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Final Report

HELCOM PreEMPT

Baltic Marine Environment Protection Commission

Wide-scope target and suspect screening of emerging contaminants and their transformation products in marine biota and sediment samples from the Baltic Sea

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List of Abbreviations

Accelerated Solvent Extraction	ASE
Atmospheric Pressure Chemical Ionization	APCI
Below the Limit of Quantification	BQL
broad-band Collision Induced Dissociation	bbCID
Data Collection Templates	DCTs
Digital Sample Freezing Platform	DSFP
Dry weight	d.w.
Electrospray Ionization	ESI
Environmental Institute	EI
Environmental Quality Standard	EQS
Frequency of Appearance	FoA
Frequency of Exceedance	FoE
Extent of Exceedance	EoE
Gas Chromatography	GC
High Resolution	HR
Limit of Detection	LOD
Limit of Quantification	LOQ
Liquid Chromatography	LC
Mass Spectrometry	MS
Measured Environmental Concentration	MEC
National and Kapodistrian University of Athens	NKUA
Not Available	NA
Not Detected	ND
Personal Care Products	PCPs
Pharmaceuticals	Pharms
Plant Protection Products	PPPs
Polychlorinated Biphenyls	PCBs
Polycyclic Aromatic Hydrocarbons	PAHs
Predicted No Effect Concentration	PNEC
Quadrupole Time of Flight Mass Spectrometer	Q-ToF MS
Quantitative Structure Activity Relationship	QSAR
Retention Time Index	RTI
Screening Detection Limit	SDL
Solid Phase Extraction	SPE
Standard Operating Procedure	SOP
Transformation Products	TPs
Ultra High Performance Liquid Chromatography	UHPLC
Water Framework Directive	WFD
Wet weight	w.w.

1. Introduction

In 2021, HELCOM initiated the PreEMPT project. The project was awarded funding by NEFCO (Nordic Environment Finance Corporation) under the Baltic Sea Action Plan Fund and supports the aims of the Baltic Sea Action Plan.
The PreEMPT project aims to support HELCOM Contracting Parties in carrying out the first Baltic Sea regional screening of hazardous substances, as well as supporting further developments of relevant hazardous substances assessment work in HELCOM. The project funds were used in conjunction with affirmed national contributions to create the largest number of screening samples at the broadest spatial coverage (and distribution) possible, while ensuring that all countries were included. The original generalised overview of samples planned to be collected and analysed is in the table below.

Country	**NEFCO funded samples**	**Nationally funded samples**
Denmark	3	13
Estonia	5	10
Finland	6	6
Germany	2	0
Lithuania	6	0
Latvia	3	2
Poland	6	0
Russia	4	0
Sweden	10	28
TOTAL	**45**	**59**

Out of the originally foreseen 104 samples, 94 have finally been received an analysed. The detected compounds were prioritised based on their frequency of occurrence in the samples and exceedance of ecotoxicological threshold values. Analysis of the collected samples has been undertaken in cooperation with the NORMAN Association using established and harmonised techniques that have been internationally developed and tested. Environmental Institute (EI) has been assigned to organise a specialized package of services, comprising screening of several thousands of organic pollutants and their transformation products by wide-scope target (>2,500 substances) and suspect (>65,000 substances) screening methodologies. For this purpose, 94 samples (30 sea sediment, 31 mussels and 33 fish) from 12 organisations representing HELCOM Contracting Parties were delivered to the Laboratory of Analytical Chemistry of the National and Kapodistrian University of Athens (NKUA).
Screening efforts of wide range chemical substances are being increasingly recognized by the EU, its services and Regional Sea Conventions as important for identifying potential contaminants' threats to the aquatic environment, sources of contamination and design of the follow up Programmes of Measures. The outcomes of the study were considered as a potential input for the development of a chemical contaminants indicator in the Baltic Sea Region.

The report is providing a summary assessment of results from all analysed samples characterising the entire Baltic Sea Region and also sub-reports discussing results and assessment of samples provided by individual countries.

2. Objectives

The specific objectives of the study were as follows:

a) Wide-scope target screening analysis of each sample for ca. 2,500 substances by LC-ESI-HRMS and GC-APCI-HRMS;
b) Suspect screening of more than 65,000 compounds in each of the samples including their semi-quantification using LC-ESI-HRMS;
c) Upload of the LC-ESI-HRMS and GC-APCI-HRMS chromatograms into NORMAN Digital Sample Freezing Platform (DSFP) for retrospective screening;
d) Prioritisation of detected compounds in order to assess their environmental toxicological relevance;
e) Report on the occurrence of targeted and suspect substances including interactive visualization tool for presentation of the results.

3. Samples

In total, 94 samples representative for the ecosystem of Baltic Sea were collected from nine countries (Denmark, Estonia, Finland, Germany, Latvia, Lithuania, Poland, Sweden, Russian Federation). The samples were delivered to NKUA in the period from November 2021 to April 2022. Information on the analyzed sediments and biota samples is provided in **Table 1** and **2,** respectively. Additional samples' metadata are available in the Data Collection Templates (DCTs) available as an Annex to this report. Samples marked with an asterisk (*) at their 'Code' were labeled as 'reference samples' (low anthropogenic pollution) by the sender. Muscle tissue was used for analysis of fish samples. Regarding mussels, the soft body was analysed.

Table 1. List of HELCOM PreEMPT sediment samples.

Code	Country	Location	Organisation	Sender's Code
13	Poland	Gdansk Basin	Institute of Meteorology and Water Management (IMGW-PIB)	P1 (station name: BMPL1)
14		Bornholm Basin		P5C (station name: PL-P5C)
15		Eastern Gotland Basin		P140 (station name: BMPK1)
63	Sweden	Bottenhavet	Swedish Agency for Marine and Water Management	a001///rfs21_a001_06_000_005
64		Urviksfjärden		c002///rfs21_c002_06_000_005
65		Bottenhavet		g003///rfs21_g003_06_000_005
66		Saltsjön		l003///rfs21_l003_06_000_005A + rfs21_l003_06_000_005B
67		Bottenhavet		i001///rfs21_i001_06_000_005A + rfs21_i001_06_000_005B
68		Östhammar		j001///rfs21_j001_06_000_005A + rfs21_j001_06_000_005B
69		Nyköping		m001///rfs21_m001_06_000_005A + rfs21_m001_06_000_005B
70		Finnagården		x002///rfs21_x002_06_000_005A + rfs21_x002_06_000_005B

71		Gothenburg		y003///rfs21_y003_06_000_005A + rfs21_y003_06_000_005B
72		Bottenhavet		h004///rfs21_h004_06_000_005A + rfs21_h004_06_000_005B
73		Innerstaden		p002///rfs21_p002_06_000_005A + rfs21_p002_06_000_005B
74		Baltic Sea		p005///rfs21_p005_06_000_005A + rfs21_p005_06_000_005B
75		Mörrums Bruk		s002///rfs21_s002_06_000_005A + rfs21_s002_06_000_005B
76		Saltkälle fjord		z003///rfs21_z003_06_000_005A + rfs21_z003_06_000_005B
77		Øresund		u004///rfs21_u004_06_000_005A + rfs21_u004_06_000_005B
78		Västervik SO		q001///rfs21_q001_06_000_005A + rfs21_q001_06_000_005B
79		Västervik SO		q002///rfs21_q002_06_000_005A + rfs21_q002_06_000_005B
80		Kattegatt		q005///rfs21_q005_06_000_005A + rfs21_q005_06_000_005B
81*		Bråviken		mos21_13001///mos21_13001_03_00_005A + mos21_13001_03_00_005B + mos21_13001_03_00_005C
82		Bråviken		n002///rfs21_n002_06_000_005A + rfs21_n002_06_000_005B
83		Bråviken		n006///rfs21_n006_06_000_005A + rfs21_n006_06_000_005B
84*		Baltic Sea		mos21_10001///mos21_11001_03_000_005A + mos21_11001_03_000_005B + mos21_11001_03_000_005C + mos21_11001_03_000_005D + mos21_11001_03_000_005E
90	Denmark	Roskilde Fjiord	Aarhus University	S0458 20161 (station FRB64)
91		Wadden Sea		S0473 20167 (station SIYJUVD5001)
92		Gamborg Fjiord		S0317 19023 (Gambrog Fj.)
93		Western Limfjorden		S0448 19927 (station LIM-372N.D.-1)
94		Skive		S0445 19929 (station Skive st 29)

Table 2. List of HELCOM PreEMPT biota samples.

Code	Specie	Country	Location	Organisation	Sender's Code
1	European perch (*Perca fluviatilis*)	Finland	Helsinki	Finnish Environment Institute	N/A
2			Kotka		N/A
3*			Parainen		N/A
4			Vaasa		N/A
5			Hailuoto		N/A
6*			Pori		N/A
7	Blue mussel (*Mytilus edulis*)		Cage 4 Kotka		N/A
8			Cage 1 Helsinki		N/A
9			Cage 2 Pori		N/A
10			Cage 3 SM		N/A
11*			Tvärminne start		N/A
12*			Hanko		N/A
16	Atlantic herring (*Clupea harengus*)	Poland	Eastern Gotland Basin	Institute of Meteorology and Water Management (IMGW-PIB)	W (station name: LWLA)
17			Bornholm Basin		KD (station name: LKOL)
18	Blue mussel (*Mytilus edulis*)		Polish coastal waters Gdansk Basin		station name: LSOP
19	European perch (*Perca fluviatilis*)	Estonia	Narva-Kunda Bay	Estonian Environmental Research Centre (EKUK)	X004
20			Pakry Bay		X010
21*	European flounder *(Platichthys flesus)*		Liivi laht		X021
22			Reigi Bay		X008
23			Pakri Bay		X009
24	Blue mussel (*Mytilus edulis*)		Aegna		X025
25*			Saaremaa		X024
26			Küdema Bay		X027
27*			Krassgrund		X026
28			Väike-Pakri		X028
29	European perch (*Perca fluviatilis*)		Matsalu Bay		X290
30			Väinameri		X291
31*			Kihelkonna Bay		X292
32			Pärnu Bay		X003
33			Liivi lath		X020
34	European flounder *(Platichthys flesus)*	Lithuania	Baltic Sea, S-3	Lithuanian Environmental Protection Agency	T-105-2021-PAV-861
35	Atlantic herring *(Clupea harengus)*		Baltic Sea, S-3		T-105-2021-PAV-863
36	Zebra mussel (*Dreissena polymorpha*)		Curonian Lagoon		T-014-2021-PAV-1087
37	Atlantic herring (*Clupea harengus*)	Latvia	Baltic Sea	Latvian Institute of Aquatic Ecology	BS-H
38			Gulf of Riga		GR-H
39	European perch (*Perca fluviatilis*)		Daugavgriva, Gulf of Riga		DG-P
40			Mersrags, Gulf of Riga		MR-P
41			Lielirbe, Baltic Sea		LI-P
42			Salacgriva, Gulf of Riga		SG-P
43			Jurmalciems, Baltic Sea		JM-P
44	Blue mussel		Pavilosta, Baltic Sea		PV-M

Code	Specie	Country	Location	Organisation	Sender's Code
45	*(Mytilus edulis)*	Sweden	Kullen	Naturhistoriska riksmuseet (Swedish Museum of Natural History)	Q2021-01349
46			Himmerfjärden		Q2021-01350
47			Malmö Hamn		Q2021-01351
48			Göteborg Hamn		Q2021-01352
49*			Gräsö		Q2021-01353
50*			Kvädöfjärden		Q2021-01354
51			Ronnebyåns mynning		Q2021-01355
52*			Sölvesborg		Q2021-01356
53			Landskrona		Q2021-01357
54			Askö		Q2021-01358
55			Oxelösund		Q2021-01023
56*	European perch *(Perca fluviatilis)*		Örefjärden		Q2021-01359
57*			Kinnbäcksfjärden		Q2021-01360
58			Skelleftehamn		Q2021-01361
59			Sundsvallsfjärden		Q2021-01362
60			Norrsundet		Q2021-01363
61*			Holmöarna		Q2021-01364
62	Blue mussel *(Mytilus edulis)*	Germany	Baltic Sea	State Office for the Environment, Nature Conservation and Geology Mecklenburg-Vorpommern (LUNG MV)	Teilprobe 13-1 & 13-2
85*			Baltic Sea: offshore Darsser Ort	German Environmental Specimen Bank	4110/0/002/06103/0/005-006, 008-010, 012-016, 018-021, 027-033, 034-042 (2/2)
86		Russian Federation	Outer Neva River estuary 1	HELCOM Secretariat	B1
87			Outer Neva River estuary 2		B2
88			Neva Bay		B3
89			Kopora Bay		B4

4. Sample preparation

4.1 Pre-treatment

The fresh biota and sediment samples were lyophilized (at -55 °C, 0.05 mbar) using a Telstar Lyoquest Freeze Dryer (**Figure 1**), and homogenized using pestle and mortar prior to analysis. The sediment samples were sieved through a 63 µm sieve for the removal of seashells and rocks.

Figure 1. LyoQuest-55 laboratory freeze dryer, Telstar®.

The % water content of HELCOM PreEMPT biota samples, used to express the results in wet weight, is provided in **Table 3**.

Table 3. %Water content of HELCOM PreEMPT biota samples. The samples marked with (*) were delivered to the analytical laboratory in dry form.

Code	% water content	Code	% water content
HELCOM PreEMPT 1	79.8	**HELCOM PreEMPT 36**	94.4
HELCOM PreEMPT 2	79.3	**HELCOM PreEMPT 37**	77.0
HELCOM PreEMPT 3	73.6	**HELCOM PreEMPT 38**	78.6
HELCOM PreEMPT 4	79.9	**HELCOM PreEMPT 39**	79.0
HELCOM PreEMPT 5	79.2	**HELCOM PreEMPT 40**	78.3
HELCOM PreEMPT 6	78.0	**HELCOM PreEMPT 41**	78.7
HELCOM PreEMPT 7	93.3	**HELCOM PreEMPT 42**	79.7
HELCOM PreEMPT 8	90.1	**HELCOM PreEMPT 43**	78.5
HELCOM PreEMPT 9	89.5	**HELCOM PreEMPT 44**	82.2
HELCOM PreEMPT 10	90.9	**HELCOM PreEMPT 45**	86.4
HELCOM PreEMPT 11	88.5	**HELCOM PreEMPT 46**	89.4
HELCOM PreEMPT 12	88.5	**HELCOM PreEMPT 47**	88.1
HELCOM PreEMPT 16	76.2	**HELCOM PreEMPT 48**	89.0
HELCOM PreEMPT 17	78.5	**HELCOM PreEMPT 49**	89.1
HELCOM PreEMPT 18	95.1	**HELCOM PreEMPT 50**	89.5
HELCOM PreEMPT 19	78.5	**HELCOM PreEMPT 51**	89.2
HELCOM PreEMPT 20	79.7	**HELCOM PreEMPT 52**	90.9
HELCOM PreEMPT 21	81.0	**HELCOM PreEMPT 53**	89.2
HELCOM PreEMPT 22	80.1	**HELCOM PreEMPT 54**	89.4
HELCOM PreEMPT 23	80.7	**HELCOM PreEMPT 55**	90.6
HELCOM PreEMPT 24	91.2	**HELCOM PreEMPT 56**	79.0
HELCOM PreEMPT 25	96.6	**HELCOM PreEMPT 57**	79.4
HELCOM PreEMPT 26	93.6	**HELCOM PreEMPT 58**	78.0

Code	% water content	Code	% water content
HELCOM PreEMPT 27	92.2	**HELCOM PreEMPT 59**	77.3
HELCOM PreEMPT 28	92.4	**HELCOM PreEMPT 60**	77.4
HELCOM PreEMPT 29	78.1	**HELCOM PreEMPT 61**	78.1
HELCOM PreEMPT 30	77.5	**HELCOM PreEMPT 62**	89.2
HELCOM PreEMPT 31	78.0	**HELCOM PreEMPT 85***	94.8
HELCOM PreEMPT 32	77.5	**HELCOM PreEMPT 86***	85.0
HELCOM PreEMPT 33	78.5	**HELCOM PreEMPT 87***	85.0
HELCOM PreEMPT 34	81.0	**HELCOM PreEMPT 88***	85.0
HELCOM PreEMPT 35	77.2	**HELCOM PreEMPT 89***	85.0

4.2 Analysis of contaminants of emerging concern

Two generic sample preparation protocols for the extraction of contaminants, suitable for wide-scope screening studies, per sample were followed. More polar, less volatile and thermally unstable compounds were extracted by the method specific for LC-amenable compounds, whereas a different sample preparation method was followed for the extraction of more volatile and thermostable GC-amenable compounds.

4.2.1 Extraction of LC-amenable contaminants from sediment samples

The extraction protocol was based on Nikolopoulou et al. (2022) study. 1 g of freeze-dried and sieved sediment sample was placed in a plastic centrifuge tube (15 mL). Polar to semi-polar contaminants of emerging concern were extracted with 2 mL Methanol/Milli-Q water (pH 2.5, formic acid 0.5 % and 0.1 % EDTA), 50/50 (v/v), by Vortex (1 min), followed by ultrasonic extraction for 15 min at 50 °C. After the extraction, the extract was centrifuged for 10 min at 4000 rpm and the supernatant was collected in a glass test tube. This procedure was repeated two more times. In total 6 mL of supernatant was collected. Then the total extract was evaporated to dryness under a gentle steam of N_2 at 40 °C. Reconstitution of the analytes was performed with 0.2 mL Methanol/Milli-Q water (50/50, v/v). Finally, the extract was filtered through a Regenerated Cellulose (RC) filter (Chromafil - pore size: 0.2 µm; filter diameter: 15 mm) and transferred to a glass vial for LC-ESI-QToF MS analysis.

4.2.2 Extraction of GC-amenable contaminants from sediment samples

10 g of each freeze-dried sediment sample was weighted into a 50 mL centrifuge tube. Two different organic mixtures of solvents were used for the extraction of the analytes. Firstly, 40 mL of dichloromethane/hexane (50/50, v/v) was added into the centrifuge tube and ultrasonic extraction was followed at 25 °C for 16 min. After centrifugation at 4000 rpm for 6 minutes, the supernatant was collected into a ground glass flask. The extraction was repeated two more times with hexane/acetone (50/50, v/v) as the extraction mixture. The three extracts (120 mL in total) were combined and evaporated to 1 mL with the use of a rotary evaporator. The remnant was cleaned-up through a glass chromatography column, packed with a glass wool plug, 3 g of silica and 3 g of aluminum

oxide. Activated anhydrous Na_2SO_4 (1 g) was added on the top of the column. Silica has been activated before use, by baking at 180 °C for 12 h, while alumina was activated at 250 °C for 3 h. A schematic illustration of the column used for the experiment is presented in **Figure 2**. The column was conditioned with 30 mL of dichloromethane/hexane (50/50, v/v) followed by 30 mL of hexane/acetone (50/50, v/v). The extract of the sample was loaded and the elution of the analytes was realized with 30 mL of dichloromethane/hexane (50/50, v/v) followed by 30 mL of hexane/acetone (50/50, v/v). 10 µL of isooctane was added as a keeper and the extract (60 mL in total) was evaporated near dryness. Finally, the sample was reconstituted to 200 µL hexane and filtered through a Regenerated Cellulose (RC) filter (Chromafil - pore size: 0.2 µm; filter diameter: 15 mm) and transferred to a glass vial for GC-APCI-QToF MS analysis.

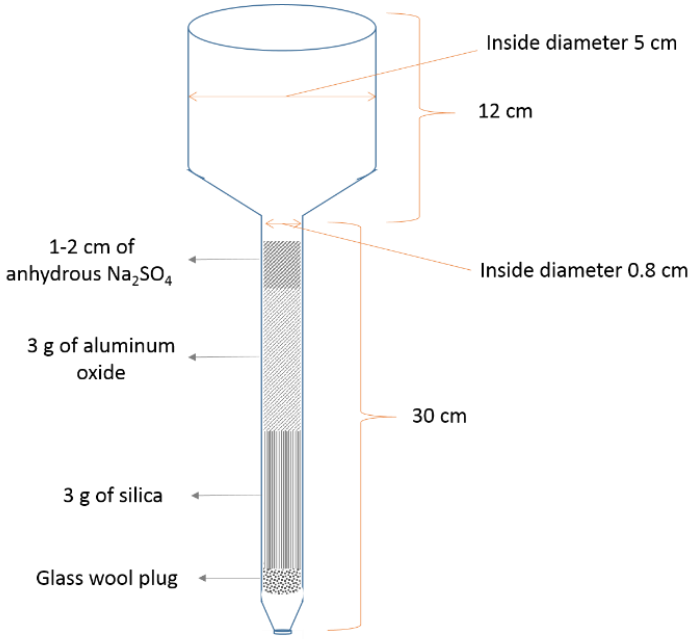


Figure 2. Glass column used for sample clean-up.

4.2.3 Extraction of LC-amenable contaminants from biota samples

Accelerated Solvent Extraction (ASE) was used for the extraction of emerging contaminants from the biota matrices, followed by a clean-up step using in-house mixed mode SPE cartridges (Gkotsis et al., 2022). Individual steps of the sample preparation protocol are presented in **Figure 6** and described below:

- ✓ 1 g of each sample was weighted and mixed with 4 g of samples' dispersant Sodium Sulfate (Na_2SO_4), using mortar and pestle.
- ✓ A mix of isotopically labelled internal standards was spiked into each sample, and left in contact with the matrix for at least 30 min prior to the extraction. Representative compounds from different classes of the LC target list of NKUA were selected.
- ✓ The samples were placed in extraction cells (**Figure 3**) and the analytes were extracted by ASE (Dionex™ ASE™ 350, Thermo Fisher Scientific, **Figure 4**). The extraction conditions are provided in **Table 4**.

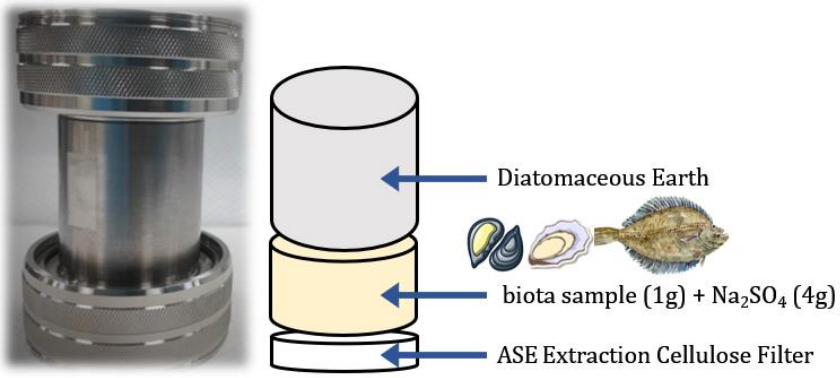


Figure 3. Samples' loading in the ASE extraction cell.

Figure 4. Dionex™ ASE™ 350, Thermo Fisher Scientific.

Table 4. ASE conditions for LC-amenable compounds.

Temperature (°C)	50
Pressure (psi)	1500
Heating Time (s)	300
Static Time (s)	420
Number of Static Cycles	3
Flush Volume (%)	60
Purge Time (s)	180
Extraction Solvent ratio	Methanol : Acetonitrile (2:1)
Total volume of extraction solvents (mL)	60

- ✓ If not transparent, the extract was filtered through a filter paper.
- ✓ The extract was pre-concentrated using rotary evaporator (at 40 °C) till reaching the final volume of 3-4 mL.
- ✓ Milli-Q water was added to adjust the final volume to 15 mL.
- ✓ Clean-Up Step 1: Defatting step. 5 mL of n-hexane were added into each sample, then the sample was mixed using Vortex stirring for 1 min and centrifuged for 10 min at 4000 rpm. Finally, the hexane layer was discarded.

- ✓ Milli-Q water was added to adjust the final volume to 50 mL.
- ✓ Clean-Up Step 2: SPE.

The samples were then cleaned-up by SPE. Layered 'mixed bed' cartridges (depicted in **Figure 5**) consisted of Oasis HLB (200 mg) and a mixture of Strata-X-AW (weak anion exchanger), Strata-X-CW (weak cation exchanger) and Isolute ENV+ (300 mg of total mixture). The conditioning of the cartridges was performed with 3 mL of methanol and 3 mL of Milli-Q water and then the samples were loaded in the SPE cartridges. The cartridges were dried by passing air through them for 0.5 to 1 h (applying vacuum facility in the SPE box; cartridges were visually inspected for complete dryness). The elution of the analytes from the adsorbent material was performed by a basic solution (6 mL of ethylacetate/methanol (50/50, v/v) containing 2% ammonia hydroxide (v/v)), followed by an acidic solution (4 mL of ethylacetate/methanol (50/50, v/v) containing 1.7% formic acid (v/v)).

