylene diisocyanate; toluene diisocyanate	No relevant articles identified on environmental monitoring. A number of studies were found in the field of material science and occupational exposure.	Diisocyanates are included as prioritized compounds in the EU human biomonitoring project HBM4EU (www.hbm4eu.eu)
96-69-5	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol	4,4′-Thiobis(2-tert-butyl-5-methylphenol); 2-tert-butyl-4-(5-tert-butyl-4-hydroxy-2-methylphenyl)sulfanyl-5-methylphenol	No relevant articles identified on environmental monitoring. Most studies are related to nanomaterials.	Biodegradability study of polymers based on CAS 96-69-5: Mallakpour et al. (2011), Colloid. Polym. Sci. 289, 93-100.
628-96-6	Ethylene dinitrate	Dinitroethylene glycol; Nitroglycol	Several articles found with links to environmental fate and monitoring	Passive samplers: McEneff et al. (2018), Scientific Reports 8: 5816; Occurrence in industrial wastewater and treatment processes: Cyplik et al. (2013), Chemosphere 93, 2823-2831; Microbial degradation: Dario et al. (2010), J. Hazard. Mat. 176, 125-130.
2451-62-9	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	Tris(2,3-epoxypropyl) isocyanurate; Triglycidyl Isocyanate	Most studies were found in the field of material science and occupational exposure.	Monitoring of workplace air: Jazewska and Kowalska (2019), Int. J. Environ. Res. Public Health 16: 4455
115-27-5	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	Chlorendic anhydride	Not much literature found, few studies on polymer manufacture and occupational exposure	Structural resemblance to dechlorane plus
2814-77-9	Pigment Red 4	-	No literature found on environmental monitoring, but it was difficult to search for this compound specifically.	Search should be repeated on CAS number

75980-60-8	Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide	2,4,6-Trimethylbenzoyldiphenyl phosphine oxide; (diphenylphosphoroso)(2,4,6-trimethylphenyl)methanone	No relevant articles identified on environmental monitoring. Most studies are related to polymers.	-
98-29-3	4-tert-butylpyrocatechol	4-tert-butylcatechol; 4-tert-Butylbenzene-1,2-diol	No relevant articles identified on environmental monitoring, some studies related to degradation.	Photochemistry: Grieco et al. (2019), J. Phys. Chem. A 123, 5356-5366; Biodegradation: Toyama et al. (2010), Appl. Environ. Microbiol. 76, 6733-6740.
693-21-0	Oxydiethylene dinitrate	Diglycol dinitrate; diethylene glycol dinitrate	Most studies found in the field of pyrotechnics, one older environmental study.	Environmental fate, focus on surface waters: Haag et al. (1991), Chemosphere 23, 215-230.
110-88-3	1,3,5-trioxane	Trioxymethylene	Many studies exist, but mainly in the field of chemical synthesis.	-

PRIORITIZATION OF EMERGING CONTAMINANTS FOR A NORDIC SCREENING STUDY

The aims of this report are 1) to identify knowledge gaps and monitoring needs for new emerging contaminants, expected to be present in the (aquatic) environment, based on lists of possibly hazardous chemical substances and 2) suggest a pan-Nordic screening study for prioritized substances. The report shall support the Joint Nordic Screening group in evaluating and prioritizing chemicals in national aquatic environmental monitoring programs.

1872 compounds identified from international lists and databases have been filtered through five filters based on PBT-profile, human and environmental profile, exposure, total use and previous environmental screening. The result of the filtering was a list of 16 chemical proposed candidates for screening studies. The report builds on a report by Woldegiorgis et al. (2019). The same method as in Woldegiogis et al. (2019) has been used, although with slight revisions

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