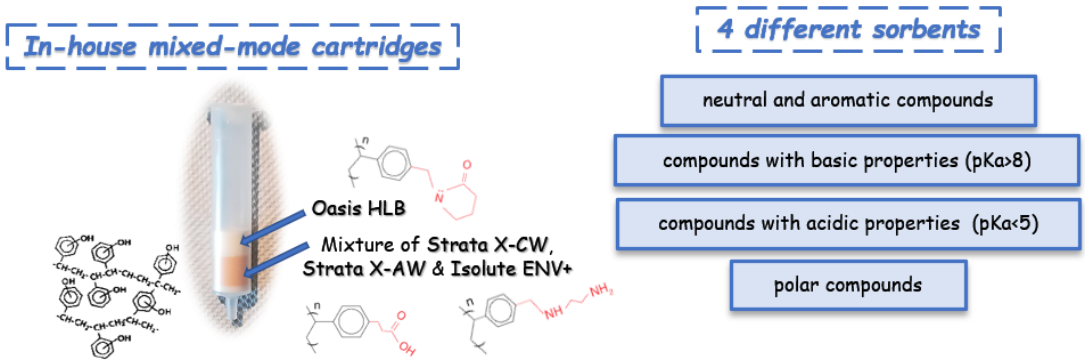


Figure 5. Mixed-mode SPE cartridges.

- ✓ The extract was evaporated using nitrogen stream at 4N.D.-45 °C till dryness.
- ✓ 250 µL of the mix of methanol (LC-MS grade) and Milli-Q water (50/50, v/v) were used for the final reconstitution of each sample and the reconstituted sample was homogenized using Vortex stirring for 1 min. During the sample preparation, a 4-fold sample enrichment was achieved.
- ✓ The final extract was filtered through the Regenerated Cellulose (RC) filter (Chromafil - pore size: 0,2 µm; filter diameter: 15 mm), using a syringe, into a 2 mL glass vial.
- ✓ After the analysis by LC-ESI-QToF MS the vials were stored in the freezer at -80 °C.

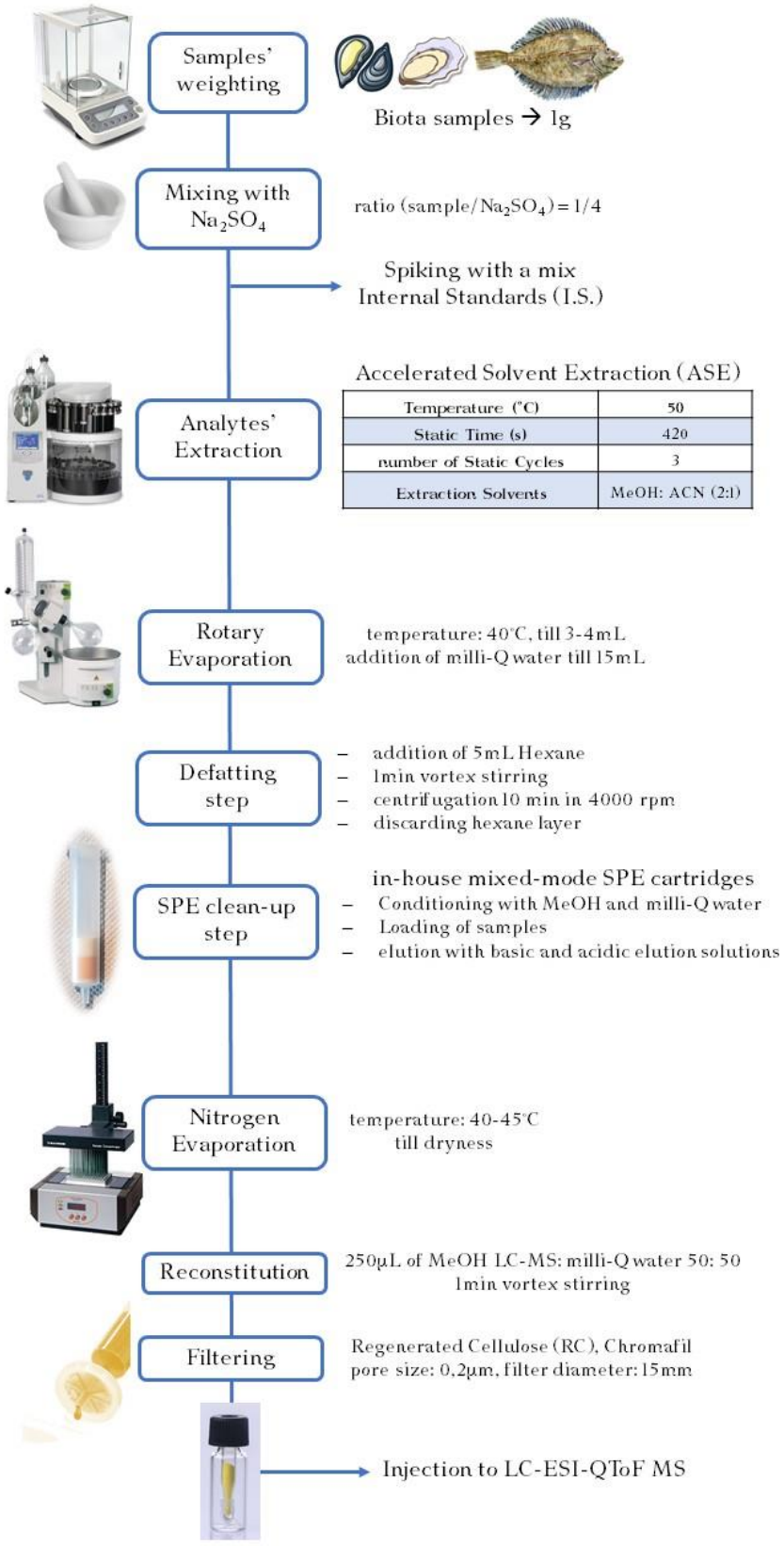


Figure 6. Sample preparation protocol for the extraction of LC-amenable compounds from biota matrices.

4.2.4 Extraction of GC-amenable contaminants from biota samples

The extraction of GC-amenable contaminants from the biota matrices was based on Badry et al. (2022) study. The individual steps of the sample preparation are presented in **Figure 7** and listed below:

- ✓ 1 g of each sample was weighted and mixed with 4 g of samples' dispersant Sodium Sulfate (Na_2SO_4) using mortar and pestle.
- ✓ A mix of isotopically labeled internal standards was spiked into each sample, and left in contact with the matrix for at least 30 min prior to the extraction. Representative compounds from different classes of the GC target list of NKUA were selected.
- ✓ The analytes were extracted by ASE (Dionex™ ASE™ 350, Thermo Fisher Scientific). The extraction conditions are provided in **Table 5**.

Table 5. ASE conditions for GC-amenable compounds.

Temperature (°C)	100
Pressure (psi)	1500
Heating Time (s)	300
Static Time (s)	300
Number of Static Cycles	3
Flush Volume (%)	60
Purge Time (s)	180
Extraction Solvent ratio	Hexane : Dichloromethane (2:1)
Total volume of extraction solvents (mL)	70

- ✓ If not transparent, the extract was filtered through a filter paper.
- ✓ 50 µL of isooctane, used as a keeper, was added.
- ✓ The extract was pre-concentrated by rotary evaporation (max. temperature 30 °C) till 10 mL.
- ✓ Clean-Up Step: SPE.

The samples were then cleaned-up by SPE. Strata® FL-PR Florisil ((170 µm, 80 Å), 5 g/ 20 mL, Giga Tubes, Phenomenex) cartridges were used. The conditioning of the cartridges was performed using 20 mL of 10% isopropanol in dichloromethane, followed by 30 mL of hexane. After conditioning, the samples were loaded in the SPE cartridges and the eluent was collected. The elution of the analytes from the adsorbent material was performed using 20 mL of dichloromethane: hexane (50/50, v/v), followed by 20 mL of hexane. The whole extract (cleaned extract and elution solvents) was placed into an evaporation flask. After that:

- ✓ 50 µL of isooctane was added.
- ✓ The extract was pre-concentrated by rotary evaporation (max. temperature 30 °C) till 10 mL.
- ✓ The extract was evaporated using nitrogen stream (max. temperature 30 °C) to a final volume of 250 µL in hexane. During the sample preparation, 4-fold enrichment of the extracts was achieved.

- ✓ The final extract was filtered through the Regenerated Cellulose (RC) filter (Chromafil - pore size: 0.2 µm; filter diameter: 15 mm), using a syringe, into a 2 mL glass vial.
- ✓ After the analysis by GC-APCI-QToF MS, the vials were stored in the freezer at -80°C.

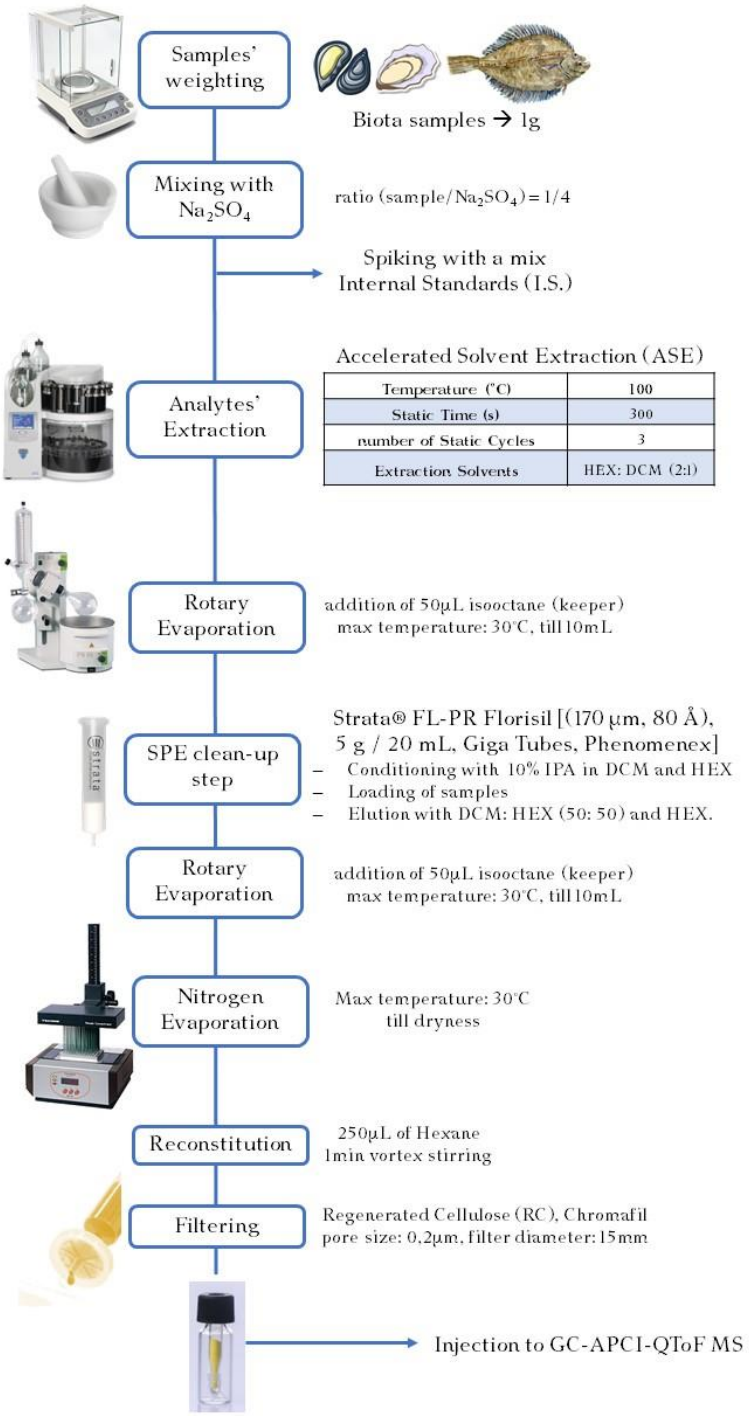


Figure 7. Sample preparation protocol for the GC-amenable compounds from biota matrices.

5. Instrumental analysis

The samples were analyzed by both liquid and gas chromatography hyphenated with a high-resolution mass spectral analyzer. Detailed information on the instrumental analysis of the RPLC-ESI-QTOF and GC-APCI-QTOF system is provided below in paragraphs 5.1 and 5.2, respectively.

5.1. Reversed-Phase Liquid Chromatography High Resolution Mass Spectrometry

Figure 8. UHPLC-ESI-QToF MS, Maxis Impact, Bruker Daltonics.

Apparatus

- *Chromatographic System*: Ultra High Performance Liquid Chromatography (UHPLC) apparatus with an HPG-3400 pump (Dionex UltiMate 3000 RSLC, Thermo Fisher Scientific) (**Figure 8**)
- *Column*: Acclaim TM RSLC 120 C18 (100 × 2.1 mm, 2.2 μm; Thermo Fisher Scientific)
- *Mass Spectrometer*: Hybrid Quadrupole Time of Flight Mass Analyzer (QTOF-MS) (Maxis Impact, Bruker Daltonics)

Solvents - Buffers

- *Ultrapure Water* by Milli-Q-UV system (Millipore)
- *Methanol*, LC-MS Grade (Merck)
- *Formic acid* - eluent additive for LC-MS (Fluka Analytical)
- *Ammonium formate,* LC-MS Ultra and *ammonium acetate* for mass spectrometry - eluent additives for UHPLC-MS (Fluka Analytical)

Gradient elution program

The gradient elution programme of the reversed-phase liquid chromatographic system, for both positive and negative ESI mode is provided in **Table 6**.

Positive Ionization:

Aqueous solvent: H_2O/methanol 90/10 (v/v), 5 mM $HCOONH_4$, 0.01% formic acid
Organic Solvent: Methanol, 5 mM $HCOONH_4$, 0.01% formic acid

Negative Ionization:

Aqueous solvent: H_2O/methanol 90/10 (v/v), 5 mM CH_3COONH_4
Organic Solvent: Methanol, 5 mM CH_3COONH_4

Table 6. RPLC gradient elution programme.

Time (min)	***Flow rate (mL min^{-1})***	***Aqueous solvent %***	***Organic solvent %***
0	0.20	99.0	1.0
1	0.20	99.0	1.0
3	0.20	61.0	39.0
14	0.40	0.1	99.9
16	0.48	0.1	99.9
16.1	0.48	99.0	1.0
19.1	0.20	99.0	1.0
20.0	0.20	99.0	1.0

Column temperature: 30 °C
Injection volume: 5 µL

Ion source

QTOF-MS was equipped with an electrospray ionization interface (ESI) operated in both positive and negative mode.

MS parameters

- *Scan mode*: a) 1st run in Data Independent mode: broad band Collision Induced Dissociation (bbCID) acquisition mode (acquisition of full scan MS spectra (4 eV) and MS/MS (25 eV) spectra in a single run) and b) 2nd run in Data Dependent mode (acquisition of full scan MS spectra and MS/MS spectra of the 5 most abundant ions per MS scan in a single run)
- *m/z (mass to charge ratio) range*: 50 - 1000 Da
- *Scan rate*: 2 Hz

External calibration of QToF-MS was performed just before analysis with 10 mM of sodium formate in a mixture of water/isopropanol (50/50, v/v). The theoretical exact masses of calibration ions with formulas $Na(NaCOOH)_{1\text{-}14}$ in the range of 50–1000 Da were used. Also, internal calibration was performed by calibrant injection at the beginning of each chromatogram (1st segment, 0.1–0.25 min).

5.2. Gas Chromatography High Resolution Mass Spectrometry

The GC-APCI-QTOF system consisted of a Bruker 450 GC, a CP-8400 AutoSampler and a hybrid quadrupole time of flight mass spectrometer (QTOF-MS) (Maxis Impact, Bruker Daltonics) (**Figures 9 and 10**).

GC was operated in splitless injection mode (Restek Split liner w/Glass Frit (4 mm x 6.3 x 78.5)) and the splitless purge valve was activated 1 min after injection. The injection volume was 1 μL. A Restek Rxi-5Sil MS column of 30 m (0.25 mm i.d. x 0.25 μm film thickness) was used with helium as a carrier gas at the constant flow of 1.5 mL min^{-1}.

The GC oven was programmed as follows: 55 °C initial hold for 3 min, increase at a rate of 15 °C min^{-1} to 180 °C, then increase with a step of 6.5 °C min^{-1} to 280 °C and hold for 5 min followed by an increase of 10 °C min^{-1} to 300 °C and hold for 5.28 min. The temperature of splitless injector port, GC-MS transfer line and MS source were maintained at 280, 290 and 250 °C, respectively.

Figure 9. GC-APCI-QToF MS, Maxis Impact, Bruker Daltonics.

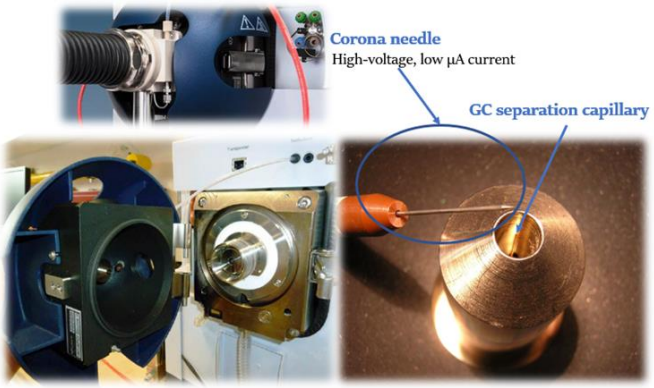


Figure 10. The APCI source.

The operating parameters of APCI interface were: capillary voltage, 5000 V; corona voltage, 2000 V; end plate offset, 500 V; nebulizer, 3.5 bar; drying gas, 1.5 L min^{-1}. The QToF MS system operated in two different acquisition modes. In broadband collision-induced dissociation (bbCID), a Data Independent Acquisition (DIA) mode, in which two sequential full scan events are triggered. The first scan at low collision energy (4 eV) results in a MS full scan over the range of m/z 50–1000. The second scan at high collision energy (25 eV) results in a MS/MS all ion fragment mode also in the range of m/z 50–1000. In Data Dependent Acquisition (DDA) mode, the first scan at low collision energy (4 eV) results in a MS full scan over the range of m/z 50–1000, whereas the second scan results in a full scan MS spectrum and in MS/MS spectra of the 5 most abundant ions per MS scan in a single run in the range of m/z 50–1000. The scan rate was 8 Hz per cycle.

The QToF mass spectrometer was calibrated with perfluorotributylamine (FC43) prior to the beginning of every analysis (external calibration) and at the first seconds (1st segment, 0.1–0.25 min) of every chromatogram (internal calibration).

6. Quality Assurance & Quality Control (QA/QC)

A thorough quality assurance and quality control (QA/QC) was applied during the sample preparation and instrumental analysis (Badry et al., 2022). A mix of internal standards was added into each sample prior to extraction to assure satisfactory recovery of the target compounds.Samples spiked with a mix of known contaminants were also analyzed in each batch of samples. Moreover, simultaneous process and monitoring of solvent blanks and procedural blanks during the analysis of all samples was realized to assess any external contamination which might have been brought in during the sample preparation of the extracts and analysis. A mix of known analytes (RTI calibrant substances) was used to assess the stability of retention time during instrumental analysis (Aalizadeh et al., 2021). A QC sample, including a representative number of contaminants included in the target list, was injected every ten injections for the evaluation of good operation and high sensitivity of the instrumentation.

7. Data treatment

7.1 Wide-scope target screening

Target screening was performed with the use of in-house developed databases of 2,528 contaminants (the LC target list is available as S21 UATHTARGETS in Suspect List Exchange https://www.norman-network.com/nds/SLE/ (Thomaidis et al., 2022), the GC target list is available as S65 UATHTARGETSGC (Damalas et al., 2020)) and the software TASQ Client 2.1 and DataAnalysis 5.1 (Bruker Daltonics, Bremen, Germany). The graphical user interface of TASQ Client 2.1 is presented in **Figure 11.** The detection was based on specific screening parameters (mass accuracy <2 mDa, retention time shift ±0.2 min, isotopic fitting <100 mSigma (only for confirmation of positive findings)), whereas

the presence of adduct and fragment ions confirmed the analytes. The Screening Detection Limit (SDL) was established as the lowest concentration level tested for which a compound is detected in all spiked samples, at the expected retention time and with specific mass error of the precursor ion. The SDL was not compound-specific, but a generic reporting value derived after method validation. Further, thorough compound-specific validation was performed for quantification purposes of the compounds detected with the screening method. Compound-specific limit of detection (LOD) and limit of quantification (LOQ) values were calculated after the treatment and analysis of samples spiked with the detected compounds and structure-related isotope labeled compounds. The contaminants that were detected in traces below the LOQ (concentration levels between the LOD and LOQ values) were reported as BQL (below the quantification limit). For statistical treatment of the results, substitution of BQL with LOQ/2 may be performed, as indicated by the QA/QC Directive (2009/90/EC).

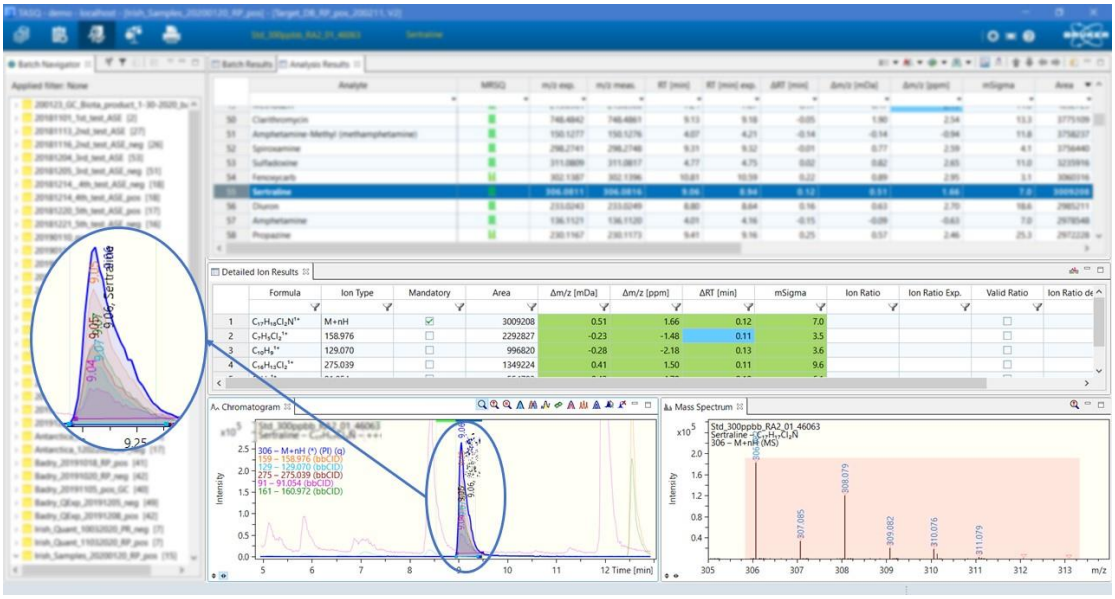


Figure 11. A typical outcome of analysis provided by the software TASQ Client 2.1 (Bruker Daltonics, Bremen, Germany).

7.2 Suspect screening

Suspect screening was performed for environmentally relevant pollutants from the NORMAN Substance Database (SusDat; https://www.norman-network.com/nds/susdat/) in all raw chromatograms which were imported into the NORMAN Digital Sample Freezing Platform (DSFP) (http://www.norman-data.eu/) - a novel tool developed for revealing the presence of suspects and identification of unknown compounds in environmental samples (Alygizakis et al., 2019). The calibrant masses were used to recalibrate the whole chromatogram using HPC fitting algorithm, which is embedded in DataAnalysis 5.1 (Bruker Daltonics, Bremen, Germany). This calibration method ensured mass accuracy below 2 mDa during the whole

chromatographic run for ions with m/z 50-1000. For exporting files in mzML format, CompassXport 3.0.9.2 (Bruker Daltonics, Bremen, Germany) was used. Chromatograms acquired under bbCID were separated in low and high collision energy layer chromatograms. All mzML files and their meta-data (instrumental, sample meta-data, matrix-specific meta-data and retention time of RTI calibrant substances) were uploaded to DSFP. DSFP is based on an integrated workflow, which follows standard operating procedure (SOP) to process the mzML files and all meta-data for generation of harmonized Data Collection Templates (DCTs). This data reduction technique resulted in an automatic generation of DCTs, which include condensed information from bulky raw LC-HRMS files.

7.3 Risk assessment

Risk assessment of the detected target and suspected compounds was based on comparing the measured concentrations of detected substances against their Predicted No-Effect Concentrations (PNECs), which represent their ecotoxicological threshold values. All PNEC values used in this project were extracted from the NORMAN Ecotoxicology database (https://www.norman-network.com/nds/ecotox/). For risk assessment purposes, the lowest PNEC was selected in the order of (a) EQS values; (b) experimental PNEC values from reference laboratories; (c) in silico predicted PNEC. The priority was evaluated based on three indicators: (i) Frequency of Appearance (FoA); (ii) Frequency of PNEC Exceedance (FoE), and (iii) Extent of PNEC Exceedance (EoE).

The first indicator expresses in how many sites the compound was detected above the limit of detection (LOD) and it is calculated using the following equation:

$$\text{FoA}\ (\%) = \frac{\text{No. of samples} > \text{LOD}}{\text{No. of samples}} * 100\%$$

The second indicator considers the frequency of monitoring sites with observations of a compound above a certain effect threshold. It is calculated using the following equation:

$$\text{FoE}\ (\%) = \frac{\text{No. of samples with concentration} > \text{PNEC}}{\text{No. of samples}} * 100\%$$

The third indicator ranks compounds with regard to the extent of the effects expected. It is calculated using the following equation:

$$\text{EoE (\%)} = \begin{cases} 1.0, \text{if } \dfrac{\text{max concentration}}{\text{PNEC}} > 1000 \\ 0.5, \quad \text{if} > 100 \dfrac{\text{max concentration}}{\text{PNEC}} \leq 1000 \\ 0.2, \text{if} > 10 \dfrac{\text{max concentration}}{\text{PNEC}} \leq 100 \\ 0.1, \text{if} \geq 1 \dfrac{\text{max concentration}}{\text{PNEC}} \leq 10 \\ 0, \text{if } \dfrac{\text{max concentration}}{\text{PNEC}} < 1 \end{cases} * 100\%$$

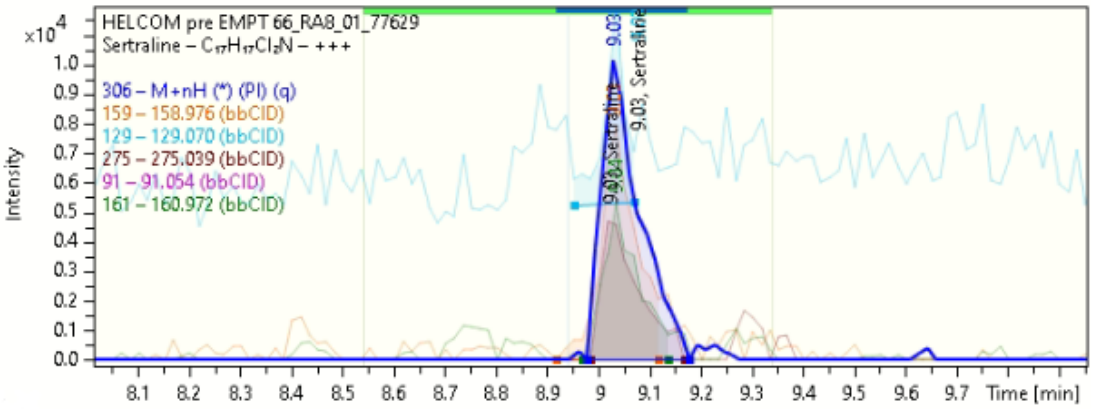
8. Results

8.1 Target screening

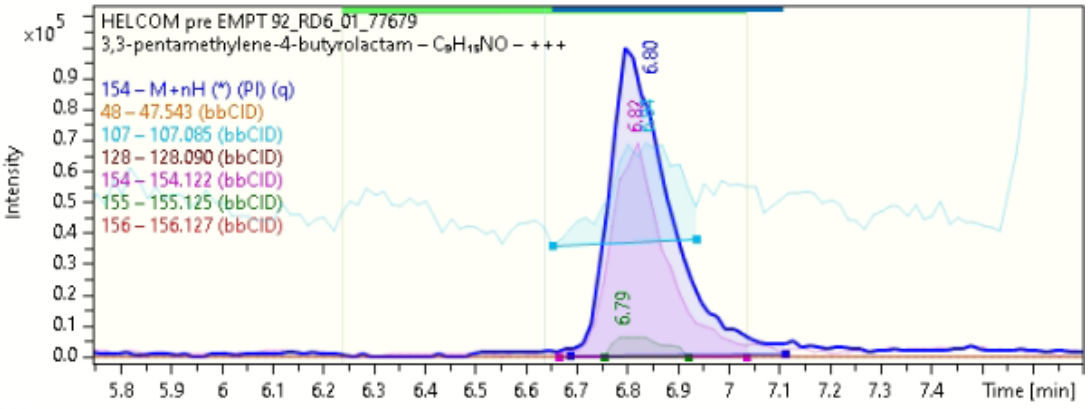
8.1.1 Wide-scope target screening of sediment samples and risk assessment

Overall, 52 contaminants were determined in the 30 analysed sediment samples. Detailed results of analyses for all samples, expressed in µg/kg dry weight, as well as the list of compounds that were below the method's Screening Detection Limit (2.00 and 0.30 µg/kg dry weight for the LC-ESI-QToF MS and GC-APCI-QToF MS analysis, respectively), are provided in the separately submitted DCTs. Extracted Ion Chromatograms for selected compounds are depicted in **Figure 12**. Data on the frequency of detection, detected concentration ranges and risk assessment are summarized in **Table 7**. Based on the available information about substances' main use, chemical class or application, their main use category was proposed, although some compounds may have multiple uses. For every detected compound, LOD and LOQ values were derived. The risk associated with the exceedance of toxicity threshold values has been assessed by comparing the measured concentrations with predicted no effect concentration (PNEC) values from the NORMAN Ecotoxicology Database (https://www.norman-network.com/nds/ecotox/lowestPnecsIndex.php). In cases where PNECs were not available, no risk assessment could be carried out. For extracting the Frequency of Appearance (FoA) for every contaminant, concentration levels above the LOD were considered (including also compounds that were detected below the limit of quantification (BQL)), while only concentrations above the LOQ were considered for the risk assessment. In cases when the PNEC value was lower than the respective method's LOD, a more sensitive method should be applied to draft reliable conclusions on the associated risk.

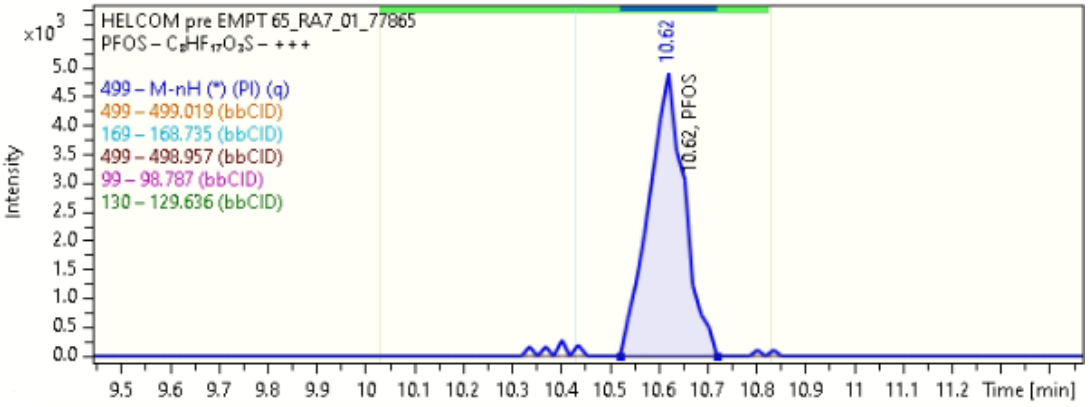
(a) Extracted Ion Chromatogram of Sertraline in HELCOM PreEMPT 66.



(b) Extracted Ion Chromatogram of 3,3-Pentamethylene-butyrolactam in HELCOM PreEMPT 92.



(c) Extracted Ion Chromatogram of PFOS in HELCOM PreEMPT 65.



(d) Extracted Ion Chromatogram of Methylparaben in HELCOM PreEMPT 72.

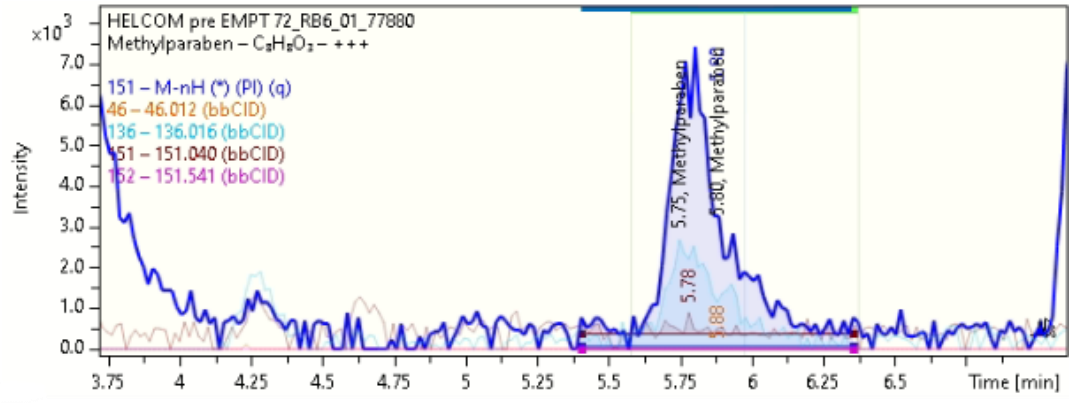


Figure 12. Extracted Ion Chromatograms of selected compounds determined in HELCOM PreEMPT sediment samples by wide-scope target analysis.

Table 7. Summary results of wide-scope target screening analyses of 30 HELCOM PreEMPT sediment samples. Compounds are ranked based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in µg/kg dry weight. The red asterisk after the name of the contaminant indicates that PNEC is lower than the LOD of the respective method.

Contaminants	Classification	Concentration range in samples where contaminant was detected	PNEC	FoA	FoE	EoE	Risk
Anthracene*	Ind. Chems-PAHs	2.17-608	0.048	0.80	0.80	1.00	2.60
Benzo(a)pyrene*	Ind. Chems-PAHs	BQL-506	2.5	1.00	0.80	0.50	2.30
Perfluorooctanesulfonic acid (PFOS)*	PFAS	0.528-20.3	0.0067	0.60	0.60	1.00	2.20
Terbumeton*	PPP & TPs	BQL-408	0.47	0.63	0.57	0.50	1.70
Methylparaben	PCPs	3.13-52.7	21.9	0.87	0.53	0.10	1.50
Prometon	PPP & TPs	12.5-534	8.51	0.60	0.60	0.20	1.40
Chrysene	Ind. Chems-PAHs	2.47-445	384	1.00	0.07	0.10	1.17
Fluorene	Ind. Chems-PAHs	0.355-273	19	0.87	0.10	0.20	1.17
Acenaphthylene	Ind. Chems-PAHs	0.587-429	44	0.90	0.07	0.10	1.07
Simazine	PPP & TPs	1.34-45.8	7.82	0.63	0.33	0.10	1.07
Benz(a)anthracene	Ind. Chems-PAHs	BQL-134	261	1.00	0.00	0.00	1.00
Fluoranthene	Ind. Chems-PAHs	1.09-147	600	1.00	0.00	0.00	1.00
Pyrene	Ind. Chems-PAHs	BQL-178	665	0.93	0.00	0.00	0.93
Fludioxonil	PPP & TPs	0.54-105	66	0.63	0.07	0.10	0.80
N-Methyldodecylamine	Ind. Chems	4.08-113	9.03	0.30	0.23	0.20	0.73
Acenaphthene	Ind. Chems-PAHs	1.88-225	16	0.37	0.13	0.20	0.70
Phenanthrene	Ind. Chems-PAHs	0.372-74.2	240	0.70	0.00	0.00	0.70
Galaxolide	PCPs	BQL-21.8	25723	0.67	0.00	0.00	0.67
2-Trifluoromethyl-benzenesulfonamide	PPP & TPs	BQL-124	90.2	0.43	0.07	0.10	0.60
Perfluorooctanoic acid (PFOA)	PFAS	BQL-4.94	6.04	0.50	0.00	0.00	0.50
p,p'-DDE	PPP & TPs	0.494-17.3	2.2	0.27	0.07	0.10	0.43
N,N-Dimethyldodecylamine	Ind. Chems	11.2-28.9	15	0.13	0.10	0.10	0.33
Caffeine	Pharms & TPs	66.5, 227	5.61	0.07	0.07	0.20	0.33
Meloxicam*	Pharms & TPs	BQL-3.01	2.6	0.13	0.07	0.10	0.30
Venlafaxine*	Antips. & Antid & TPs	20.8	1.29	0.03	0.03	0.20	0.27
Dibenz(a,h)anthracene	Ind. Chems-PAHs	41.0-76.7	63.4	0.10	0.03	0.10	0.23
Indeno(1,2,3-cd)pyrene	Ind. Chems-PAHs	154-296	240	0.10	0.03	0.10	0.23
3,3-Pentamethylene-4-butyrolactam	Pharms & TPs	7.21-29.0	860	0.23	0.00	0.00	0.23
2-Hydroxy-benzothiazole	Ind. Chems	BQL-12.5	323	0.17	0.00	0.00	0.17
Benzotriazole (BTR)	Ind. Chems	BQL-2.92	31.2	0.17	0.00	0.00	0.17
Diuron	PPP & TPs	1.94	0.98	0.03	0.03	0.10	0.17
Lamotrigine	Pharms & TPs	BQL-0.645	104	0.13	0.00	0.00	0.13
Metoprolol	Pharms & TPs	1.02-21.7	557	0.13	0.00	0.00	0.13

Contaminants	Classification	Concentration range in samples where contaminant was detected	PNEC	FoA	FoE	EoE	Risk
Amitriptyline	Antips. & Antid. & TPs	BQL-3.50	44.3	0.10	0.00	0.00	0.10
Sertraline	Antips. & Antid. & TPs	BQL-7.05	20.2	0.10	0.00	0.00	0.10
Tributylamine	Ind. Chems	1.35-2.94	1803	0.10	0.00	0.00	0.10
Oxprenolol	Pharms & TPs	0.176-0.509	101	0.10	0.00	0.00	0.10
Cyromazine	PPP & TPs	BQL-0.996	1.12	0.10	0.00	0.00	0.10
o,p'-DDT	PPP & TPs	BQL	156	0.10	0.00	0.00	0.10
Citalopram	Antips. & Antid. & TPs	0.193, 0.328	1923	0.07	0.00	0.00	0.07
Propranolol	Pharms & TPs	1.27, 1.47	5.76	0.07	0.00	0.00	0.07
Tramadol	Pharms & TPs	1.92, 4.14	256	0.07	0.00	0.00	0.07
Desmethyl-Citalopram (Nor-Citalopram)	Antips. & Antid & TPs	2.72	24	0.03	0.00	0.00	0.03
O-Desmethyl-venlafaxine (Desvenlafaxine)	Antips. & Antid & TPs	4.39	642	0.03	0.00	0.00	0.03
Perfluorohexanoic acid (PFHxA)	PFAS	BQL	7602	0.03	0.00	0.00	0.03
Flecainide	Pharms & TPs	0.63	63.1	0.03	0.00	0.00	0.03
Levamisol	Pharms & TPs	4.12	25.1	0.03	0.00	0.00	0.03
Meptazinol	Pharms & TPs	0.0981	74.3	0.03	0.00	0.00	0.03
4-Hydroxy-benzenesulfonate	Ind. Chems	BQL	N/A	0.067	N/A		
Benzododecinium (Benzyl-dimethyl-dodecylammonium)	Ind. Chems	4.44-9.47	N/A	0.100	N/A		
Irgarol	PPP & TPs	1.22-3.80	N/A	0.133	N/A		
Phthalamic acid	PPP & TPs	BQL	N/A	0.033	N/A		

BQL: Below the Limit of Quantification, TPs: Transformation products, Pharms: Pharmaceuticals, PCPs: Personal Care Products, Antips.: Antipsychotics, Antid: Antidepressants, PPP: Plant Protection Product, PFAS: Per- and Polyfluoroalkyl Substances, Ind. Chems: Industrial Chemicals, PAHs: Polycyclic Aromatic Hydrocarbons, N.D.: Not detected, N.A.: Not available, FoA: Frequency of Appearance, FoE: Frequency of Exceedance, EoE: Extent of Exceedance.

Most of the detected compounds were Industrial chemicals (including PAHs and PFAS, n=22), Personal Care Products (PCPs), Pharmaceuticals and their TPs (n=13). The other categories (antipsychotic and antidepressant drugs, Plant Protection Products (PPPs) and their TPs), overall accounted for 33% of the detected compounds (n=17). The PAHs Benz(a)anthracene, Benzo(a)pyrene, Chrysene and Fluoranthene were omnipresent in the tested samples (FoA: 1), while Acenaphthylene, Anthracene, Fluorene, Phenanthrene and Pyrene were detected in more than 21 samples (FoA: 0.70-0.93). High frequency of detection was also observed for PPPs Prometon, Simazine, Terbumeton and Fludioxonil (FoA: 0.60-0.63), PCPs Methylparben and Galaxolide (FoA: 0.87 and 0.67, respectively) and Perfluorooctanesulfonic acid (PFOS) (FoA: 0.6).

Overall, 22 compounds were detected in >6 samples (FoA >0.2). The six detected antipsychotic and antidepressant drugs were present only in three samples from Sweden

(HELCOM PreEMPT 66, 69 and 72) while HELCOM PreEMPT 82 was the most contaminated sample considering concentrations of PAHs. The highest number of detected compounds (n=35) was observed in the sample collected from Saltsjön, Sweden (HELCOM PreEMPT 66). Most of the compounds were detected at BQL levels or at concentrations below 50 μg/kg d.w.

Analysis of the 30 sediment samples revealed the presence of 22 compounds, which exceeded their ecotoxicological threshold value in at least one sample (**Table 7**). Most of the compounds exceeded their PNEC values (Frequency of Exceedance; FoE) in less than 5 samples (FoE: 0.17). However, Anthracene and Benzo(a)pyrene seem to be of high environmental concern, as their concentration exceeded respective PNEC values in 24 samples. Perfluorooctanesulfonic acid (PFOS) and Prometon exceeded their ecotoxicological threshold in 18 samples (FoE: 0.60), whereas Terbumeton and Methylparaben were detected at concentration levels above their PNECs in 17 and 16 samples, respectively. Regarding the Extent of PNEC Exceedance (EoE), EoE≥0.5 were observed for 4 compounds. The highest EoE was recorded for Anthracene and PFOS (EoE: 1.00). For 12 compounds the maximum detected concentrations were up to ten times higher than their respective PNEC, whereas for 6 compounds (Prometon, Fluorene, N-Methyldodecylamine, Acenaphthene, Caffeine and Venlafaxine) the maximum detected concentrations varied in the range from 13 to 63-fold higher levels compared to their respective PNECs.

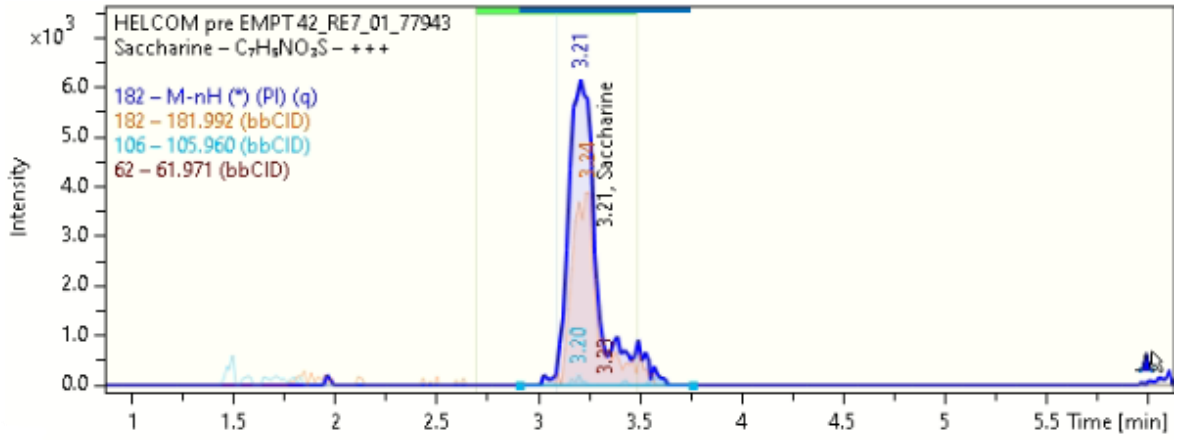
One should note, that the used lowest PNECs for majority of the aforementioned compounds used for the risk assessment were at low-ppb and ppt levels. A careful scrutiny of the ecotoxicological threshold values and further experimental toxicity evidence is suggested to support the outcomes of this risk assessment.

8.1.2 Wide-scope target screening of biota samples and risk assessment

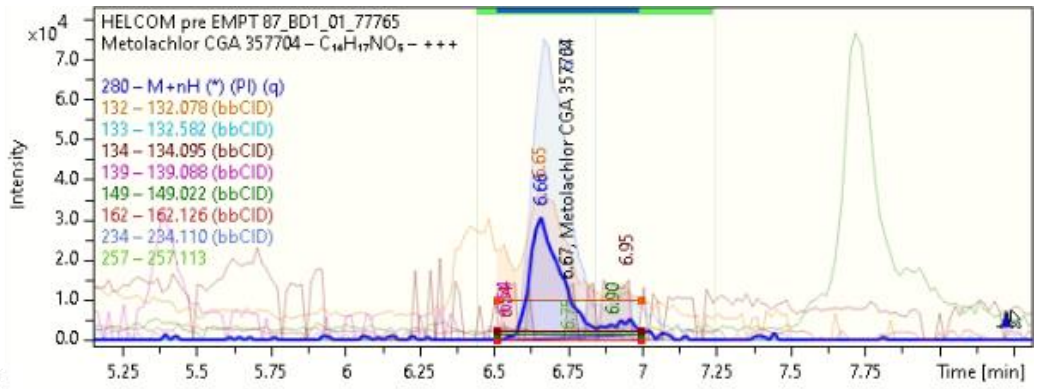
Overall, 75 contaminants were determined in the 64 tested biota samples (33 fish and 31 mussels samples). Detailed results of analyses for all samples, expressed in μg/kg wet weight, as well as the list of compounds that were below the method's Screening Detection Limit (0.25 μg/kg wet weight for both LC-ESI-QToF MS and GC-APCI-QToF MS analysis), were provided in the separately submitted DCTs. Data on the frequency of detection and determined concentration ranges are included in **Table 8**. Risk assessment results are summarized in **Tables 9** and **10** for fish and mussels samples, respectively. Extracted Ion Chromatograms for selected compounds are depicted in **Figure 13**. Based on the available information about substances' main use, chemical class or application, their main use category was proposed, although some compounds may have multiple uses. For every detected compound, LOD and LOQ values were derived. The risk associated with the exceedance of toxicity threshold values has been assessed by comparing the measured concentrations with the environmental quality standards (EQS) for biota as in the Directive 2013/39/EU and PNEC values from the NORMAN

Ecotoxicology Database (https://www.norman-network.com/nds/ecotox/lowestPnecsIndex.php). PNEC values for biota were derived from existing PNECs for freshwater (PNECfw; available in the NORMAN Ecotoxicity Database), using the equation PNECfw*BCF/10 (fish) and PNECfw*BCF/10/4 (for mussels); where BCF is the bioconcentration factor for fish from the US EPA CompTox Database (for values, see NORMAN Substance Factsheets at https://www.norman-network.com/nds/factsheets/). Please, note that for some compounds either PNECs or BCFs were not available and, consequently, no risk assessment could be carried out. For extracting the Frequency of Appearance (FoA) for every contaminant, concentration levels above the LOD were considered (including also compounds that were detected below the limit of quantification (BQL)) while only concentrations above the LOQ were considered for the risk assessment. In cases where the PNEC value was lower than the respective method LOD, a more sensitive method should be applied to provide more reliable conclusions on the associated risk.

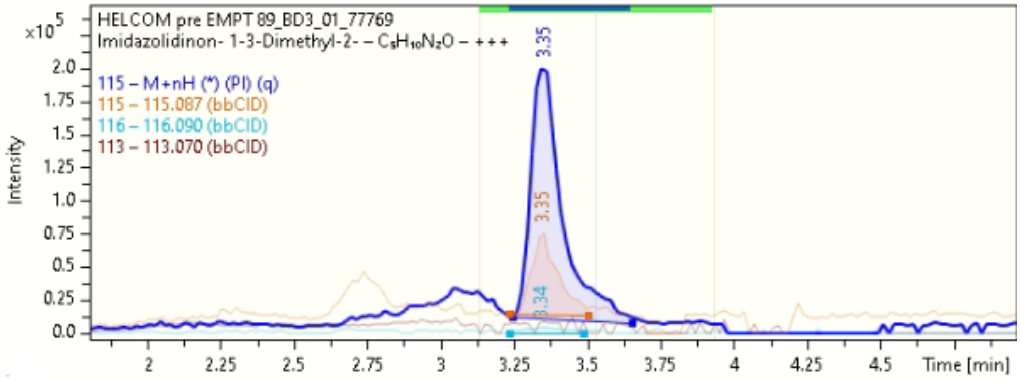
(a) Extracted Ion Chromatogram of Saccharine in HELCOM PreEMPT 42.



(b) Extracted Ion Chromatogram of Metolachlor CGA 357704 in HELCOM PreEMPT 87.



(c) Extracted Ion Chromatogram of 1,3-Dimethyl-2-imidazolidinon in HELCOM PreEMPT 89.



(d) Extracted Ion Chromatogram of 4,4-DDE in HELCOM PreEMPT 37.

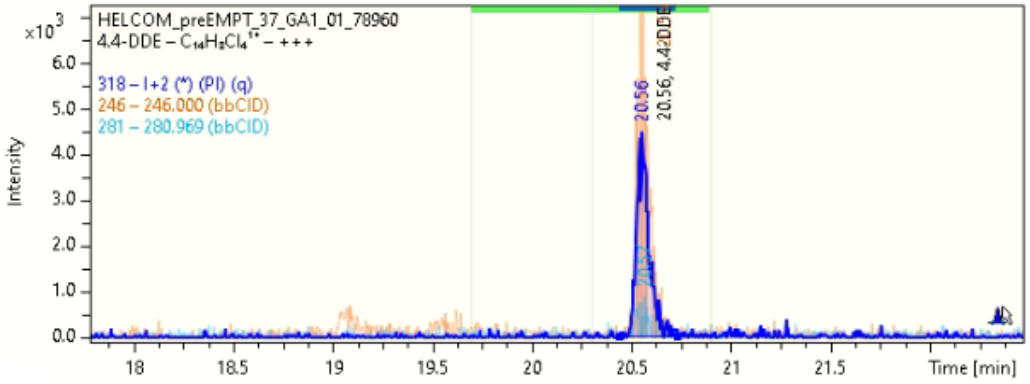


Figure 13. Extracted Ion Chromatograms of selected compounds determined in HELCOM PreEMPT biota samples by wide-scope target analysis.

Table 8. Summary results of wide-scope target screening analyses of 33 fish and 31 mussels HELCOM PreEMPT samples. Concentrations are expressed in µg/kg wet weight.

Contaminants	***Classification***	***Fish (n=33)***				***Mussels (n=31)***			
		Conc. Range	***%FoA***	***LOD***	***LOQ***	***Conc. Range***	***%FoA***	***LOD***	***LOQ***
Amisulpride	Antidepressant & Antipsychotic Drugs	BQL - 0.82	9	0.18	0.54	Not Detected		0.265	0.794
Amitriptyline		Not Detected		0.012	0.040	0.462	3	0.0737	0.243
Venlafaxine		BQL - 10.8	9	0.34	1.01	Not Detected		0.498	1.49
Caffeine	Coffee related ECs	BQL - 16.0	12	1.8	5.5	BQL - 9.03	19	2.84	8.51
Theobromine		BQL	9	2.0	6.1	BQL	3	1.02	3.07
1,2-Benzisothiazolinone	Industrial Chemicals	BQL - 7.52	27	1.0	3.4	Not Detected		0.652	2.15
2-Amino-benzothiazole		Not Detected		0.36	1.21	BQL	3	0.0283	0.0935
2-Hydroxy-benzothiazole		Not Detected		1.1	3.3	BQL	10	1.61	4.83
1-Hydroxy-benzotriazole		11.1, 17.6	6	1.1	3.4	BQL	3	1.67	5.00
5-Carboxylic acid-benzotriazole		Not Detected		0.05	0.17	BQL	3	0.073	0.241
Benzododecinium (Benzyl-dimethyl-dodecylammonium)		3.68, 5.03	6	0.4	1.3	3.40 - 9.53	19	1.00	3.01
N,N-Dimethyldecylamine		16.7 - 121.1	15	0.7	2.5	Not Detected		3.24	10.7
Triphenylphosphate		13.1	3	1.8	5.5	Not Detected		1.25	3.74
Triethyl phosphate		BQL	6	0.33	0.98	Not Detected		0.482	1.45
Tributylamine		0.938	3	0.095	0.28	BQL - 2.78	58	0.14	0.42
Acenaphthene	Ind. Chems - PAHs	BQL	3	0.14	0.41	Not Detected		0.2	0.6

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Contaminants	***Classification***	***Fish (n=33)***				***Mussels (n=31)***			
		Conc. Range	***%FoA***	***LOD***	***LOQ***	***Conc. Range***	***%FoA***	***LOD***	***LOQ***
Acenaphthylene		Not Detected		0.17	0.52	Not Detected		0.259	0.777
Anthracene		BQL - 0.289	6	0.093	0.280	BQL	13	0.095	0.285
Benzo(a)pyrene		Not Detected		2.1	6.4	Not Detected		3.14	9.42
Benzo(a)anthracene		Not Detected		0.32	0.97	Not Detected		0.368	1.103
Chrysene		Not Detected		0.12	0.36	Not Detected		0.176	0.527
Fluoranthene		5.60	3	0.05	0.15	BQL - 6.35	23	0.074	0.222
Fluorene		BQL - 2.66	64	0.03	0.10	BQL - 1.98	26	0.0494	0.148
Phenanthrene		2.23, 6.46	6	0.041	0.125	BQL - 17.6	39	0.0617	0.185
Pyrene		0.263 -5.57	36	0.043	0.130	BQL - 50.6	32	0.0642	0.192
2,2,4,5,5'-Pentochlorobiphenyl (PCB 101)	Ind. Chems - PCBs	0.837 - 3.81	21	0.17	0.52	Not Detected		0.183	0.550
2,2',3,4,4',5'-Hexachlorobiphenyl (PCB 138)		0.575 - 2.37	18	0.13	0.39	Not Detected		0.194	0.581
2,2',4,4',5,5'-Hexachlorobiphenyl (PCB 153)		1.22 - 3.37	15	0.16	0.49	Not Detected		0.226	0.679
2,2',5,5'-Tetrachlorobiphenyl (PCB 52)		Not Detected		0.0058	0.0173	BQL - 0.0349	10	0.00684	0.0205
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octanesulfonic acid	Ind. Chems - PFAS	Not Detected		0.29	0.88	1.44 - 4.85	13	0.436	1.31
Perfluorohexanoic acid (PFHxA)		0.656	3	0.18	0.55	BQL	13	0.173	0.519
Perfluorooctanoic acid (PFOA)		1.600	3	0.38	1.15	Not Detected		0.567	1.70
Perfluorononanoic acid (PFNA)		BQL - 2.01	91	0.07	0.22	BQL - 0.368	26	0.0488	0.146
Perfluorodecanoic acid (PFDeA)		BQL	48	0.85	2.54	Not Detected		1.25	3.76

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Contaminants	***Classification***	***Fish (n=33)***				***Mussels (n=31)***			
		Conc. Range	***%FoA***	***LOD***	***LOQ***	***Conc. Range***	***%FoA***	***LOD***	***LOQ***
Perfluoroundecanoic acid (PFUnA)		BQL - 1.68	42	0.43	1.30	BQL	10	0.259	0.778
Perfluorohexanesulfonic acid (PFHxS)		BQL - 0.138	6	0.026	0.077	Not Detected		0.0378	0.113
Perfluorooctanesulfonic acid (PFOS)		2.81 - 58.6	97	0.19	0.56	BQL - 7.09	23	0.148	0.443
Butylparaben	Personal Care Products & TPs	Not Detected		0.69	2.08	BQL - 21.9	29	1.03	3.08
Ethylparaben		Not Detected		1.1	3.2	BQL - 5.64	26	1.58	4.74
Methylparaben		BQL - 50.7	88	0.38	1.14	2.23 - 270	100	0.617	1.85
Galaxolide		Not Detected		0.55	1.66	2.01, 50.1	6	0.82	2.46
Galaxolidone		6.30	3	0.56	1.85	Not Detected		2.44	8.06
Imidazolidinon- 1-3-dimethyl-2-		Not Detected		0.28	0.91	23.4 - 46.6	13	0.382	1.26
3,3-Pentamethylene-4-butyrolactam	Pharmaceuticals & TPs	BQL - 7.09	88	0.27	0.82	BQL - 19.8	71	0.407	1.22
Brinzolamide		Not Detected		0.33	0.99	BQL	3	0.489	1.47
Deprenyl / Selegiline		Not Detected		0.26	0.77	9.75	3	0.382	1.15
Florfenicol		0.300	3	0.062	0.188	Not Detected		0.092	0.278
Lopinavir		BQL - 1.33	9	0.24	0.71	Not Detected		0.35	1.05
Mepindolol		Not Detected		0.45	1.36	BQL	10	0.67	2.01
Naproxen		Not Detected		2.98	8.93	BQL - 25.9	10	4.41	13.2
O-Desmethyldinor-tramadol		Not Detected		0.10	0.32	BQL - 0.936	6	0.156	0.468
Pilocarpine		BQL - 22.2	12	0.55	1.66	3.39 - 12.5	16	0.29	0.87

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Contaminants	***Classification***	***Fish (n=33)***				***Mussels (n=31)***			
		Conc. Range	***%FoA***	***LOD***	***LOQ***	***Conc. Range***	***%FoA***	***LOD***	***LOQ***
Pindolol		Not Detected		0.50	1.49	BQL - 4.26	10	1.21	3.62
Propyphenazone		BQL	3	0.11	0.33	BQL	3	0.163	0.490
Salicylic acid		2.71 - 17.8	18	0.82	2.47	3.64 - 13.7	26	0.255	0.765
o,p'-DDT	Plant Protection Products & TPs	BQL	3	0.38	1.14	Not Detected		0.562	1.68
p,p'-DDE		BQL - 5.55	61	0.22	0.67	BQL, 1.69	16	0.33	0.99
Alachlor-ESA		6.54, 10.7	6	1.7	5.0	Not Detected		2.48	7.45
Clomazone		Not Detected		0.33	1.01	209	3	0.497	1.49
Diethofencarb		Not Detected		2.5	7.5	BQL - 20.7	16	1.08	3.25
Diethyltoluamide (DEET)		4.80	3	0.15	0.44	0.181 - 0.479	10	0.0238	0.0785
Diphenylamine		BQL - 7.10	33	0.30	0.89	0.519	3	0.144	0.433
Endothal		Not Detected		1.49	4.47	10.6	3	2.21	6.63
Fipronil		0.170	3	0.034	0.103	Not Detected		0.0508	0.152
Fludioxonil		0.0336 - 0.0839	9	0.001	0.030	Not Detected		0.0118	0.0353
Hexachlorobenzene		BQL - 0.225	18	0.064	0.192	Not Detected		0.0947	0.284
Metolachlor CGA 357704		Not Detected		0.04	0.15	2.49 - 3.74	6	0.195	0.645
Metolachlor-ESA		BQL	12	0.3	0.9	Not Detected		0.447	1.34
Pyrimethanil		0.0551 - 0.106	12	0.011	0.034	BQL - 0.449	23	0.0438	0.131
Anabasine	Tobacco related ECs	BQL - 14.1	9	0.82	2.46	BQL - 72.7	16	0.310	0.929

Contaminants	***Classification***	***Fish (n=33)***				***Mussels (n=31)***			
		Conc. Range	***%FoA***	***LOD***	***LOQ***	***Conc. Range***	***%FoA***	***LOD***	***LOQ***
Cotinine		BQL - 2.02	6	0.30	0.91	Not Detected		0.45	1.35
Nicotine		21.5	3	0.83	2.50	BQL - 8.07	6	0.71	2.12
Nor-nicotine		BQL	3	1.8	5.3	2.73	3	0.84	2.53
Benzamidine	Other	Not Detected		0.045	0.135	0.280 - 1.56	6	0.067	0.20
Saccharine		8.22 - 20.8	9	2.2	6.5	Not Detected		6.2	20.4

BQL: Below the Limit of Quantification, TPs: Transformation products.

Table 9. Ranking of the contaminants determined in fish samples based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in μg/kg wet weight. The red asterisk after the name of the contaminant indicates that PNEC is lower than LOD of the respective method, while the double asterisk after the respective PNEC indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC.

Contaminants	Classification	*Conc. Range*	*PNEC*	FoA	FoE	EoE	Risk
p,p'-DDE*	PPP & TPs	BQL - 5.55	0.005	0.61	0.42	1.00	2.03
Perfluorooctanesulfonic acid (PFOS)	PFAS	2.8 - 58.6	9.1**	0.97	0.67	0.10	1.74
Methylparaben	PCPs & TPs	BQL - 50.7	2.56	0.88	0.36	0.20	1.44
Pyrene*	PAHs	0.26 -5.57	0.11	0.36	0.36	0.20	0.93
Perfluorononanoic acid (PFNA)	PFAS	BQL - 2.01	16.5	0.91	0.00	0.00	0.91
3,3-Pentamethylene-4-butyrolactam	Pharms & TPs	BQL - 7.09	66.7	0.88	0.00	0.00	0.88
Pilocarpine*	Pharms & TPs	BQL - 22.2	0.034	0.12	0.09	0.50	0.71
Fluorene	PAHs	BQL - 2.66	11.7	0.64	0.00	0.00	0.64
2,2,4,5,5'-Pentochlorobiphenyl (PCB 101)*	PCBs	0.84 - 3.81	0.08	0.21	0.21	0.20	0.62
2,2',3,4,4',5'-Hexachlorobiphenyl (PCB 138)*	PCBs	0.57 - 2.37	0.1	0.18	0.18	0.20	0.56
2,2',4,4',5,5'-Hexachlorobiphenyl (PCB 153)*	PCBs	1.22 - 3.37	0.05	0.15	0.15	0.20	0.50
N,N-Dimethyldecylamine	Ind. Chems	16.7 - 121.1	2.6	0.15	0.15	0.20	0.50
Perfluorodecanoic acid (PFDeA)	PFAS	BQL	0.82	0.48	0.00	0.00	0.48
1,2-Benzisothiazolinone*	Ind. Chems	BQL - 7.52	2.81	0.27	0.06	0.10	0.43
Perfluoroundecanoic acid (PFUnA)	PFAS	BQL - 1.68	22.3	0.42	0.00	0.00	0.42
Caffeine*	Coffee related CECs	BQL - 16.0	0.19	0.12	0.06	0.20	0.38
Venlafaxine*	Antid. & Antips. Drugs	BQL - 10.8	0.32	0.09	0.06	0.20	0.35
Diphenylamine	PPP & TPs	BQL - 7.1	10.9	0.33	0.00	0.00	0.33
Lopinavir*	Pharms & TPs	BQL, 1.3	0.014	0.09	0.03	0.20	0.32
Saccharine	Sweeteners	8.2 - 20.8	6.63	0.09	0.09	0.10	0.28
Fipronil*	PPP & TPs	0.17	0.002	0.03	0.03	0.20	0.26
Perfluorooctanoic acid (PFOA)*	PFAS	1.6	0.041	0.03	0.03	0.20	0.26
Amisulpride	Antid. & Antips. Drugs	BQL - 0.82	0.37	0.09	0.06	0.10	0.25
1-Hydroxy-benzotriazole	Ind. Chems	11.1, 17.6	4.09	0.06	0.06	0.10	0.22
Alachlor-ESA	PPP & TPs	6.5, 10.7	8.56	0.06	0.03	0.10	0.19
Anthracene*	PAHs	BQL, 0.29	0.13	0.06	0.03	0.10	0.19
Hexachlorobenzene*	PPP & TPs	BQL, 0.22	10**	0.18	0.00	0.00	0.18
Salicylic acid	Pharms & TPs	2.7 - 17.8	2160	0.18	0.00	0.00	0.18

Contaminants	Classification	*Conc. Range*	*PNEC*	FoA	FoE	EoE	Risk
Nicotine	Tobacco related CECs	21.5	4.69	0.03	0.03	0.10	0.16
Galaxolidone	PCPs & TPs	6.3	6.17	0.03	0.03	0.10	0.16
Metolachlor-ESA	PPP & TPs	BQL	8.44	0.12	0.00	0.00	0.12
Pyrimethanil	PPP & TPs	0.055 - 0.106	3.87	0.12	0.00	0.00	0.12
Theobromine	Coffee related CECs	BQL	12.6	0.09	0.00	0.00	0.09
Fludioxonil	PPP & TPs	0.034 - 0.084	14.6	0.09	0.00	0.00	0.09
Cotinine	Tobacco related CECs	BQL, 2.02	2.76	0.06	0.00	0.00	0.06
Triethyl phosphate	Ind. Chems	BQL	81.4	0.06	0.00	0.00	0.06
Perfluorohexanesulfonic acid (PFHxS)	PFAS	BQL, 0.14	15.3	0.06	0.00	0.00	0.06
Phenanthrene	PAHs	2.23, 6.46	8.8	0.06	0.00	0.00	0.06
Nor-Nicotine	Tobacco related CECs	BQL	21.0	0.03	0.00	0.00	0.03
Triphenyl phosphate	Ind. Chems	13.1	202	0.03	0.00	0.00	0.03
Propyphenazone	Pharms & TPs	BQL	2.02	0.03	0.00	0.00	0.03
Tributylamine	Ind. Chems	0.94	221	0.03	0.00	0.00	0.03
Florfenicol	Pharms & TPs	0.3	1.63	0.03	0.00	0.00	0.03
Perfluorohexanoic acid (PFHxA)	PFAS	0.66	690	0.03	0.00	0.00	0.03
o,p'-DDT	PPP & TPs	BQL	31.0	0.03	0.00	0.00	0.03
Acenaphthene	PAHs	BQL	189	0.03	0.00	0.00	0.03
Fluoranthene	PAHs	5.6	120	0.03	0.00	0.00	0.03
Diethyltoluamide (DEET)	PPP & TPs	4.8	21.1	0.03	0.00	0.00	0.03
Anabasine	Tobacco related CECs	BQL, 14.1	N/A	0.09	N/A		
Benzododecinium (Benzyl-dimethyl-dodecylammonium)	Ind. Chems	3.68, 5.03	N/A	0.06	N/A		

BQL: Below the Limit of Quantification, TPs: Transformation products, Pharms: Pharmaceuticals, PCPs: Personal Care Products, Antips.: Antipsychotics, Antid.: Antidepressants, PPP: Plant Protection Product, PFAS: Per- and Polyfluoroalkyl Substances, Ind. Chems: Industrial Chemicals, PAHs: Polycyclic Aromatic Hydrocarbons, CECs: contaminants of emerging concern, N.A.: Not available, FoA: Frequency of appearance, FoE: Frequency of Exceedance, EoE: Extent of Exceedance.

Table 10. Ranking of the contaminants determined in mussels samples based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in μg/kg wet weight. The red asterisk after the name of the contaminant indicates that PNEC is lower than LOD of the respective method, while the double asterisk after the respective PNEC indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC.

Analytes	Classification	*Conc. Range*	*PNEC*	FoA	FoE	EoE	Risk
Methylparaben*	PCPs & TPs	2.23 - 270	0.64	1.00	1.00	0.50	2.50
Pyrene*	PAHs	BQL - 50.6	0.0275	0.32	0.26	1.00	1.58
Pilocarpine*	Pharms & TPs	3.39 - 12.5	0.0085	0.16	0.15	1.00	1.31
p,p'-DDE*	PPP & TPs	BQL, 1.69	0.00125	0.16	0.03	1.00	1.19
3,3-Pentamethylene-4-butyrolactam	Pharms & TPs	BQL - 19.8	16.7	0.71	0.03	0.10	0.84
Caffeine*	Coffee related CECs	BQL - 9.03	0.0475	0.19	0.06	0.50	0.75
Phenanthrene	PAHs	BQL - 17.6	2.2	0.39	0.23	0.10	0.71
Naproxen*	Pharms & TPs	BQL - 25.9	0.24	0.10	0.06	0.50	0.66
Butylparaben*	PCPs & TPs	BQL - 21.9	1.1	0.29	0.16	0.20	0.65
Tributylamine	Ind Chems	BQL - 2.8	55.3	0.58	0.00	0.00	0.58
1-3-Dimethyl-2-imidazolidinon	PCPs & TPs	23.4 - 46.6	3.1	0.13	0.13	0.20	0.46
Ethylparaben*	PCPs & TPs	BQL - 5.6	1.8	0.26	0.06	0.10	0.42
Diethofencarb*	PPP & TPs	BQL, 20.7	1.5	0.16	0.03	0.20	0.39
Perfluorooctanesulfonic acid (PFOS)	PFAS	BQL - 7.1	2.3	0.23	0.06	0.10	0.39
Pindolol*	Pharms & TPs	BQL - 4.3	0.2	0.10	0.03	0.20	0.33
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octanesulfonic acid	Ind Chems	1.4 - 4.8	2.9	0.13	0.10	0.10	0.33
Clomazone	PPP & TPs	209	15.4	0.03	0.03	0.20	0.26
Perfluorononanoic acid (PFNA)	PFAS	BQL, 0.37	4.13	0.26	0.00	0.00	0.26
Fluorene	PAHs	BQL - 1.98	2.93	0.26	0.00	0.00	0.26
Salicylic acid	Pharms & TPs	3.6 - 13.7	540	0.26	0.00	0.00	0.26
2,2',5,5'-Tetrachlorobiphenyl (PCB 52)*	PCBs	BQL - 0.035	0.02	0.10	0.06	0.10	0.26
Fluoranthene	PAHs	BQL - 6.3	30**	0.23	0.00	0.00	0.23
Pyrimethanil	PPP & TPs	BQL - 0.45	0.97	0.23	0.00	0.00	0.23
Metolachlor CGA 357704*	PPP & TPs	2.49, 3.74	0.41	0.06	0.06	0.10	0.23
Nicotine*	Tobacco related CECs	BQL, 8.07	1.17	0.06	0.03	0.10	0.19
Endothal*	PPP & TPs	10.6	2.1	0.03	0.03	0.10	0.16
Perfluorohexanoic acid (PFHxA)	PFAS	BQL	173	0.13	0.00	0.00	0.13
Anthracene	PAHs	BQL	0.0325	0.13	0.00	0.00	0.13

Analytes	Classification	*Conc. Range*	*PNEC*	FoA	FoE	EoE	Risk
2-Hydroxy-benzothiazole	Ind Chems	BQL	2.2	0.10	0.00	0.00	0.10
Perfluoroundecanoic acid (PFUnA)	PFAS	BQL	5.6	0.10	0.00	0.00	0.10
Diethyltoluamide (DEET)	PPP & TPs	0.18 - 0.48	5.28	0.10	0.00	0.00	0.10
Benzamidine	Other	0.28, 1.56	3.05	0.06	0.00	0.00	0.06
Galaxolide	PCPs & TPs	2.01, 50.1	215	0.06	0.00	0.00	0.06
Nor-nicotine	Tobacco related CECs	2.73	5.25	0.03	0.00	0.00	0.03
Deprenyl / Selegiline	Pharms & TPs	9.7	21.3	0.03	0.00	0.00	0.03
Propyphenazone	Pharms & TPs	BQL	0.505	0.03	0.00	0.00	0.03
Theobromine	Coffee related CECs	BQL	3.15	0.03	0.00	0.00	0.03
1-Hydroxy-benzotriazole	Ind Chems	BQL	1.02	0.03	0.00	0.00	0.03
Brinzolamide	Pharms & TPs	BQL	0.66	0.03	0.00	0.00	0.03
Diphenylamine	PPP & TPs	0.52	2.73	0.03	0.00	0.00	0.03
Amitriptyline	Antidepr & Antips Drugs	0.46	1.16	0.03	0.00	0.00	0.03
2-Amino-benzothiazole	Ind Chems	BQL	0.12	0.03	0.00	0.00	0.03
5-Carboxylic acid-benzotriazole	Ind Chems	BQL	1.4	0.03	0.00	0.00	0.03
Anabasine	Tobacco related CECs	BQL - 72.7	N/A	0.16	N/A		
Benzododecinium (Benzyl-dimethyl-dodecylammonium)	Ind Chems	3.40 - 9.53	N/A	0.19	N/A		
Mepindolol	Pharms & TPs	BQL	N/A	0.10	N/A		
O-Desmethyldinor-tramadol	Pharms & TPs	BQL, 0.936	N/A	0.06	N/A		

BQL: Below the Limit of Quantification, TPs: Transformation products, Pharms: Pharmaceuticals, PCPs: Personal Care Products, Antips.: Antipsychotics, Antid.: Antidepressants, PPP: Plant Protection Products, PFAS: Per- and Polyfluoroalkyl Substances, Ind. Chems: Industrial Chemicals, PAHs: Polycyclic Aromatic Hydrocarbons, N.A.: Not available, FoA: Frequency of appearance, FoE: Frequenct of exceedance, EoE: Extent of exceedance.

In total, 50 compounds were determined by wide-scope target analysis in the 33 fish samples. Most of the detected compounds were industrial chemicals (including PAHs, PCBs and PFAS, n=23), followed by plant protection products (n=10) and pharmaceuticals (including antipsychotic and antidepressant drugs), PCPs and their TPs (n=10). The other contaminants were linked to coffee and tobacco related CEC and artificial sweeteners and were detected in less than four fish samples in low concentration levels in contrast to the majority of the detected compounds. PFOS was omnipresent (FoA: 0.97) in the tested fish samples, followed by PFNA, Methylparaben and 3,3-Pentamethylene-4-butyrolactam (FoA >0.88). Fluorene and p,p'-DDE, were determined in more than 60% of the tested samples. Concentration levels below 25 µg/kg w.w. were observed for the majority of the detected compounds.

The analysis of 33 fish samples revealed the presence of 23 compounds, which exceeded their ecotoxicological threshold value in at least one sample (**Table 9**). The majority of determined compounds exceeded their PNEC values (Frequency of Exceedance; FoE) in less than five samples (FoE: 0.15). Concentration levels, observed for chemicals known for their persistent, bioaccumulative and toxic (PBT) properties, exceeded the respective PNEC values in the majority of the analyzed fish samples. Perfluorooctanesulfonic acid (PFOS) seems to be of high environmental concern, as in 22 fish samples the concentration levels were higher than its respective EQS (9.1 μg/kg w.w.), established by Directive 2013/39/EU for fish tissue, while p,p'-DDE, PCB 101, PCB 138 and PCB 153 exceeded their ecotoxicological threshold in 14 (FoE: 0.42), 7 (FoE: 0.21), 6 (FoE: 0.18) and 5 (FoE: 0.15) samples, respectively. The rest of the compounds that exceeded their ecotoxicological threshold value were Methylparaben (n=12, FoE: 0.3), Pyrene (n=12, FoE: 0.36) and N,N-Dimethyldecylamine (n=5, FoE: 0.15). Regarding the Extent of PNEC Exceedance (EoE), EoE≥0.5 were observed for two compounds (p,p'-DDE, Pilocarpine) and the highest EoE was recorded for p,p'-DDE (EoE: 1.00). For 10 compounds the maximum detected concentrations were up to ten times higher than their respective PNECs, whereas for 13 compounds (Lopinavir, Pilocarpine, Caffeine, Venlafaxine, Fipronil, Methylparaben, PFOA, p,p'-DDE, Pyrene, PCB 101, PCB138, PCB 153, N,N-Dimethyldecylamine) the maximum detected concentrations varied in the range from 20 (Methylparaben) to 1110 (p,p'-DDE)-fold higher levels compared to their respective PNECs.

Regarding the mussels samples, 47 compounds were determined by the wide-scope target analysis. Most of the detected compounds were industrial chemicals (including PAHs, PCBs and PFAS, n=17), followed by personal care products and their TPs (n=16), pharmaceuticals (including antipsychotic and antidepressant drugs, n=10) and PPPs (n=8). The other contaminants were linked to coffee and tobacco related CECs and they were detected in less than five blue mussel samples. Methylparaben was omnipresent (FoA: 1.00) in the analyzed mussels samples, followed by 3,3-Pentamethylene-4-butyrolactam (FoA: 0.71) and Tributylamine, which was detected in almost 60% of the samples (FoA: 0.58). The majority of the compounds were detected at BQL levels or at concentrations below 20 μg/kg w.w.

The analysis of 31 blue mussels samples revealed the presence of 20 compounds, which exceeded their ecotoxicological threshold value in at least one sample (**Table 10**). The majority of the compounds exceeded their PNEC values (Frequency of Exceedance; FoE) in less than five samples (FoE: 0.16).

Methylparaben seems to be of high environmental concern, as the observed concentration levels exceeded the ecotoxicological threshold value in all analyzed blue mussels samples (FoE: 1.00). The PAHs Pyrene and Phenanthrene, exceeded their ecotoxicological threshold in 8 (FoE: 0.26) and 7 (FoE: 0.23) samples, respectively, while

Pilocarpine and Butylparaben exceeded their ecotoxicological threshold value in 5 samples (FoE: 0.16). Regarding the Extent of PNEC Exceedance (EoE), EoE≥0.5 were observed for 6 compounds (Methylparaben, Pyrene, Pilocarpine, p,p'-DDE, Caffeine, Naproxen) and the highest EoE (EoE: 1.00) was recorded for 3 compounds (Pyrene, Pilocarpine, p,p'-DDE). For 9 compounds the maximum detected concentrations were up to ten times higher than the respective PNEC, whereas for 11 compounds (Diethofencarb, Pilocarpine, Pindolol, Caffeine, Butylparaben, Methylparaben, Naproxen, p,p'-DDE, Clomazone, Pyrene, 1-3-Dimethyl-2-imidazolidinon) the maximum detected concentrations varied in the range from 14 (Clomazone) to 1839 (Pyrene)-fold higher levels compared to their respective PNECs.

One should note, that the lowest PNECs for the majority of the aforementioned compounds used for the risk assessment were at low-ppb and ppt levels. A careful scrutiny of the ecotoxicological threshold values and further experimental toxicity evidence is suggested to support the outcomes of this risk assessment. It should also be assured that more sensitive targeted analytical methods with LODs lower than respective PNECs are used in parallel with the screening analysis. There is a general need for more data covering the entire Baltic Sea Region over a longer period of time to support more conclusive and robust risk assessment.

8.2 Target screening results and risk assessment by sample provider

8.2.1 Swedish Agency for Marine and Water Management

Within the context of the HELCOM PreEMPT project, the Swedish Agency for Marine and Water Management provided 22 sediment samples (HELCOM PreEMPT 63-84), collected within 2021. The detailed wide-scope target analysis results are provided in **Table 11.**

Among the 52 contaminants that were detected in all HELCOM PreEMPT sediment samples, 45 were present in the Swedish samples, whereas 18 compounds (Amitriptyline, Citalopram, Citalopram-Nor, Sertraline, Venlafaxine, Desvenlafaxine, Flecainide, Levamisol, Meptazinol, Metoprolol, Propranolol, Tramadol, Benzododecinium, Benzotriazole, N,N-Dimethyldodecylamine, Tributylamine, Diuron and Irgarol) were detected only in the samples collected in Sweden. Antidepressant & Antipsychotic Drugs & TPs were present only in the 3 Swedish samples, HELCOM PreEMPT 66, 69 and 72. The sample HELCOM PreEMPT 66, collected at Saltsjön was the most contaminated sediment sample of this project with 34 determined contaminants. Significantly higher levels of PAHs compared to the rest of the samples were determined in HELCOM PreEMPT 82 sample from Bråviken, collected on 13 October 2021.

The detected compounds were ranked based on their calculated environmental risk and the results are provided in **Table 12**. 17 contaminants were detected in more than 50% of the tested Swedish samples (FoA ≥0.50). PAHs were the most frequently detected contaminants. Benzo(a)pyrene, Chrysene, Benz(a)anthracene, Fluoranthene and Pyrene were omnipresent in the samples from Sweden (FoA: 1.00). Overall, 20 contaminants exceeded their PNEC value in at least one Swedish sample, while the highest frequency of

exceedance was observed for Benzo(a)pyrene (FoE: 0.82). The concentration levels of Anthracene and PFOS exceeded greatly their respective PNEC values, reaching EoE equal to 1 (*i.e.,* exceeding the PNEC more than 1,000-fold). The highest risk was calculated for Anthracene (Risk: 2.45), followed by Benzo(a)pyrene and PFOS (Risk: 2.32 and 2.27, respectively). The sediment HELCOM PreEMPT 78, sampled at Västervik SO, was highly contaminated. In total, 14 compounds were determined at concentration levels exceeding their ecotoxicological thresholds.

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Table 11. Summary results for HELCOM PreEMPT sediment samples 63-84. Results are expressed in µg/kg dry weight. Concentrations exceeding respective PNECs are highlighted in red colour.

Contaminant	Samples (sampling location, year of sampling and sample code)																					LOD	LOQ
	Bottenhavet	Urviksfjärden	Bottenhavet	Saltsjön	Bottenhavet	Östhammar	Nyköping	Finnagården	Gothenburg	Bottenhavet	Innerstaden	Baltic Sea	Mörrums Bruk	Saltkälle fjord	Øresund	Västervik SO	Västervik SO	Kattegatt	Bråviken	Bråviken	Bråviken	Baltic Sea		
	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021		
	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84		
Amitriptyline	<LOD	<LOD	<LOD	3.16	<LOD	<LOD	3.50	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.64	2.11
Citalopram	<LOD	<LOD	<LOD	0.328	<LOD	<LOD	0.193	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.025	0.084
Desmethyl-citalopram (Nor-Citalopram)	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	2.72	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.39	1.29
Sertraline	<LOD	<LOD	<LOD	7.05	<LOD	<LOD	4.73	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.82	2.71
Venlafaxine	<LOD	<LOD	<LOD	**20.8**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.02	3.36
Desmethyl-venlafaxine (Desvenlafaxine)	<LOD	<LOD	<LOD	4.39	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.67	2.20
Acenaphthene	<LOD	<LOD	**20.0**	<LOD	2.85	<LOD	1.88	<LOD	<LOD	**89.1**	2.77	3.50	<LOD	<LOD	<LOD	**22.1**	<LOD	<LOD	<LOD	**226**	<LOD	<LOD	0.06	0.19
Acenaphthylene	0.881	0.587	8.32	5.32	2.73	<LOD	3.56	<LOD	3.43	<LOD	10.4	31.0	9.66	4.26	18.7	**186**	6.09	4.34	4.48	**429**	2.93	2.69	0.16	0.47
Anthracene	<LOD	<LOD	**45.8**	**7.12**	**5.26**	<LOD	**14.2**	<LOD	**4.90**	**130**	**23.4**	**88**	**7.32**	**4.36**	**20.0**	**228**	**5.11**	<LOD	**8.63**	**608**	<LOD	**2.17**	0.074	0.223
Benzo(a)anthracene	BQL	2.51	85.0	6.68	1.88	5.48	11.0	BQL	2.54	134	13.3	62.9	10.1	4.01	15.2	85.0	2.17	4.2	3.50	115	2.63	2.21	0.4	1.3
Benzo(a)pyrene	BQL	**6.29**	**145**	**23.7**	BQL	**9.12**	**15.9**	BQL	**10.8**	**288**	**23.2**	**64.2**	**12.8**	**18.2**	**30.0**	**214**	**7.77**	**10.8**	**9.07**	**506**	BQL	**11.4**	1.7	5.2
Chrysene	3.02	12.1	**419**	19.6	5.66	17.0	29.1	2.47	8.15	256	75.7	170	170	13.7	93.1	**445**	9.32	19.1	16.3	309	8.51	7.96	0.075	0.225
Fluoranthene	1.17	2.17	56.4	11.6	2.84	3.96	6.00	1.09	5.81	64.5	24.5	59.5	25.2	11.3	37.7	107	6.07	5.84	7.79	71.6	1.80	7.34	0.13	0.38
Fluorene	1.06	0.355	11.3	2.53	0.616	<LOD	1.36	4.51	1.28	**75.8**	4.00	10.6	2.69	10.8	4.10	**76.5**	<LOD	<LOD	4.70	**274**	2.33	4.21	0.07	0.21

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Contaminant	Samples (sampling location, year of sampling and sample code)																					LOD	LOQ
	Bottenhavet	Urviksfjärden	Bottenhavet	Saltsjön	Bottenhavet	Östhammar	Nyköping	Finnagården	Gothenburg	Bottenhavet	Innerstaden	Baltic Sea	Mörrums Bruk	Saltkälle fjord	Øresund	Västervik SO	Västervik SO	Kattegatt	Bråviken	Bråviken	Bråviken	Baltic Sea		
	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021		
	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84		
Phenanthrene	<LOD	<LOD	17.2	9.83	<LOD	<LOD	<LOD	<LOD	6.56	21.9	4.37	32.1	3.24	8.41	26.8	64.8	<LOD	0.372	4.00	74.2	<LOD	<LOD	0.045	0.136
Pyrene	BQL	2.41	25.2	10.2	BQL	3.04	4.62	BQL	4.69	29.2	10.0	24.9	10.0	9.83	15.6	49.6	2.21	2.48	3.14	5.31	1.56	BQL	0.46	1.37
Benzododecinium	<LOD	<LOD	<LOD	<LOD	9.33	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	9.47	<LOD	4.43	<LOD	<LOD	0.108	0.355
2-OH-Benzothiazole	<LOD	<LOD	<LOD	12.5	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	3.34	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.50	1.51
Benzotriazole	<LOD	<LOD	BQL	2.94	<LOD	<LOD	BQL	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	0.81	2.67
N,N-Dimethyl dodecylamine	**28.9**	**20.1**	<LOD	11.2	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**20.5**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.194	0.641
N-Methyldodecylamine	**114**	**69.7**	<LOD	**56.3**	**40.8**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**9.38**	4.08	<LOD	**102**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.206	0.678
Tributylamine	<LOD	<LOD	1.85	2.94	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.35	<LOD	<LOD	<LOD	<LOD	<LOD	0.56	1.84
Perfluorooctanesulfonic acid (PFOS)	**6.77**	**0.885**	**7.40**	**1.02**	<LOD	**13.7**	**1.49**	<LOD	<LOD	<LOD	**0.842**	**3.47**	**9.79**	**5.26**	<LOD	**6.53**	<LOD	**20.3**	**7.17**	<LOD	**6.51**	<LOD	0.126	0.377
Perfluorooctanoic acid (PFOA)	<LOD	2.23	2.38	1.08	2.20	1.74	1.03	<LOD	<LOD	BQL	1.06	BQL	1.86	<LOD	BQL	2.43	<LOD	4.94	<LOD	<LOD	<LOD	<LOD	0.34	1.01
Galaxolide	12.8	7.26	8.19	21.7	<LOD	9.11	10.9	4.26	<LOD	<LOD	3.83	13.2	5.67	<LOD	10.7	12.4	8.93	<LOD	<LOD	<LOD	12.4	<LOD	0.35	1.05
Methylparaben	**30.9**	**26.9**	**25.0**	**31.9**	19.3	18.2	15.9	**32.1**	11.9	18.0	8.73	3.13	**23.3**	**23.0**	4.02	**36.3**	**26.1**	**33.7**	<LOD	10.3	**24.8**	**25.4**	1.03	3.09
3,3-Pentamethylene-4-butyrolactam	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	18.8	<LOD	12.3	<LOD	<LOD	<LOD	28.8	<LOD	<LOD	<LOD	<LOD	<LOD	7.21	<LOD	29.0	0.35	1.14
Caffeine	<LOD	<LOD	**227**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.31	1.02
Flecainide	<LOD	<LOD	<LOD	0.634	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.12	0.40

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	Bottenhavet	Urviksfjärden	Bottenhavet	Saltsjön	Bottenhavet	Östhammar	Nyköping	Finnagården	Gothenburg	Bottenhavet	Innerstaden	Baltic Sea	Mörrums Bruk	Saltkälle fjord	Øresund	Västervik SO	Västervik SO	Kattegatt	Bråviken	Bråviken	Bråviken	Baltic Sea		
	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021		
	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84		
Lamotrigine	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	0.645	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.18	0.60
Levamisol	<LOD	<LOD	<LOD	4.12	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.66	2.17
Meloxicam	<LOD	<LOD	BQL	**3.01**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.91	2.73
Meptazinol	<LOD	0.0981	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.028	0.093
Metoprolol	<LOD	<LOD	<LOD	21.7	<LOD	<LOD	3.06	<LOD	<LOD	1.02	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	6.57	<LOD	<LOD	0.26	0.86
Propranolol	<LOD	<LOD	<LOD	1.27	<LOD	<LOD	1.47	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.23	0.75
Tramadol	<LOD	<LOD	<LOD	4.14	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.92	<LOD	<LOD	0.39	1.29
2-Trifluoromethyl-benzenesulfonamide	42.4	<LOD	21.9	**97.9**	32.8	73.7	15.9	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**125**	82.2	<LOD	<LOD	<LOD	<LOD	81.5	1.97	5.90
Diuron	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**1.94**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.25	0.84
Fludioxonil	7.49	0.540	18.0	1.30	2.46	39.6	<LOD	18.5	<LOD	<LOD	5.61	<LOD	32.5	3.94	0.568	5.09	<LOD	**72.8**	<LOD	1.82	**106**	10.8	0.087	0.261
Irgarol	<LOD	<LOD	<LOD	1.81	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	3.80	1.82	1.23	<LOD	<LOD	<LOD	<LOD	<LOD	0.15	0.50
p,p'-DDE	<LOD	<LOD	**17.3**	1.94	<LOD	0.527	**4.49**	<LOD	<LOD	<LOD	<LOD	1.54	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.08	0.24
Phthalamic acid	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.7	2.1
Prometon	**12.5**	<LOD	<LOD	<LOD	**17.2**	<LOD	<LOD	<LOD	<LOD	<LOD	**53.4**	<LOD	**35.4**	**31.4**	**14.4**	**79.0**	**189**	**534**	**409**	**96.7**	**12.8**	**13.5**	1.3	3.9
Simazine	<LOD	<LOD	<LOD	3.27	<LOD	7.73	<LOD	<LOD	<LOD	<LOD	4.86	**12.3**	**14.2**	1.34	**9.39**	**15.9**	5.48	**33.0**	6.36	**15.7**	**45.8**	5.71	0.4	1.2
Terbumeton	**39.1**	<LOD	<LOD	<LOD	**13.2**	<LOD	<LOD	<LOD	<LOD	<LOD	**39.0**	**44.0**	**26.1**	**84.5**	**7.62**	**50.9**	**55.9**	**217**	**408**	**48.2**	BQL	**8.40**	2.4	7.2

Table 12. Ranking of the detected contaminants in the Swedish sediment samples based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in μg/kg dry weight.

Contaminants	PNEC	FoA	FoE	EoE	Risk
Anthracene	0.048	0.73	0.73	1.00	2.45
Benzo(a)pyrene	2.5	1.00	0.82	0.50	2.32
Perfluorooctanesulfonic acid (PFOS)	0.0067	0.64	0.64	1.00	2.27
Terbumeton	0.47	0.64	0.59	0.50	1.73
Methylparaben	21.9	0.95	0.55	0.10	1.60
Prometon	8.5	0.59	0.59	0.20	1.38
Chrysene	384	1.00	0.09	0.10	1.19
Fluorene	19	0.86	0.14	0.10	1.10
Acenaphthylene	44	0.86	0.09	0.10	1.05
Simazine	7.8	0.64	0.32	0.10	1.05
Benzo(a)anthracene	261	1.00	0.00	0.00	1.00
Fluoranthene	600	1.00	0.00	0.00	1.00
Pyrene	665	1.00	0.00	0.00	1.00
Fludioxonil	66	0.73	0.09	0.10	0.92
N-Methyldodecylamine	9.0	0.32	0.27	0.20	0.79
Acenaphthene	16	0.36	0.18	0.20	0.75
Galaxolide	25723	0.64	0.00	0.00	0.64
2-Trifluoromethyl-benzenesulfonamide	90.2	0.41	0.09	0.10	0.60
Phenanthrene	240	0.59	0.00	0.00	0.59
Perfluorooctanoic acid (PFOA)	6.0	0.59	0.00	0.00	0.59
N,N-Dimethyldodecylamine	15	0.18	0.14	0.10	0.42
p,p'-DDE	2.2	0.23	0.09	0.10	0.42
Venlafaxine	1.3	0.05	0.05	0.20	0.29
Caffeine	5.6	0.05	0.05	0.20	0.29
Meloxicam	2.6	0.09	0.05	0.10	0.24
Benzotriazole (BTR)	31.2	0.23	0.00	0.00	0.23
3,3-Pentamethylene-4-butyrolactam	860	0.23	0.00	0.00	0.23
Diuron	0.98	0.05	0.05	0.10	0.19
Metoprolol	557	0.18	0.00	0.00	0.18
Amitriptyline	44.3	0.14	0.00	0.00	0.14
Sertraline	20.2	0.14	0.00	0.00	0.14
Tributylamine	1803	0.14	0.00	0.00	0.14
Lamotrigine	104	0.14	0.00	0.00	0.14
Citalopram	1923	0.09	0.00	0.00	0.09
2-OH-Benzothiazole	323	0.09	0.00	0.00	0.09
Propranolol	5.8	0.09	0.00	0.00	0.09
Tramadol	256	0.09	0.00	0.00	0.09
N-Desmethyl-citalopram(Nor-Citalopram)	24	0.05	0.00	0.00	0.05
O-Desmethyl-Venlafaxine (Desvenlafaxine)	642	0.05	0.00	0.00	0.05
Flecainide	63.1	0.05	0.00	0.00	0.05

Contaminants	PNEC	FoA	FoE	EoE	Risk
Levamisol	25.1	0.05	0.00	0.00	0.05
Meptazinol	74.3	0.05	0.00	0.00	0.05
Benzododecinium (Benzyl-dimethyl-dodecylammonium)	N/A	0.14	N/A		
Irgarol	N/A	0.18			
Phthalamic acid	N/A	0.00			

8.2.2 Swedish Museum of Natural History

Within the context of the HELCOM PreEMPT project, the Swedish Museum of Natural History provided 17 biota samples (HELCOM PreEMPT 45-61), including 11 fish and 6 blue mussel samples, sampled within 2017 and 2021.

Fish samples

Six pooled samples of muscle tissue of European perch, collected in Sweden, were analyzed and the detailed wide-scope target analysis results are provided in **Table 13.** Overall, 11 contaminants were detected in the Swedish fish samples. Industrial chemicals, including PAHs, PFAS and surfactants, were the dominating classes of determined compounds. All of the compounds detected in the samples from Sweden, were also present in at least one sample, provided by other HELCOM PreEMPT partners. Most of the detected compounds were present at low µg/kg w.w. levels. N,N-Dimethyldecylamine and PFOS were the most abundant compounds, reaching maximum concentrations at 53.3 and 52.8 low µg/kg w.w., respectively, whereas Anabasine and 1,2-Benzisothiazolinone were present only at concentrations below their respective method LoQ.

PFOS, PFNA and 3,3-Pentamethylene-4-butyrolactam were detected in all Swedish fish samples (FoA: 1.00), whereas 7 contaminants were present in less than 50% of the tested samples (FoA ≤ 0.50). Based on the risk assessment results, provided in **Table 14**, the concentrations of PFOS, N,N-Dimethyldecylamine, Methylparaben and PFOA, exceeded their respective PNEC values in at least one sample, whereas the highest extent of PNEC exceedance was observed for N,N-Dimethyldecylamine. Two PFAS, PFOS and PFNA, and 3,3-Pentamethylene-4-butyrolactam, were on the top of the list when ranking compounds based on the overall environmental risk. The determined levels of PFOS were higher than the EQS in 5 out of 6 analyzed samples. The sample HELCOM PreEMPT 58, collected in Skelleftehamn in 2017, was the most contaminated considering both the number of detected compounds and the number of compounds determined at levels exceeding their ecotoxicological thresholds.

Table 13. Summary results for HELCOM PreEMPT fish samples 56-61. Results are expressed in µg/kg wet weight. Concentrations exceeding the respective PNEC/EQS are highlighted in red colour.

Contaminant	Samples (sampling location, year of sampling and sample code)						LOD	LOQ
	Örefjärden	Kinnbäcksfjärden	Skelleftehamn	Sundsvallsfjärden	Norrsundet	Holmöarna		
	2021	2021	2017	2017	2017	2017		
	56	57	58	59	60	61		
Salicylic acid	<LOD	8.05	2.71	<LOD	<LOD	<LOD	0.82	2.47
3,3-Pentamethylene-4-butyrolactam	1.66	1.97	1.92	BQL	BQL	BQL	0.27	0.82
Anabasine	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	0.82	2.46
Methylparaben	<LOD	<LOD	**2.79**	<LOD	<LOD	BQL	0.38	1.14
Perfluorononanoic acid (PFNA)	0.388	BQL	0.461	BQL	BQL	BQL	0.07	0.22
Perfluorooctanoic acid (PFOA)	<LOD	<LOD	<LOD	<LOD	<LOD	**1.60**	0.38	1.15
Perfluorooctanesulfonic acid (PFOS)	**52.8**	**15.5**	**26.2**	**19.9**	**13.6**	7.78	0.19	0.56
Fluorene	0.478	<LOD	<LOD	<LOD	<LOD	<LOD	0.033	0.100
Phenanthrene	2.22	<LOD	<LOD	<LOD	<LOD	<LOD	0.042	0.125
1,2-Benzisothiazolinone	BQL	BQL	BQL	BQL	BQL	<LOD	1.04	3.42
N,N-Dimethyldecylamine	<LOD	**16.7**	**53.3**	<LOD	<LOD	<LOD	0.74	2.46

Table 14. Ranking of the contaminants determined in the Swedish fish samples based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in μg/kg wet weight. The red asterisk indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC.

Contaminant	PNEC	FoA	FoE	EoE	Risk
Perfluorooctanesulfonic acid (PFOS)	9.1*	1.00	0.83	0.10	1.93
Perfluorononanoic acid (PFNA)	16.5	1.00	0.00	0.00	1.00
3,3-Pentamethylene-4-butyrolactam	66.7	1.00	0.00	0.00	1.00
N,N-Dimethyldecylamine	2.6	0.33	0.33	0.20	0.87
Methylparaben	2.56	0.33	0.17	0.10	0.60
Perfluorooctanoic acid (PFOA)	0.041	0.17	0.17	0.20	0.53
Salicylic acid	2160	0.33	0.00	0.00	0.33
Fluorene	11.7	0.17	0.00	0.00	0.17
Phenanthrene	8.8	0.17	0.00	0.00	0.17
Anabasine	N/A	0.17	N/A		
1,2-Benzisothiazolinone	2.81	0.83	Detected only at BQL levels		

Mussels samples

The detailed wide-scope target analysis results for the 17 contaminants that were detected in the 11 blue mussels samples collected from different locations in Sweden in 2021 are provided in **Table 15.**

The majority of detected compounds belong to industrial chemicals, including PAHs, PFAS and Benzotriazoles & Benzothiazoles. Almost all contaminants were detected at low concentration levels (from below the method limit of quantification to 10 μg/kg w.w.), except for Salicylic acid and Methylparaben, which were detected at maximum concentrations of 13.7 and 270 μg/kg w.w., respectively. Amitriptyline and Benzotriazole-5-carboxylic acid were detected only in the mussels samples from Sweden, HELCOM PreEMPT 48 and 53, respectively.

The PNECs, calculated FoA, FoE, EoE and overall risk are presented in **Table 16**. Methylparaben, 3,3-Pentamethylene-4-butyrolactam and Tributylamine were omnipresent in the tested Swedish mussels, whereas Phenanthrene and Salicylic acid were detected in more than 50% of the tested samples (FoA ≥ 0.50). Methylparaben, Phenanthrene, Pyrene and PFOS exceeded their ecotoxicological thresholds in at least one Swedish mussel sample. The highest frequency and extent of PNEC exceedance was recoded for Methylparaben.

Table 15. Summary results for HELCOM PreEMPT mussels samples 45-55. Results are expressed in µg/kg wet weight. Concentrations exceeding respective PNEC/EQS are highlighted in red colour.

Contaminant	Samples (sampling location, year of sampling and sample code)											LOD	LOQ
	Kullen	Himmerfjärden	Malmö Hamn	Göteborg Hamn	Gräsö	Kvädöfjärden	Ronnebyåns mynning	Sölvesborg	Landskrona	Askö	Oxelösund		
	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021		
	45	46	47	48	49	50	51	52	53	54	55		
Methylparaben	240	116	270	177	125	50.4	81.9	41.9	202	109	7.71	0.62	1.85
Salicylic acid	6.70	12.7	<LOD	<LOD	10.7	13.7	12.9	3.64	<LOD	4.17	<LOD	0.25	0.76
3,3-Pentamethylene-4-butyrolactam	2.92	4.59	2.50	1.72	6.36	5.96	7.45	4.45	2.89	5.10	6.07	0.41	1.22
Amitriptyline	<LOD	<LOD	<LOD	0.462	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.074	0.243
Anabasine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	0.31	0.93
Benzamidine	<LOD	<LOD	1.56	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.067	0.200
Benzotriazole-5-carboxylic acid	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	0.073	0.24
Benzododecinium (Benzyl-dimethyl-dodecylammonium)	5.74	<LOD	<LOD	<LOD	<LOD	<LOD	4.44	<LOD	4.32	9.53	3.40	1.0	3.0
2-OH-Benzothiazole	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	1.6	4.8
Tributylamine	1.54	1.04	1.65	1.12	1.37	1.11	1.01	0.546	0.789	1.23	BQL	0.14	0.42
Perfluorooctanesulfonic acid (PFOS)	<LOD	7.09	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.15	0.44
Fluoranthene	<LOD	<LOD	<LOD	5.39	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.25	0.074	0.22
Fluorene	<LOD	<LOD	0.226	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	0.629	0.049	0.148
Phenanthrene	<LOD	<LOD	0.720	1.95	<LOD	0.255	BQL	<LOD	3.09	<LOD	2.58	0.062	0.185
Pyrene	<LOD	<LOD	1.99	<LOD	<LOD	<LOD	1.34	<LOD	1.23	<LOD	1.25	0.064	0.192
Pyrimethanil	<LOD	<LOD	0.207	0.180	0.449	BQL	BQL	<LOD	<LOD	<LOD	<LOD	0.044	0.131
p,p'-DDE	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.33	0.99

Table 16. Ranking of the detected contaminants in the Swedish mussels samples based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in μg/kg wet weight. The red asterisk indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC.

Contaminant	PNEC	FoA	FoE	EoE	Risk
Methylparaben	0.64	1.00	1.00	0.50	2.50
3,3-Pentamethylene-4-butyrolactam	16.7	1.00	0.00	0.00	1.00
Tributylamine	55.3	1.00	0.00	0.00	1.00
Pyrene	0.0275	0.36	0.36	0.20	0.93
Phenanthrene	2.2	0.55	0.18	0.10	0.83
Salicylic acid	540	0.64	0.00	0.00	0.64
Pyrimethanil	0.97	0.45	0.00	0.00	0.45
Perfluorooctanesulfonic acid (PFOS)	2.275*	0.09	0.09	0.10	0.28
Fluorene	2.93	0.27	0.00	0.00	0.27
Fluoranthene	7.50*	0.18	0.00	0.00	0.18
Amitriptyline	1.16	0.09	0.00	0.00	0.09
Benzamidine	3.05	0.09	0.00	0.00	0.09
Anabasine	N/A	0.09	N/A		
Benzododecinium (Benzyl-dimethyl-dodecylammonium)	N/A	0.45			
Benzotriazole-5-carboxylic acid	1.40	0.09	Detected only at BQL levels		
2-OH-Benzothiazole	2.22	0.09			
p,p'-DDE	0.00125	0.09			

8.2.3 Estonian Environmental Research Centre

Within the context of the HELCOM PreEMPT project, the Estonian Environmental Research Centre (EKUK) provided 10 pooled fish samples (HELCOM PreEMPT 19-23 and 29-33), including 3 European flounder (*Platichthys flesus*) and 7 European perch (*Perca fluviatilis*) samples, gathered in 2021 and 5 pooled blue mussel samples (HELCOM PreEMPT 24-28), collected in Estonian sea water region in 2021.

Fish samples

Ten pooled muscle tissue samples of European flounder (*Platichthys flesus*) and European perch (*Perca fluviatilis*), collected in Estonian waters, were analyzed using HRMS techniques. The detailed wide-scope target analysis results are provided in **Table 17.** Overall, 29 contaminants were detected in the Estonian fish samples. Industrial chemicals, including PAHs, PCBs and PFAS, was the dominating class of detected compounds, followed by Pharmaceuticals and PPPs. The least contaminated fish sample, concerning the number of the detected compounds, was HELCOM PreEMPT 33 (n=9), whereas the most contaminated fish sample was HELCOM PreEMPT 20 (n=12), collected from Liivi lath and Pakry Bay in 2021, respectively. PFOS, PFNA, Methylparaben and PFDeA were omnipresent in the analyzed fish samples (FoA: 1.00). p,p'-DDE, Fluorene, PFUnA and 3,3-Pentamethylene-4-butyrolactam were determined in more than 70% of

the tested Estonian fish samples. Most of the detected compounds were present at low µg/kg w.w. levels. PFOS was the most abundant compound, reaching maximum concentration of 53.0 µg/kg w.w., whereas 11 compounds were present only at concentration levels below their respective method LOQ.
Based on the risk assessment results, summarized in **Table 17**, the concentrations of 10 compounds (p,p'-DDE, PFOS, Methylparaben, Pyrene, Lopinavir, PCB 101, Amisulpride, Caffeine, Venlafaxine and Fipronil), exceeded their respective PNEC values in at least one sample, whereas the highest extent of PNEC exceedance was measured for p,p'-DDE. Two PFAS (PFOS, PFNA), the transformation product of the banned insecticide DDT (p,p'-DDE) and the widely used PCP Methylparaben were on the top of the list of the ranked contaminants based on the overall environmental risk. The highest EoE was observed for PFOS, with the determined concentration levels higher than its respective EQS in 60% of the analyzed fish samples.

Mussels samples

Five pooled blue mussel (*Mytilus edulis*) samples, collected in Estonian sea waters, were analyzed using HRMS techniques. Results of the detailed wide-scope target analysis are provided in **Table 18.** In total, 17 contaminants were detected. Per- and polyfluoroalkyl substances (PFAS), was the dominating class of detected compounds, followed by Personal Care Products. The least contaminated blue mussel sample, concerning the number of the detected compounds, was HELCOM PreEMPT 25 (n=4), collected at Saaremaa in 2021. The most contaminated blue mussel sample was HELCOM PreEMPT 28 (n=12), gathered at Väike-Pakri. Methylparaben was omnipresent in the analyzed mussels samples (FoA: 1.00), Butylparaben and Anabasine were determined in 4 out of the 5 samples, whereas the rest of the compounds were determined in less than 60% of the Estonian blue mussels samples. Most of the compounds were determined at concentration levels below the method LOQ. Methylparaben was the most abundant compound, reaching maximum concentration of 53.3 µg/kg w.w.
Based on the risk assessment results, summarized in **Table 18**, the concentrations of 5 compounds (Methylparaben, Naproxen, 3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octanesulfonic acid, Butylparaben and Pindolol), exceeded their respective PNEC values in at least one sample, whereas the highest extent of PNEC exceedance was measured for Naproxen. The highest risk was calculated for Methylparaben (Risk: 2.20), followed by Pindolol (Risk: 1.50).

Table 17. Summary results for Estonian HELCOM PreEMPT fish samples 19-23 and 29-33. Results are expressed in μg/kg wet weight. Concentrations exceeding the respective PNEC/EQS are highlighted in red colour. The detected contaminants were ranked based on their final score (Sum of FoA+EoE+FoE). The red asterisk indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC.

Contaminant	Samples (species, sampling location, year of sampling and sample code)										*LOD*	*LOQ*	*PNEC*	FoA	FoE	EoE	Risk
	European perch		European flounder			European perch											
	Narva-Kunda Bay	Pakry Bay	Liivi laht	Reigi Bay	Pakri Bay	Matsalu Bay	Väinameri	Kihelkonna Bay	Pärnu Bay	Liivi lath							
	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021							
	19	**20**	**21**	**22**	**23**	**29**	**30**	**31**	**32**	**33**							
p,p'-DDE	BQL	BQL	**1.41**	**0.677**	**0.672**	BQL	BQL	<LOD	**0.852**	**1.33**	**0.22**	**0.67**	0.005	0.90	0.50	0.50	1.90
Perfluorooctanesulfonic acid (PFOS)	**23.4**	**30.6**	7.17	3.75	**10.5**	**21.5**	**53.0**	**35.2**	5.30	9.04	**0.19**	**0.56**	9.1*	1.00	0.60	0.10	1.70
Methylparaben	BQL	BQL	1.37	**15.0**	**2.63**	1.86	BQL	BQL	BQL	BQL	**0.38**	**1.14**	2.56	1.00	0.20	0.10	1.30
Perfluorononanoic acid (PFNA)	0.551	2.01	0.348	0.226	BQL	0.424	0.351	0.345	0.539	1.11	**0.07**	**0.22**	16.5	1.00	0.00	0.00	1.00
Fluorene	0.787	0.888	0.713	1.23	1.14	1.19	1.79	1.32	0.976	<LOD	**0.03**	**0.10**	11.7	0.90	0.00	0.00	0.90
Perfluoroundecanoic acid (PFUnA)	1.68	1.46	<LOD	<LOD	1.38	1.41	1.53	1.46	BQL	1.49	**0.43**	**1.30**	22.3	0.80	0.00	0.00	0.80
Pyrene	<LOD	<LOD	**0.846**	<LOD	**0.760**	**2.73**	<LOD	<LOD	<LOD	<LOD	**0.043**	**0.130**	0.11	0.30	0.30	0.20	0.80
3,3-Pentamethylene-4-butyrolactam	<LOD	<LOD	<LOD	BQL	BQL	1.17	0.972	BQL	BQL	BQL	**0.27**	**0.82**	66.7	0.70	0.00	0.00	0.70
Lopinavir	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	BQL	**1.33**	**0.24**	**0.71**	0.014	0.30	0.10	0.20	0.60
2,2,4,5,5'-Pentochlorobiphenyl (PCB 101)	**1.86**	**0.837**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**0.17**	**0.52**	0.08	0.20	0.20	0.20	0.60
Amisulpride	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**0.822**	BQL	**0.788**	**0.18**	**0.54**	0.37	0.30	0.20	0.10	0.60
Caffeine	<LOD	BQL	**6.78**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**1.8**	**5.5**	0.19	0.20	0.10	0.20	0.50
Venlafaxine	<LOD	<LOD	<LOD	**1.11**	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	**0.34**	**1.01**	0.32	0.20	0.10	0.10	0.40
Fipronil	<LOD	<LOD	<LOD	**0.175**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**0.034**	**0.103**	0.002	0.10	0.10	0.20	0.40
Tributylamine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.938	<LOD	<LOD	<LOD	**0.095**	**0.284**	221	0.10	0.00	0.00	0.10
Florfenicol	<LOD	0.300	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**0.062**	**0.188**	1.63	0.10	0.00	0.00	0.10
Perfluorohexanoic acid (PFHxA)	<LOD	<LOD	<LOD	0.656	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**0.18**	**0.55**	690	0.10	0.00	0.00	0.10
Cotinine	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	**0.30**	**0.91**	2.76	0.10			

Contaminant	Samples (species, sampling location, year of sampling and sample code)										LOD	LOQ	PNEC	FoA	FoE	EoE	Risk
	European perch		European flounder			European perch											
	Narva-Kunda Bay	Pakry Bay	Liivi laht	Reigi Bay	Pakri Bay	Matsalu Bay	Väinameri	Kihelkonna Bay	Pärnu Bay	Liivi lath							
	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021							
	19	**20**	**21**	**22**	**23**	**29**	**30**	**31**	**32**	**33**							
Metolachlor-ESA	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	**0.30**	**0.91**	8.44	0.10	Detected only at BQL levels		
Phosphate-triethyl	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	**0.33**	**0.98**	81.4	0.10			
Propyphenazone	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**0.11**	**0.33**	2.02	0.10			
Theobromine	<LOD	BQL	BQL	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	**2.0**	**6.1**	12.6	0.30			
Perfluorodecanoic acid (PFDA)	BQL	BQL	BQL	BQL	BQL	BQL	BQL	BQL	BQL	BQL	**0.85**	**2.54**	0.82	1.00			
Acenaphthene	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	**0.14**	**0.41**	189	0.10			
Anthracene	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	**0.09**	**0.28**	0.13	0.10			
Diphenylamine	BQL	BQL	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	**0.30**	**0.89**	10.9	0.40			
Hexachlorobenzene	BQL	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**0.064**	**0.192**	10	0.20			
Anabasine	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**0.82**	**2.46**	N/A	0.10	N/A		
Benzododecinium (Benzyl-dimethyl-dodecylammonium)	<LOD	<LOD	<LOD	3.68	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**0.44**	**1.31**	N/A	0.10			

Table 18. Summary results of Estonian HELCOM PreEMPT mussels samples 24-28. Results are expressed in µg/kg wet weight. Concentrations exceeding respective PNEC/EQS are highlighted in red colour. The detected contaminants are ranked based on their final score (Sum of FoA+EoE+FoE).

Contaminant	Samples (sampling location, year of sampling and sample code)					LOD	LOQ	PNEC	FoA	FoE	EoE	Risk
	Aegna	Saaremaa	Küdema Bay	Krassgrund	Väike-Pakri							
	2021	2021	2021	2021	2021							
	24	***25***	***26***	***27***	***28***							
Methylparaben	**14.9**	**3.15**	**53.3**	**34.2**	**14.1**	**0.62**	**1.85**	0.64	1.00	1.00	0.20	2.20
Naproxen	<LOD	<LOD	**25.9**	BQL	**16.7**	**4.4**	**13.2**	0.24	0.60	0.40	0.50	1.50
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octanesulfonic acid	**4.06**	1.44	<LOD	<LOD	**4.85**	**0.44**	**1.31**	2.925	0.60	0.4	0.10	1.10

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Contaminant	**Samples (sampling location, year of sampling and sample code)**					***LOD***	***LOQ***	***PNEC***	***FoA***	***FoE***	***EoE***	***Risk***
	Aegna	Saaremaa	Küdema Bay	Krassgrund	Väike-Pakri							
	2021	2021	2021	2021	2021							
	24	***25***	***26***	***27***	***28***							
Butylparaben	**4.51**	<LOD	BQL	BQL	BQL	**1.03**	**3.08**	1.08	0.80	0.20	0.10	1.10
Pindolol	<LOD	<LOD	BQL	**4.26**	BQL	**1.21**	**3.62**	0.20	0.60	0.20	0.20	1.00
Perfluorononanoic acid (PFNA)	BQL	<LOD	<LOD	BQL	0.368	**0.05**	**0.15**	4.12	0.60	0.00	0.00	0.60
Perfluorooctanesulfonic acid (PFOS)	0.716	BQL	<LOD	0.87	<LOD	**0.15**	**0.44**	2.275*	0.60	0.00	0.00	0.60
Galaxolide	<LOD	<LOD	<LOD	50.2	2.0	**0.82**	**2.46**	214.7	0.40	0.00	0.00	0.4
Benzamidine	0.28	<LOD	<LOD	<LOD	<LOD	**0.07**	**0.20**	3.0	0.20	0.00	0.00	0.200
Mepindolol	<LOD	<LOD	BQL	BQL	BQL	**0.67**	**2.01**	N/A	0.60	Detected only at BQL levels		
Caffeine	<LOD	<LOD	BQL	<LOD	<LOD	**2.84**	**8.51**	0.047	0.20			
Ethylparaben	BQL	<LOD	BQL	BQL	<LOD	**1.58**	**4.74**	1.79	0.60			
Perfluorohexanoic acid (PFHxA)	BQL	BQL	BQL	<LOD	<LOD	**0.17**	**0.52**	172.5	0.60			
Perfluoroundecanoic acid (PFUnA)	BQL	<LOD	<LOD	<LOD	BQL	**0.26**	**0.78**	5.57	0.40			
Anthracene	<LOD	<LOD	BQL	<LOD	BQL	**0.095**	**0.285**	0.032	0.40			
Diethofencarb	BQL	<LOD	BQL	<LOD	BQL	**1.08**	**3.25**	1.5	0.60			
Anabasine	72.7	<LOD	6.13	10.4	24.4	**0.31**	**0.93**	N/A	0.80	N/A		

8.2.4 Finnish Environment Institute and Ministry of Natural Resources and Environment of the Russian Federation

Within the context of the HELCOM PreEMPT project, the Finnish Environment Institute provided 12 biota (HELCOM PreEMPT 1-12 samples), including six fish and six blue mussel samples, sampled within 2021. Additional four blue mussels samples (HELCOM PreEMPT 86-90 samples), collected in 2021 in the sea waters of Russian Federation.

Fish samples

The detailed wide-scope target analysis results for the six Finnish fish samples are provided in **Table 19.** Overall, 22 contaminants were detected in at least one sample, while industrial chemicals, including PAHs, PCBs and PFAS, was the most frequently detected class of contaminants (n=11). The tobacco related compounds, Nicotine, Cotinine and Anabasine were present only in HELCOM PreEMPT 6 sample, which was marked as reference site by the sample provider. Among all analyzed fish samples within HELCOM PreEMPT project, Phosphate-triphenyl was detected only in one Finnish sample (HELCOM PreEMPT 2). PCB 153 presented high frequency of detection only in the samples provided by the Finnish Environment Institute. HELCOM PreEMPT 3 sample (collected from a reference site) was the least contaminated sample in terms of the number of detected contaminants (n=7). Altough HELCOM PreEMPT 6 sample was reportedly collected from a reference site as well, it was highly contaminated, considering the highest number of determined contaminants from among all Finnish samples (n=16). In addition, 7 contaminants determined in this sample exceeded their respective PNEC/EQS values.

The highest FoA (1.00) was recorded for p,p'-DDE, PFOS, PFDA, Methylparaben and Fluorene, whereas PCB 138, PCB 153, PFNA, PFUdA, Diphenylamine and 3,3-Pentamethylene-4-butyrolactam were detected in 5 out of 6 analyzed samples. The detected concentration levels for 9 contaminants exceeded their respective ecotoxicological threshold in at least one sample, while the measured concentrations for PFOS exceeded the respective Directive 2013/39/EU EQS of 9.1 µg/kg w.w. in all tested samples (FoE: 1.00). The highest EoE was calculated for p,p'-DDE (EoE: 0.50), considering that very low PNEC at ng/kg levels was used for the risk assessment. Based on the risk assessment results, provided in **Table 20**, the highest total scores were calculated for p,p'-DDE and PFOS, followed by PCB 138 and PCB 153.

Table 19. Summary results for Finnish HELCOM PreEMPT fish samples 1-6. Results are expressed in µg/kg wet weight. Concentrations exceeding respective PNEC/EQS are highlighted in red colour.

Contaminant	Samples (sampling location, year of sampling and sample code)						LOD	LOQ
	Helsinki	Kotka	Parainen	Vaasa	Hailuoto	Pori		
	2021	2021	2021	2021	2021	2021		
	1	**2**	**3**	**4**	**5**	**6**		
Caffeine	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	1.84	5.51
3,3-Pentamethylene-4-butyrolactam	<LOD	BQL	1.14	0.884	1.48	BQL	0.275	0.824
Methylparaben	1.32	BQL	**4.53**	1.23	BQL	BQL	0.38	1.14
Anabasine	<LOD	<LOD	<LOD	<LOD	<LOD	14.1	0.82	2.46
Cotinine	<LOD	<LOD	<LOD	<LOD	<LOD	2.02	0.30	0.91
Nicotine	<LOD	<LOD	<LOD	<LOD	<LOD	**21.5**	0.83	2.50
Metolachlor-ESA	<LOD	BQL	<LOD	BQL	BQL	<LOD	0.30	0.91
Alachlor-ESA	<LOD	<LOD	<LOD	<LOD	**10.8**	<LOD	1.68	5.03
Hexachlorobenzene	BQL	BQL	<LOD	<LOD	<LOD	<LOD	0.064	0.192
Perfluorodecanoic acid (PFDA)	BQL	BQL	BQL	BQL	BQL	BQL	0.85	2.54
Perfluorononanoic acid (PFNA)	0.325	<LOD	0.304	BQL	0.426	0.292	0.07	0.22
Perfluorooctanesulfonic acid (PFOS)	**58.6**	**25.8**	**26.3**	**28.9**	**25.6**	**22.9**	0.19	0.56
Perfluoroundecanoic acid (PFUdA)	1.67	1.41	<LOD	BQL	1.52	1.41	0.43	1.30
p,p'-DDE	BQL	**0.726**	**1.45**	**0.943**	**1.97**	**1.15**	0.22	0.67
Diphenylamine	BQL	BQL	<LOD	BQL	BQL	4.51	0.30	0.89
Triphenyl phosphate	<LOD	13.1	<LOD	<LOD	<LOD	<LOD	1.85	5.54
Triethyl phosphate	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	0.33	0.98
Pyrene	**1.12**	<LOD	<LOD	**0.819**	**0.735**	**1.22**	0.043	0.130
Fluorene	0.677	0.694	1.07	BQL	0.600	0.936	0.033	0.100
2,2,4,5,5'-Pentochlorobiphenyl (PCB 101)	**3.81**	**3.67**	<LOD	**2.47**	<LOD	**2.17**	0.17	0.52

Contaminant	**Samples (sampling location, year of sampling and sample code)**						**LOD**	**LOQ**
	Helsinki	Kotka	Parainen	Vaasa	Hailuoto	Pori		
	2021	2021	2021	2021	2021	2021		
	1	**2**	**3**	**4**	**5**	**6**		
2,2',3,4,4',5'-Hexachlorobiphenyl (PCB 138)	**2.37**	**1.50**	<LOD	**1.52**	**1.32**	**1.95**	0.13	0.39
2,2',4,4',5,5'-Hexachlorobiphenyl (PCB 153)	**3.37**	**1.74**	<LOD	**1.23**	**1.21**	**2.42**	0.16	0.49

Table 20. Ranking of the detected contaminants in the Finnish fish samples based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in μg/kg wet weight. The red asterisk indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC.

Contaminant	PNEC	FoA	FoE	EoE	Risk
p,p'-DDE	0.005	1.00	0.83	0.50	2.33
Perfluorooctanesulfonic acid (PFOS)	9.1*	1.00	1.00	0.10	2.10
2,2',3,4,4',5'-Hexachlorobiphenyl (PCB 138)	0.1	0.83	0.83	0.20	1.87
2,2',4,4',5,5'-Hexachlorobiphenyl (PCB 153)	0.05	0.83	0.83	0.20	1.87
Pyrene	0.11	0.67	0.67	0.20	1.53
2,2,4,5,5'-Pentochlorobiphenyl (PCB 101)	0.08	0.67	0.67	0.20	1.53
Methylparaben	2.56	1.00	0.17	0.10	1.27
Fluorene	11.7	1.00	0.00	0.00	1.00
3,3-Pentamethylene-4-butyrolactam	66.7	0.83	0.00	0.00	0.83
Perfluorononanoic acid (PFNA)	16.5	0.83	0.00	0.00	0.83
Perfluoroundecanoic acid (PFUdA)	22.3	0.83	0.00	0.00	0.83
Diphenylamine	10.9	0.83	0.00	0.00	0.83
Nicotine	4.69	0.17	0.17	0.10	0.43
Alachlor-ESA	8.56	0.17	0.17	0.10	0.43
Cotinine	2.76	0.17	0.00	0.00	0.17
Triphenyl phosphate	202	0.17	0.00	0.00	0.17
Caffeine	0.19	0.17	Detected only at BQL levels		
Metolachlor-ESA	8.44	0.50			
Hexachlorobenzene	10	0.33			
Perfluorodecanoic acid (PFDA)	0.82	1.00			
Triethyl phosphate	81.4	0.17			
Anabasine	N/A	0.17	N/A		

Mussels samples

The wide-scope target analysis results for the 10 blue mussels samples are presented in **Table 21**. The screening results revealed the presence of 28 contaminants from various chemical classes, such as Industrial Chemicals (n=11, including PFAS, PAHs and PCBs) and Plant Protection Products &TPs (n=6). Most of the detected compounds in these samples, were also detected in at least one mussel sample provided by another HELCOM Contracting Party, except for Nicotine-Nor, Deprenyl, Endothal, Benzotriazole-1-hydroxy, Clomazone, Benzothiazole- 2-amino, DEET, Metolachlor CGA 357704, PCB 52, Pilocarpine and 1,3-Dimethyl-2-imidazolidinon that were detected only in the mussels collected in Finland. The highest number of contaminants (n=14) was detected in HELCOM PreEMPT 86 sample, whereas only 4 and 3 contaminants were present in HELCOM PreEMPT 11 and 12 samples that were collected from reference sites.

High frequency of detection was noticed in the mussels samples from the Russian Federation, and especially in HELCOM PreEMPT 87, 86 and 88. At least two contaminants

exceeded their respective ecotoxicological thresholds in each sample, while the highest frequency of PNEC exceedance was recorded for 6 compounds in HELCOM PreEMPT 86 and 87, both collected from the Outer Neva River estuary.

Methylparaben was the only contaminant that was detected in all Finnish mussel samples, followed by 3,3-Pentamethylene-4-butyrolactam that presented high FoA at 0.80. As shown in **Table 22**, most of the detected compounds (85%) were present in less than 50% of the analyzed samples (FoA <0.50) and for 14 contaminants the measured concentrations exceeded their respective PNEC values in at least one sample. The highest FoE was recorded for Methylparaben (FoE: 1.00), while Pilocarpine levels exceeded the EQS value in 5 samples. Pilocarpine and Pyrene reached a maximum value of EoE (EoE: 1.00), which may be attributed to the low PNEC values at ng/kg levels. The highest risk score was calculated for Methylparaben (Risk: 2.20), followed by Pilocarpine (Risk: 2.00), Pyrene (Risk: 1.70) and Caffeine (Risk: 1.00).

Table 21. Summary results for HELCOM PreEMPT mussels samples 7-12 and 86-89. Results are expressed in µg/kg wet weight. Concentrations exceeding the respective PNEC/EQS are highlighted in red colour.

Contaminant	Samples (sampling location, year of sampling and sample code)										LOD	LOQ
	Cage 4 Kotka	Cage 1 Helsinki	Cage 2 Pori	Cage 3 SM	Tvärminne start	Hanko	Outer Neva River estuary	Outer Neva River estuary	Neva Bay	Kopora Bay		
	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021		
	7	**8**	**9**	**10**	**11**	**12**	**86**	**87**	**88**	**89**		
Deprenyl / Selegiline	<LOD	<LOD	<LOD	<LOD	<LOD	**9.75**	<LOD	<LOD	<LOD	<LOD	0.38	1.15
Pilocarpine	**5.03**	**3.39**	**10.7**	**6.02**	**12.5**	<LOD	<LOD	<LOD	<LOD	<LOD	0.29	0.87
3,3-Pentamethylene-4-butyrolactam	**2.27**	**2.90**	**3.64**	**2.04**	**6.42**	<LOD	**1.32**	<LOD	**2.10**	BQL	0.41	1.22
O-Desmethyldinor-tramadol	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	0.16	0.47
1-3-Dimethyl-2-imidazolidinon	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**40.2**	**29.2**	**23.4**	**46.6**	0.38	1.26
Butylparaben	<LOD	<LOD	**13.5**	**21.9**	<LOD	**14.9**	<LOD	<LOD	<LOD	<LOD	1.0	3.1
Ethylparaben	BQL	**5.64**	BQL	BQL	4.85	<LOD	<LOD	<LOD	<LOD	<LOD	1.6	4.7
Methylparaben	**21.5**	**56.2**	**23.6**	**50.0**	**38.4**	**28.6**	**5.15**	**3.88**	**23.3**	**2.23**	0.62	1.85
Nicotine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	0.71	2.12
Nor-nicotine	<LOD	<LOD	<LOD	<LOD	<LOD	**2.73**	<LOD	<LOD	<LOD	<LOD	0.84	2.53
Caffeine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**8.80**	BQL	BQL	**9.03**	2.8	8.5
Perfluorononanoic acid (PFNA)	<LOD	BQL	BQL	BQL	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	0.049	0.146
Perfluorooctanesulfonic acid (PFOS)	<LOD	**5.22**	**1.65**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.15	0.44
Tributylamine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	BQL	**0.779**	BQL	0.14	0.42
2-OH-Benzothiazole	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	1.6	4.8
1-Hydroxy-benzotriazole	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.7	5.0
2-Amino-benzothiazole	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	0.028	0.093
Fluoranthene	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**1.90**	**6.35**	**2.97**	<LOD	0.074	0.222
Fluorene	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**1.06**	**0.895**	**1.11**	0.049	0.148
Phenanthrene	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**10.6**	**17.6**	**11.7**	**17.2**	0.062	0.185

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Contaminant	**Samples (sampling location, year of sampling and sample code)**										**LOD**	**LOQ**
	Cage 4 Kotka	Cage 1 Helsinki	Cage 2 Pori	Cage 3 SM	Tvärminne start	Hanko	Outer Neva River estuary	Outer Neva River estuary	Neva Bay	Kopora Bay		
	2021	2021	2021	2021	2021	2021	2021	2021	2021	2021		
	7	**8**	**9**	**10**	**11**	**12**	**86**	**87**	**88**	**89**		
Pyrene	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**12.4**	**50.6**	**6.62**	BQL	0.064	0.192
PCB 52	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	**0.0349**	**0.0209**	<LOD	0.0068	0.0205
DEET	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**0.479**	**0.181**	<LOD	**0.206**	0.024	0.078
Metolachlor CGA 357704	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**2.49**	**3.74**	<LOD	<LOD	0.19	0.64
p,p'-DDE	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	BQL	<LOD	0.33	0.99
Clomazone	<LOD	<LOD	<LOD	**209**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.50	1.49
Diethofencarb	<LOD	<LOD	<LOD	<LOD	<LOD	**20.6**	<LOD	<LOD	<LOD	<LOD	1.1	3.2
Endothal	<LOD	**10.6**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	2.2	6.6

Table 22. Ranking of the contaminants determined in the Finnish and Russian Federation mussels samples based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in μg/kg wet weight. The red asterisk indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC (divided by factor 4 as in the NORMAN Prioritisation framework).

Contaminants	PNEC	FoA	FoE	EoE	Risk
Methylparaben	0.64	1.00	1.00	0.20	2.20
Pilocarpine	0.0085	0.50	0.50	1.00	2.00
Pyrene	0.027	0.40	0.30	1.00	1.70
Caffeine	0.047	0.40	0.20	0.50	1.10
1-3-Dimethyl-2-imidazolidinon	3.1	0.40	0.40	0.20	1.00
Phenanthrene	2.2	0.40	0.40	0.10	0.90
3,3-Pentamethylene-4-butyrolactam	16.7	0.80	0.00	0.00	0.80
Butylparaben	1.1	0.30	0.30	0.20	0.80
Ethylparaben	1.8	0.50	0.20	0.10	0.80
PCB 52	0.02	0.30	0.20	0.10	0.60
Metolachlor CGA 357704	0.41	0.20	0.20	0.10	0.50
Perfluorooctanesulfonic acid (PFOS)	2.3*	0.20	0.10	0.10	0.40
Tributylamine	55.2	0.40	0.00	0.00	0.40
Clomazone	15.4	0.10	0.10	0.20	0.40
Diethofencarb	1.5	0.10	0.10	0.20	0.40
Endothal	2.1	0.10	0.10	0.10	0.30
Fluoranthene	7.5*	0.30	0.00	0.00	0.30
Fluorene	2.9	0.30	0.00	0.00	0.30
DEET	5.3	0.30	0.00	0.00	0.30
Deprenyl	21.3	0.10	0.00	0.00	0.10
Nor-nicotine	5.2	0.10	0.00	0.00	0.10
Nicotine	1.2	0.10	Detected only at BQL levels		
2-OH-Benzothiazole	2.2	0.10			
Perfluorononanoic acid (PFNA)	4.1	0.40			
1-Hydroxy-benzotriazole	1.0	0.10			
2-Amino-benzothiazole	0.12	0.10			
p,p'-DDE	0.0012	0.20			
O-Desmethyldinor-tramadol	N/A	0.10	N/A		

8.2.5 Latvian Institute of Aquatic Ecology

Within the context of the HELCOM PreEMPT project, the Latvian Institute of Aquatic Ecology provided 7 pooled fish samples (HELCOM PreEMPT 37-43), including 2 Atlantic herring (*Clupea harengus*) and 5 European perch (*Perca fluviatilis*) samples, gathered within 2018 and 2021 and 1 pooled blue mussel sample (HELCOM PreEMPT 44), collected from Pavilosta, Baltic Sea in 2021.

Fish samples

Seven pooled samples of muscle tissue of Atlantic herring (*Clupea harengus*) and European perch (*Perca fluviatilis*), collected in Latvian sea waters, were analyzed using HRMS techniques. The detailed wide-scope target analysis results are provided in **Table 23.** Overall, 21 contaminants were detected in the Latvian fish samples. Industrial chemicals, including PAHs, PFAS and surfactants, was the dominating class of detected compounds. The least contaminated fish sample, concerning the number of detected compounds, was HELCOM PreEMPT 41 (n=6), whereas the most contaminated fish sample was HELCOM PreEMPT 39 (n=13). 3,3-Pentamethylene-4-butyrolactam and Methylparaben were omnipresent in the fish samples (FoA=1.00), while PFOS and PFNA were detected in 6 and 5 samples, respectively. Pyrene, Salicylic acid and Pyrimethanil were present in more than the 50% of the analyzed fish samples. Most of detected compounds were present at low µg/kg w.w. levels. N,N-Dimethyldecylamine and PFOS were the most abundant compounds, reaching maximum concentrations of 121 and 24.1 µg/kg w.w., respectively, whereas p,p'-DDE was present only at concentrations below the respective method LOQ.
Based on the risk assessment results, summarized in **Table 23**, the measured concentrations for 10 compounds (Methylparaben, PFOS, Pyrene, N,N-Dimethyldecylamine, 1,2-Benzisothiazolinone, Saccharine, 1-Hydroxy-benzotriazole, Pilocarpine, PCB 138, Galaxolidone), exceeded their respective PNEC/EQS values in at least one sample, whereas the highest extent of PNEC exceedance was observed for N,N-Dimethyldecylamine and Pyrene. Methylparaben, PFOS and Pyrene are on the top of the list, where compounds were ranked based on their overall environmental risk. The concentration levels of PFOS exceeded the EQS in 4 out of 7 analyzed samples.

Mussels samples

The detailed wide-scope target analysis results for 4 contaminants (Methylparaben, 3,3-Pentamethylene-4-butyrolactam, Tributylamine and Salicylic acid) that were determined in the analyzed blue mussels collected from Latvian sea waters are summarized in **Table 24**. The highest concentration was observed for Methylparaben (103 µg/kg w.w.), whereas the lowest concentration was observed for Tributylamine (2.78 µg/kg w.w.). Based on the risk assessment results, the measured concentrations for Methylparaben and 3,3-Pentamethylene-4-butyrolactam exceeded their respective PNEC values. The highest extent of PNEC exceedance was assessed for Methylparaben.

Table 23. Summary results for Latvian HELCOM PreEMPT fish samples 37-43. Results are expressed in μg/kg wet weight. Concentrations exceeding respective PNEC/EQS are highlighted in red colour. The detected contaminants were ranked based on their final score (Sum of FoA+EoE+FoE). The red asterisk indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC.

Contaminant	Samples (species, sampling location, year of sampling and sample code)							*LOD*	*LOQ*	*PNEC*	FoA	FoE	EoE	Risk
	Atlantic herring (Clupea harengus)		European perch (Perca fluviatilis)											
	Baltic Sea	Gulf of Riga	Daugavgriva	Mersrags	Lielirbe	Salacgriva	Jurmalciems							
	2020	2021	2018	2018	2018	2020	2019							
	37	*38*	*39*	*40*	*41*	*42*	*43*							
Methylparaben	**7.63**	**10.1**	**4.20**	1.38	**4.95**	2.46	BQL	0.38	1.14	2.56	1.00	0.57	0.10	1.67
Perfluorooctanesulfonic acid (PFOS)	<LOD	5.34	8.72	**21.1**	**24.1**	**17.2**	**19.3**	0.19	0.56	9.1*	0.86	0.57	0.10	1.53
Pyrene	**1.57**	**1.03**	**5.57**	<LOD	<LOD	<LOD	**0.263**	0.043	0.130	0.11	0.57	0.57	0.20	1.34
N,N-Dimethyldecylamine	<LOD	**91.9**	**121**	<LOD	<LOD	**61.9**	<LOD	0.74	2.46	2.6	0.43	0.43	0.20	1.06
3,3-Pentamethylene-4-butyrolactam	7.09	4.83	1.52	1.74	1.91	2.41	1.40	0.27	0.82	66.7	1.00	0.00	0.00	1.00
1,2-Benzisothiazolinone	<LOD	<LOD	**7.52**	BQL	<LOD	**4.19**	BQL	1.0	3.4	2.81	0.57	0.29	0.10	0.96
Saccharine	<LOD	**12.4**	**20.8**	<LOD	<LOD	**8.22**	<LOD	2.2	6.5	6.63	0.43	0.43	0.10	0.96
Perfluorononanoic acid (PFNA)	<LOD	<LOD	0.259	0.410	0.321	0.316	BQL	0.074	0.220	16.5	0.71	0.00	0.00	0.71
1-Hydroxy-benzotriazole	**17.6**	**11.1**	<LOD	<LOD	<LOD	<LOD	<LOD	1.1	3.4	4.09	0.29	0.29	0.10	0.67
Pilocarpine	<LOD	<LOD	**2.22**	<LOD	<LOD	BQL	<LOD	0.55	1.66	0.034	0.29	0.14	0.20	0.63
Salicylic acid	17.8	16.8	<LOD	<LOD	<LOD	5.63	4.90	0.82	2.47	2160	0.57	0.00	0.00	0.57
Pyrimethanil	<LOD	0.0969	<LOD	0.0551	0.0597	<LOD	0.106	0.011	0.034	3.87	0.57	0.00	0.00	0.57
Fludioxonil	0.0595	0.0336	0.0839	<LOD	<LOD	<LOD	<LOD	0.0099	0.0297	14.6	0.43	0.00	0.00	0.43
2,2',3,4,4',5'-Hexachlorobiphenyl (PCB 138)	**0.575**	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.13	0.39	0.1	0.14	0.14	0.10	0.39
Galaxolidone	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	**6.30**	0.56	1.85	6.17	0.14	0.14	0.10	0.39
Fluoranthene	<LOD	<LOD	5.60	<LOD	<LOD	<LOD	<LOD	0.05	0.15	30*	0.14	0.00	0.00	0.14
Fluorene	<LOD	<LOD	2.66	<LOD	<LOD	<LOD	<LOD	0.033	0.100	11.7	0.14	0.00	0.00	0.14
Phenanthrene	<LOD	<LOD	6.46	<LOD	<LOD	<LOD	<LOD	0.042	0.12	8.8	0.14	0.00	0.00	0.14
DEET	<LOD	<LOD	<LOD	<LOD	4.80	<LOD	<LOD	0.15	0.44	21.1	0.14	0.00	0.00	0.14

Contaminant	Samples (species, sampling location, year of sampling and sample code)							*LOD*	*LOQ*	*PNEC*	FoA	FoE	EoE	Risk
	Atlantic herring (Clupea harengus)		European perch (Perca fluviatilis)											
	Baltic Sea	Gulf of Riga	Daugavgriva	Mersrags	Lielirbe	Salacgriva	Jurmalciems							
	2020	2021	2018	2018	2018	2020	2019							
	37	*38*	*39*	*40*	*41*	*42*	*43*							
p,p'-DDE	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.22	0.67	0.005	0.14	Detected only at BQL levels		
Benzododecinium (Benzyl-dimethyl-dodecylammonium)	<LOD	<LOD	<LOD	5.03	<LOD	<LOD	<LOD	0.44	1.31	N/A	0.14	N/A		

Table 24. Summary results for HELCOM PreEMPT mussel sample 44. Results are expressed in µg/kg wet weight. Concentrations exceeding the respective PNEC/EQS are highlighted in red colour. The detected contaminants were ranked based on their final score (Sum of FoA+EoE+FoE).

Contaminants	Pavilosta, Baltic Sea	*LOD (µg/kg w.w.)*	*LOQ (µg/kg w.w.)*	*PNEC*	FoA	FoE	EoE	Risk
	2021							
	44							
Methylparaben	**103**	0.617	1.85	0.64	1.00	1.00	0.50	2.50
3,3-Pentamethylene-4-butyrolactam	**19.8**	0.407	1.22	16.7	1.00	1.00	0.10	2.10
Tributylamine	2.78	0.140	0.420	55.3	1.00	0.00	0.00	1.00
Salicylic acid	10.6	0.255	0.765	540	1.00	0.00	0.00	1.00

8.2.6 Institute of Meteorology and Water Management (IMGW-PIB)

Within the context of HELCOM PreEMPT project, the Institute of Meteorology and Water Management (IMGW-PIB) provided 3 sediment samples (top layer (slice 0-5 cm), HELCOM PreEMPT 13-15), 2 pooled Atlantic herring (*Clupea harengus*) samples (HELCOM PreEMPT 16,17), and 1 pooled blue mussel (*Mytilus edulis*) sample (HELCOM PreEMPT 18), collected in Polish sea waters in 2021.

Sediment samples

The three sediment samples were analyzed using HRMS techniques; the detailed wide-scope target analysis results are provided in **Table 25.** Overall, 24 contaminants were detected. Industrial chemicals, including PAHs (n=12) and PFAS, was the dominating class of determined compounds, including more than 50% of the overally detected compounds. The least contaminated sediment sample, regarding the number of detected compounds, was HELCOM PreEMPT 14 (n=18; Bornholm), whereas the most contaminated sample was HELCOM PreEMPT 15 (n=22; eastern Gotland Basin). 17 contaminants (11 PAHs, 2-OH-Benzothiazole, Galaxolide, Oxprenolol, 2-Trifluoromethyl-benzenesulfonamide, Cypromazine, p,p'-DDE) were omnipresent in the 3 analyzed samples (FoA=1.00). Most of the detected compounds were present at low µg/kg d.w. levels. The highest concentration levels were observed for PAHs, reaching maximum cumulative concentration of 1.07 mg/kg d.w. at HELCOM PreEMPT 13, which was also the most contaminated sample regarding the number of PAHs.

Based on the risk assessment results, summarized in **Table 25**, the concentrations of 5 compounds (Anthracene, Benzo(a)pyrene, Dibenzo(a,h)anthracene, Indeno(1,2,3-cd)pyrene and PFOS), exceeded their respective PNEC values in at least one sample, whereas the highest extent of PNEC exceedance was observed for Anthracene. Anthracene and Benzo(a)pyrene exceeded their respective PNEC values in all of the tested sediment samples. The highest risk was calculated for Anthracene (Risk: 2.50), followed by Benzo(a)pyrene (Risk: 2.20).

Table 25. Summary results for Polish HELCOM PreEMPT sediment samples 13-15. Results are expressed in µg/kg dry weight. Concentrations exceeding respective PNEC are highlighted in red colour. The detected contaminants were ranked based on their final score (Sum of FoA+EoE+FoE).

Contaminant	**Samples (sampling location, year of sampling and sample code)**			***LOD***	***LOQ***	***PNEC***	***FoA***	***FoE***	***EoE***	***Risk***
	Gdansk Basin	Bornholm Basin	Eastern Gotland Basin							
	2021	2021	2021							
	13	***14***	***15***							
Anthracene	**18.5**	**8.00**	**7.63**	**0.074**	**0.22**	0.048	1.00	1.00	0.50	2.50
Benzo(a)pyrene	**74.9**	**37.4**	**30.8**	**1.7**	**5.2**	2.5	1.00	1.00	0.20	2.20
Dibenzo(a,h)anthracene	**76.7**	55.2	41.0	**2.1**	**6.2**	63.4	1.00	0.33	0.10	1.43

Contaminant	Samples (sampling location, year of sampling and sample code)			*LOD*	*LOQ*	*PNEC*	*FoA*	*FoE*	*EoE*	*Risk*
	Gdansk Basin	Bornholm Basin	Eastern Gotland Basin							
	2021	2021	2021							
	13	***14***	***15***							
Indeno(1,2,3-cd)pyrene	**296**	155	201	**0.38**	**1.15**	240	1.00	0.33	0.10	1.43
Acenaphthene	4.83	2.21	2.13	**0.063**	**0.19**	16	1.00	0.00	0.00	1.00
Acenaphthylene	19.0	7.94	4.77	**0.16**	**0.47**	44	1.00	0.00	0.00	1.00
Benz(a)anthracene	88.7	45.2	35.7	**0.44**	**1.33**	261	1.00	0.00	0.00	1.00
Chrysene	123	56.1	46.2	**0.075**	**0.22**	384	1.00	0.00	0.00	1.00
Fluoranthene	147	69.8	73.5	**0.13**	**0.38**	600	1.00	0.00	0.00	1.00
Fluorene	13.1	3.90	3.77	**0.07**	**0.21**	19	1.00	0.00	0.00	1.00
Phenanthrene	32.0	13.1	11.5	**0.045**	**0.136**	240	1.00	0.00	0.00	1.00
2-OH-Benzothiazole	5.68	4.88	BQL	**0.50**	**1.51**	323	1.00	0.00	0.00	1.00
Galaxolide	6.08	BQL	BQL	**0.35**	**1.05**	25723	1.00	0.00	0.00	1.00
Oxprenolol	0.509	0.176	0.181	**0.053**	**0.160**	101	1.00	0.00	0.00	1.00
2-Trifluoromethyl-benzenesulfonamide	9.07	BQL	BQL	**2.0**	**5.9**	90.2	1.00	0.00	0.00	1.00
Cyromazine	0.996	BQL	BQL	**0.17**	**0.47**	1.12	1.00	0.00	0.00	1.00
p,p'-DDE	1.73	0.808	0.494	**0.08**	**0.24**	2.2	1.00	0.00	0.00	1.00
Perfluorooctanesulfonic acid (PFOS)	<LOD	<LOD	**0.528**	**0.13**	**0.38**	0.0067	0.33	0.33	0.20	0.87
Pyrene	178	<LOD	<LOD	**0.46**	**1.37**	665	0.33	0.00	0.00	0.33
Perfluorohexanoic acid (PFHxA)	BQL	<LOD	<LOD	**0.36**	**1.09**	7602	0.33	Detected only at BQL levels		
Perfluorooctanoic acid (PFOA)	<LOD	<LOD	BQL	**0.34**	**1.01**	6.04	0.33			
o,p'-DDT	BQL	BQL	BQL	**0.51**	**1.53**	156	1.00			
Phthalamic acid	<LOD	<LOD	BQL	**0.70**	**2.10**	N/A	1.00	N/A		
4-OH-Benzenesulfonate	BQL	<LOD	BQL	**13.9**	**41.6**	N/A	0.67			

Fish samples

Two pooled Atlantic herring (*Clupea harengus*) samples, collected in Polish sea waters in 2021, were analyzed using HRMS techniques and the detailed wide-scope target analysis results are provided in **Table 26.** Overall, 13 contaminants were detected. Industrial chemicals, including PAHs, PCBs and PFAS, was the dominating class of determined compounds, followed by Plant Protection Products. The most contaminated fish sample, concerning the cumulative concentration of the detected compounds, was HELCOM PreEMPT 16, collected from eastern Gotland Basin in 2021 (∑Conc= 76.1 μg/kg w.w., n=10), while the total contaminants' concentration in HELCOM PreEMPT 17 was 28.4 μg/kg w.w. (n=11). Most of the detected compounds were present at low μg/kg w.w. levels. Based on the risk assessment results, summarized in **Table 26**, the concentrations of 5 compounds (p,p'-DDE, Methylparaben, Pilocarpine, PCB 101 and Pyrene), exceeded

their respective PNEC values in at least one sample, whereas the highest extent of PNEC exceedance was measured for p,p'-DDE and Pilocarpine. The highest risk was calculated for p,p'-DDE (Risk: 2.50), followed by Methylparaben (Risk: 2.20).

Table 26. Summary results for Polish HELCOM PreEMPT fish samples 16 and 17. Results are expressed in µg/kg wet weight. Concentrations exceeding respective PNEC/EQS are highlighted in red colour. The detected contaminants were ranked based on their final score (Sum of FoA+EoE+FoE). The red asterisk indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC.

Contaminant	**Samples (sampling location, year of sampling and sample code)**		***LOD***	***LOQ***	***PNEC***	***FoA***	***FoE***	***EoE***	***Risk***
	Eastern Gotland Basin	Bornholm Basin							
	2021	2021							
	16	**17**							
p,p'-DDE	**5.00**	**3.99**	**0.22**	**0.67**	0.005	1.00	1.00	0.50	2.50
Methylparaben	**34.0**	**3.95**	**0.38**	**1.14**	2.56	1.00	1.00	0.20	2.20
Pilocarpine	**22.2**	<LOD	**0.55**	**1.66**	0.034	0.50	0.50	0.50	1.50
2,2,4,5,5'-Pentochlorobiphenyl (PCB 101)	<LOD	**3.00**	**0.17**	**0.52**	0.08	0.50	0.50	0.20	1.20
Pyrene	<LOD	**2.36**	**0.043**	**0.130**	0.11	0.50	0.50	0.20	1.20
Diphenylamine	4.6	7.1	**0.30**	**0.89**	10.9	1.00	0.00	0.00	1.00
Fluorene	1.48	1.25	**0.033**	**0.100**	11.7	1.00	0.00	0.00	1.00
Hexachlorobenzene	0.225	BQL	**0.064**	**0.192**	10	1.00	0.00	0.00	1.00
Perfluorononanoic acid (PFNA)	0.87	1.00	**0.074**	**0.220**	16.5	1.00	0.00	0.00	1.00
Perfluorooctanesulfonic acid (PFOS)	3.11	4.60	**0.19**	**0.56**	9.1*	1.00	0.00	0.00	1.00
3,3-Pentamethylene-4-butyrolactam	2.02	BQL	**0.27**	**0.82**	66.7	1.00	0.00	0.00	1.00
Nicotine-nor	BQL	<LOD	**1.8**	**5.3**	21	0.50	Detected only at BQL levels		
Perfluoroundecanoic acid (PFUnA)	<LOD	BQL	**0.43**	**1.30**	22.3	0.50			

Mussels samples

Overall, 6 contaminants were determined in the analyzed Polish blue mussel sample by wide-scope target analysis. The targeted results are summarized in **Table 27**. The detected compounds belong to different chemical classes, based on their main use; 2 PFAS (PFNA, PFUnA), 2 Personal Care Products (Methylparaben, Butylparaben), 1 PAH (Athracene) and 1 Plant Protection Product (Diethofencarb). Methylparaben was the most abundant compound, reaching maximum concentration of 4.28 µg/kg w.w., whereas the rest of the contaminants were present only below their respective method LOQ. Based on the risk assessment results, summarized in **Table 27**, the measured concentration exceeded respective PNEC value only for Methylparaben (Risk: 2.10).

Table 27. Summary results for Polish HELCOM PreEMPT blue mussel sample 18. Results are expressed in µg/kg wet weight. Concentrations exceeding the respective PNEC/EQS are highlighted in red colour. The detected contaminants were ranked based on their final score (Sum of FoA+EoE+FoE).

Contaminant	Gdansk Basin 2021 **18**	***LOD***	***LOQ***	***PNEC***	**FoA**	**FoE**	**EoE**	**Risk**
Methylparaben	**4.28**	**0.62**	**1.85**	0.64	1.00	1.00	0.10	2.10
Diethofencarb	BQL	**1.1**	**3.2**	1.50	1.00	Detected only at BQL levels		
Butylparaben	BQL	**1.0**	**3.1**	1.09	1.00			
Perfluorononanoic acid (PFNA)	BQL	**0.049**	**0.15**	4.13	1.00			
Perfluoroundecanoic acid (PFUnA)	BQL	**0.26**	**0.79**	5.58	1.00			
Anthracene	BQL	**0.095**	**0.285**	0.0325	1.00			

8.2.7 Aarhus University

Within the context of the HELCOM PreEMPT project, Aarhus University provided 5 sediment samples [top layer (slice 0-5 cm)], collected within 2020 and 2021.
In total, 23 contaminants were determined in the five Danish sediment samples by wide-scope target analysis. The detailed results are summarized in **Table 28**. Industrial chemicals classes of PFAS and PAHs were the dominating groups of detected compounds. The least contaminated sediment sample, regarding the number of the detected compounds, was HELCOM PreEMPT 94 (n=13), whereas the most contaminated sediment samples were HELCOM PreEMPT 90 and 92 (n=18). Eight PAHs were omnipresent in the tested Danish sediment samples (Acenaphthylene, Anthracene, Benz(a)anthracene, Benzo(a)pyrene, Chrysene, Fluoranthene, Phenanthrene, Pyrene); Fluorene was detected in 4 out of the 5 analyzed samples. Methylparaben, as well as the Plant Protection Products Prometon, Simazine and Terbumeton occurred in all tested sediment samples. Most of the detected compounds were present at low µg/kg d.w. levels. Prometon was the most abundant contaminant, reaching maximum concentration of 477 µg/kg d.w, while Methylparaben, Caffeine and Terbumeton were present at high concentration levels (maximum concentration higher than 50 µg/kg d.w.).

Based on the risk assessment results, summarized in **Table 29**, the concentrations for 10 compounds (Anthracene, Benzo(a)pyrene, N-Methyldodecylamine, PFOS, Methylparaben, Caffeine, Meloxicam, Prometon, Simazine, Terbumeton), exceeded their respective PNEC values in at least one sample. The highest extent of PNEC exceedance was observed for Anthracene and PFOS. Anthracene, Prometon and Terbumeton were on the top of the list, when compounds were ranked based on their overall environmental risk.

Table 28. Summary results for the Danish HELCOM PreEMPT sediment samples 90-94. Results are expressed in µg/kg dry weight. Concentrations exceeding the respective PNEC/EQS are highlighted in red colour.

Contaminant	**Samples (sampling location, year of sampling and sample code)**					***LOD***	***LOQ***
	Roskilde Fjiord	Wadden Sea	Gamborg Fjiord	Western Limfjorden	Skive		
	2021	2021	2021	2021	2021		
	90	***91***	***92***	***93***	***94***		
Acenaphthylene	5.90	5.18	15.5	5.21	9.26	0.16	0.47
Anthracene	**5.97**	**4.96**	**12.6**	**7.55**	**17.9**	0.074	0.223
Benz(a)anthracene	2.61	5.96	4.55	3.45	5.43	0.44	1.33
Benzo(a)pyrene	BQL	BQL	**8.57**	**5.85**	**9.53**	1.7	5.2
Chrysene	11.4	23.9	22.6	14.5	15.6	0.075	0.225
Fluoranthene	5.78	11.3	13.1	7.79	8.59	0.13	0.38
Fluorene	<LOD	9.14	6.69	7.93	4.61	0.07	0.21
Phenanthrene	0.714	4.27	5.22	3.26	3.88	0.045	0.136

Contaminant	Samples (sampling location, year of sampling and sample code)					*LOD*	*LOQ*
	Roskilde Fjiord	Wadden Sea	Gamborg Fjiord	Western Limfjorden	Skive		
	2021	2021	2021	2021	2021		
	90	***91***	***92***	***93***	***94***		
Pyrene	2.54	3.20	5.76	2.79	5.01	0.46	1.37
N-Methyldodecylamine	**10.3**	5.28	<LOD	<LOD	<LOD	0.21	0.68
Perfluorooctanesulfonic acid (PFOS)	**5.77**	**3.72**	<LOD	**2.71**	<LOD	0.13	0.38
Perfluorooctanoic acid (PFOA)	2.64	<LOD	<LOD	<LOD	<LOD	0.34	1.01
Galaxolide	11.6	<LOD	7.27	3.19	<LOD	0.35	1.05
Methylparaben	15.9	**25.0**	**33.0**	**26.3**	**52.7**	1.0	3.1
3,3-Pentamethylene-4-butyrolactam	<LOD	8.85	18.0	<LOD	<LOD	0.35	1.14
Caffeine	<LOD	<LOD	<LOD	**66.5**	<LOD	0.31	1.02
Lamotrigine	BQL	<LOD	<LOD	<LOD	<LOD	0.18	0.60
Meloxicam	**2.79**	<LOD	BQL	<LOD	<LOD	0.91	2.73
2-Trifluoromethyl-benzenesulfonamide	<LOD	<LOD	44.4	<LOD	<LOD	2.0	5.9
Fludioxonil	<LOD	10.5	7.33	3.85	<LOD	0.087	0.26
Prometon	**26.2**	**328**	**162**	**477**	**322**	1.3	3.9
Simazine	**17.1**	6.42	**14.8**	5.10	**8.14**	0.40	1.21
Terbumeton	BQL	**329**	**66.2**	**390**	**135**	2.4	7.2

Table 29. Ranking of the detected contaminants in the Danish sediment samples based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in µg/kg dry weight.

Contaminant	*PNEC*	FoA	FoE	EoE	Risk
Anthracene	0.048	1.00	1.00	0.50	2.50
Terbumeton	0.47	1.00	0.80	0.50	2.30
Prometon	8.51	1.00	1.00	0.20	2.20
Methylparaben	21.9	1.00	0.80	0.10	1.90
Simazine	7.82	1.00	0.60	0.10	1.70
Perfluorooctanesulfonic acid (PFOS)	0.0067	0.60	0.60	0.50	1.70
Benzo(a)pyrene	2.5	1.00	0.60	0.10	1.70
Acenaphthylene	44	1.00	0.00	0.00	1.00
Benz(a)anthracene	261	1.00	0.00	0.00	1.00
Chrysene	384	1.00	0.00	0.00	1.00
Fluoranthene	600	1.00	0.00	0.00	1.00
Phenanthrene	240	1.00	0.00	0.00	1.00
Pyrene	665	1.00	0.00	0.00	1.00
Fluorene	19	0.80	0.00	0.00	0.80
N-Methyldodecylamine	9.03	0.40	0.20	0.10	0.70
Meloxicam	2.6	0.40	0.20	0.10	0.70

Contaminant	*PNEC*	FoA	FoE	EoE	Risk
Caffeine	5.61	0.20	0.20	0.20	0.60
Galaxolide	25723	0.60	0.00	0.00	0.60
Fludioxonil	66	0.60	0.00	0.00	0.60
3,3-Pentamethylene-4-butyrolactam	860	0.40	0.00	0.00	0.40
Perfluorooctanoic acid (PFOA)	6.04	0.20	0.00	0.00	0.20
2-Trifluoromethyl-benzenesulfonamide	90.2	0.20	0.00	0.00	0.20
Lamotrigine	104	0.20	Detected only at BQL levels		

8.2.8 Lithuanian Environmental Protection Agency

Within the context of the HELCOM PreEMPT project, the Lithuanian Environmental Protection Agency provided 3 biota samples (HELCOM PreEMPT 33-36), 2 fish samples - European flounder (*Platichthys flesus*) and Atlantic herring (*Clupea harengus*) – and 1 zebra mussel (*Dreissena polymorpha*), gathered in Lithuanian sea waters in 2021.

Fish samples

Two pooled fish samples, collected from the Baltic Sea, Lithuania in 2021, were analyzed using HRMS techniques and the detailed wide-scope target analysis results are provided in **Table 30.** Overall, 13 contaminants were detected in the Lithuanian fish samples. The detected compounds were mainly Industrial Chemicals, including PFAS and PAHs, whereas the other compounds belong to different chemical classes, based on their main use; Plant Protection Products, Pharmaceuticals, PCPs and coffee related compounds. The most contaminated fish sample, concerning the cumulative concentration and the number of the detected compounds, was the European flounder (*Platichthys flesus*) pooled HELCOM PreEMPT sample 34 (∑Conc= 90.3 μg/kg w.w., n=10), while the total contaminants' concentration in Atlantic herring (*Clupea harengus*) pooled HELCOM PreEMPT sample 35 was 63.1 μg/kg w.w. (n=9). Methylparaben was the most abundant compound, reaching maximum concentration of 50.7 μg/kg w.w., whereas the rest of the detected compounds were present at low μg/kg w.w. levels. Based on the risk assessment results, summarized in **Table 30**, the concentrations of 7 compounds (p,p'-DDE, Methylparaben, PFOS, Pilocarpine, Caffeine and Venlafaxine), exceeded their respective PNEC values in at least one sample. The highest extent of PNEC exceedance was measured for p,p'-DDE and Pilocarpine. The highest risk was calculated for p,p'-DDE (Risk: 3.00), followed by Methylparaben (Risk: 2.20). The concentration level of PFOS was higher than its respective EQS in the sample HELCOM PreEMPT 34.

Table 30. Summary results for Lithuanian HELCOM PreEMPT fish samples 34 and 35. Results are expressed in μg/kg wet weight. Concentrations exceeding the respective PNEC/EQS are

highlighted in red colour. The detected contaminants were ranked based on their final score (Sum of FoA+EoE+FoE). The red asterisk indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC.

Contaminant	Baltic Sea, S-3 2021		*LOD*	*LOQ*	*PNEC*	FoA	FoE	EoE	Risk
	34	35							
p,p'-DDE	0.75	5.55	0.22	0.67	0.005	1.00	1.00	1.00	3.00
Methylparaben	50.7	24.7	0.38	1.14	2.56	1.00	1.00	0.20	2.20
Perfluorooctanesulfonic acid (PFOS)	11.7	2.8	0.19	0.56	9.1*	1.00	0.50	0.10	1.60
Pilocarpine	<LOD	13.8	0.55	1.66	0.034	0.50	0.50	0.50	1.50
Caffeine	16.0	<LOD	1.8	5.5	0.19	0.50	0.50	0.20	1.20
Venlafaxine	<LOD	10.8	0.34	1.01	0.32	0.50	0.50	0.20	1.20
Anthracene	0.29	<LOD	0.093	0.280	0.13	0.50	0.50	0.10	1.10
3,3-Pentamethylene-4-butyrolactam	1.85	2.55	0.27	0.82	66.7	1.00	0.00	0.00	1.00
Perfluorononanoic acid (PFNA)	0.317	BQL	0.07	0.22	16.5	1.00	0.00	0.00	1.00
Fluorene	1.98	2.30	0.033	0.100	11.7	1.00	0.00	0.00	1.00
Alachlor-ESA	6.54	<LOD	1.7	5.0	8.56	0.50	0.00	0.00	0.50
Perfluorohexanesulfonic acid (PFHxS)	0.138	<LOD	0.026	0.076	15.3	0.50	0.00	0.00	0.50
o,p'-DDT	<LOD	BQL	0.38	1.14	31	0.50	Detected only at BQL levels		

Mussels samples

Overall, 14 contaminants were determined in the analyzed Lithuanian zebra mussel sample by wide-scope target analysis. The targeted results are summarized in **Table 31**. The detected compounds were mainly Industrial Chemicals, including PFAS and PAHs, whereas the other compounds belong to different chemical classes, based on their main use; PCPs (Methylparaben, Butylparaben), coffee and tobacco related compounds (Nicotine, Caffeine, Theobromine), Pharmaceuticals and PPPs. Nicotine was the most abundant compound, reaching maximum concentration of 8.1 µg/kg w.w., whereas the total cumulative concentration of the detected contaminants was 33.1 µg/kg w.w. Eight contaminants were present only below their respective method LOQ. Based on the risk assessment results, summarized in **Table 31**, the measured concentrations exceeded respective PNEC values for 4 compounds (Methylparaben, Nicotine, 3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octanesulfonic acid and Butylparaben) in the analyzed zebra mussel sample. The highest risk was calculated for Methylparaben (Risk: 2.20).

Table 31. Summary results for Lithuanian HELCOM PreEMPT mussel sample 36. Results are expressed in µg/kg wet weight. Concentrations exceeding the respective PNEC/EQS are

highlighted in red colour. The detected contaminants ranked based on their final score (Sum of FoA+EoE+FoE). The red asterisk indicates that the EQS, as reported in Directive 2013/39/EU, was used instead of PNEC.

Contaminant	Curonian Lagoon 2021 36	*LOD*	*LOQ*	*PNEC*	FoA	FoE	EoE	Risk
Methylparaben	**6.68**	***0.62***	***1.85***	0.64	1.00	1.00	0.20	2.20
Nicotine	**8.07**	***0.71***	***2.12***	1.17	1.00	1.00	0.10	2.10
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluoro-1-octanesulfonic acid	**3.77**	***0.44***	***1.31***	2.9	1.00	1.00	0.10	2.10
Butylparaben	**3.32**	***1.03***	***3.08***	1.08	1.00	1.00	0.10	2.10
Diphenylamine	0.519	***0.14***	***0.43***	2.72	1.00	0.00	0.00	1.00
2-OH-Benzothiazole	BQL	***1.61***	***4.83***	2.2	1.00	Detected only at BQL levels		
Propyphenazone	BQL	***0.16***	***0.49***	0.5	1.00			
Caffeine	BQL	***2.84***	***8.51***	0.047	1.00			
Theobromine	BQL	***1.0***	***3.1***	3.15	1.00			
Brinzolamide	BQL	***0.49***	***1.47***	0.66	1.00			
Perfluorohexanoic acid (PFHxA)	BQL	***0.17***	***0.52***	172.5	1.00			
Perfluorooctanesulfonic acid (PFOS)	BQL	***0.15***	***0.44***	9.1*	1.00			
Anthracene	BQL	***0.095***	***0.285***	0.03	1.00			
O-Desmethyldinor-tramadol	0.936	***0.16***	***0.47***	N/A	1.00	N/A		

8.2.9 German Environmental Specimen Bank and Landesamt für Umwelt, Naturschutz und Geologie Mecklenburg-Vorpommern

Within the context of the HELCOM PreEMPT project, two mussel samples from Germany were analyzed. The State Office for the Environment, Nature Conservation and Geology Mecklenburg-Vorpommern (LUNG MV) provided HELCOM PreEMPT 62 sample and the German Environmental Specimen Bank provided HELCOM PreEMPT 85 sample, collected from the National Park.

The results of wide-scope target analysis, as well as the risk assessment outcomes are presented in **Table 32**. Ten contaminants, mainly industrial chemicals, were detected in the German samples. All contaminants were present in both samples (some of them below the LOQ levels). Benzododecinium was found with FoA of 0.50. Phenanthrene, Pyrene and p,p'-DDE concentrations exceeded their respective PNEC values in at least one sample, whereas Methylparaben was determined in both German samples at concentration levels two orders of magnitude higher that its EQS. The highest EoE was calculated for p,p'-DDE (EoE: 1.00), followed by Methylparaben (EoE: 0.500). The top three contaminants detected in the German samples based on the calculated final risk score were Methylparaben, p,p'-DDE and Pyrene.

Table 32. Summary results for HELCOM PreEMPT mussel samples 62 and 85. Results are expressed in µg/kg wet weight. Concentrations exceeding respective PNEC/EQS are highlighted in red colour. Contaminants were ranked based on their final score (Sum of FoA+EoE+FoE).

Contaminant	Samples (sampling location, year of sampling and sample code)		LOD	LOQ	PNEC	FoA	FoE	EoE	Risk
	Baltic Sea	Baltic Sea: offshore Darsser Ort							
	2021	2002							
	62	**85**							
Methylparaben	**72.6**	**29.3**	0.62	1.85	0.64	1.00	1.00	0.50	2.50
p,p'-DDE	**1.69**	BQL	0.33	0.99	0.00125	1.00	0.50	1.00	2.50
Pyrene	BQL	**1.34**	0.064	0.19	0.0275	1.00	0.50	0.20	1.70
Phenanthrene	**2.25**	1.34	0.062	0.185	2.20	1.00	0.50	0.10	1.60
3,3-Pentamethylene-4-butyrolactam	1.87	BQL	0.41	1.22	16.675	1.00	0.00	0.00	1.00
Pyrimethanil	0.254	0.183	0.044	0.13	0.9675	1.00	0.00	0.00	1.00
Tributylamine	1.19	BQL	0.14	0.42	55.25	1.00	0.00	0.00	1.00
Fluoranthene	1.43	BQL	0.074	0.222	7.5*	1.00	0.00	0.00	1.00
Fluorene	1.98	1.91	0.049	0.148	2.925	1.00	0.00	0.00	1.00
Benzododecinium (Benzyl-dimethyl-dodecylammonium)	6.94	<LOD	1.0	3.0	N/A	0.50	N/A		

8.3 Suspect screening

8.3.1 Suspect screening results of sediment samples and risk assessment

98 contaminants were tentatively identified in the 30 analysed sediment samples. Detailed results of analyses for all samples, expressed in µg/kg dry weight are provided in the separately submitted DCTs. Data on the frequency of appearance, chemical classification, concentration range, PNECs and risk assessment are summarized in **Table 33**. Based on the available information about substances' main use, chemical class or application, their main use category was proposed, although some compounds may have multiple uses. The risk associated with the exceedance of toxicity threshold values has been assessed by comparing the measured concentrations with PNEC values from the NORMAN Ecotoxicology Database. In cases were PNECs were not available, no risk assessment could be carried out.

Table 33. Summary results of suspect screening analyses of the 30 HELCOM PreEMPT sediment samples. Compounds are ranked based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in µg/kg dry weight.

Contaminant	Classification	Detection Range	PNEC	FoA	FoE	EoE	Risk
3a,4,5,6,7,7a-Hexahydro-4,7-methano-1H-inden-5-yl propionate	PCP	2.9-135	269	1.00	1.00	0.00	2.00
Musk	PCP	35-416	4.75	0.90	0.90	0.20	2.00
Dacarbazine	Pharmaceutical	1-31	9.75	1.00	0.87	0.10	1.97
4-Morpholinecarboxaldehyde	Ind. chemical	2.3-35	131	0.97	0.97	0.00	1.93
Methacrylamide	Plasticizer	4.9-252	135	0.93	0.87	0.10	1.90
4,4-Dimethyl oxazolidine	PPP	3.6-116	164	0.97	0.93	0.00	1.90
TP3/Trimethylolpropane trimethacrylate	Ind. chemical	2.9-39	1653	0.90	0.90	0.00	1.80
4-tert-Butylbenzoic acid	Ind. chemical	24-271	20.1	0.80	0.70	0.20	1.70
3,5-Di-tert-butyl-4-hydroxybenzaldehyde	Ind. chemical	24-504	72.9	0.77	0.77	0.10	1.63
Threonate	Pharmaceutical	1-61	1253	0.83	0.80	0.00	1.63
Hexa-2,4-dienoic acid	PPP	36-471	24.6	0.70	0.70	0.20	1.60
Piperonal	PPP	0.01-4.8	133	0.80	0.70	0.00	1.50
N-Methyl-2-pyrrolidone	Plasticizer	2.5-141	359	0.97	0.50	0.00	1.47
2-Allyloxymethyl-2-ethylpropanediol	Plasticizer	0.8-23	499	0.70	0.70	0.00	1.40
Methylhexahydrophthalic anhydride	Plasticizer	0.9-22	743	0.70	0.70	0.00	1.40
2-Naphthylamine	Dyes	8.4-384	5.61	0.87	0.27	0.20	1.33
Miristalkonium	Surfactant	2.9-4.2	35.7	0.67	0.67	0.00	1.33
Jasmonic acid	PPP	1.2-15	79.1	0.67	0.67	0.00	1.33
2H-1-Benzopyran-2-one, 7-amino-4-methyl-	Dyes	0.7-115	66.2	0.60	0.60	0.10	1.30
5'-Methylthioadenosine	Pharmaceutical	1.5-23	1.31	1.00	0.00	0.20	1.20
Cetylpyridinium	Surfactant	4.5-22	6.71	0.77	0.20	0.10	1.07
N,N-Dimethylformamide	Ind. chemical	6.4-21	37856	0.50	0.50	0.00	1.00
2-[2-(Dimethylamino)ethoxy]ethanol	Plasticizer	1.6-29	400	0.97	0.00	0.00	0.97
TP2/Pentanedioic acid, bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] ester	Surfactant	0.3-12	354	0.97	0.00	0.00	0.97
Tricyclodecanedimethanol	PCP	31-159	2018	0.47	0.47	0.00	0.93
Benzoic acid, 4-(1,1-dimethylethyl)-, 1-methylethyl ester	Ind. chemical	7.7-23	10.7	0.83	0.00	0.10	0.93
1,3-Diphenylguanidine	Plasticizer	2.8-41	12.3	0.80	0.00	0.10	0.90
CGA 353042	PPP	0.4-6.4	-	0.90	-	-	0.90
Sodium hydroxy- methane sulfonate	Ind. chemical	5-159	361	0.90	0.00	0.00	0.90
TP3/tert-Butyl phenyl glycidyl ether	Dyes	21-531	-	0.87	-	-	0.87
Hexaprofen	Pharmaceutical	0.01-6.9	-	0.87	-	-	0.87
TP1/Dimethyl succinate	Ind. chemical	1.5-30	172	0.53	0.30	0.00	0.83
Cyclohexylamine	Ind. chemical	0.9-3.5	80.1	0.40	0.40	0.00	0.80
N-(2,4-Dimethylphenyl)formamide	PPP	0.8-21	93.2	0.63	0.17	0.00	0.80
N-Hexyl-N-(3-phenylpropyl)hexan-1-amine	Surfactant	4.5-22	-	0.77	-	-	0.77
N-Vinyl-2-pyrrolidone	Plasticizer	1.6-5.7	225	0.37	0.37	0.00	0.73
Octadecanamide	Plasticizer	9-148	3.93	0.50	0.00	0.20	0.70
2-Propen-1-yl 2-(cyclohexyloxy)acetate	PCP	0.01-9.2	49.7	0.70	0.00	0.00	0.70
Penicillic acid	Pharmaceutical	37-142	41.8	0.60	0.00	0.10	0.70
3-Methylbenzoic acid	Ind. chemical	0.01-11	151	0.40	0.30	0.00	0.70
Sodium levulinate	PCP	14-47	730	0.67	0.00	0.00	0.67

Contaminant	Classification	Detection Range	PNEC	FoA	FoE	EoE	Risk
2,2,6,6-Tetramethyl-4-oxopiperidinooxy	Ind. chemical	1.8-151	48.5	0.57	0.00	0.10	0.67
Bis(2-chloro-1-methylethyl) 2-chloropropyl phosphate	Plasticizer	7.4-40	0.21	0.13	0.00	0.50	0.63
Octinoxate	PCP	11-31	283	0.63	0.00	0.00	0.63
Erucamide	Plasticizer	0.04-9.7	4.85	0.50	0.00	0.10	0.60
TP1/Hydroxycitronellal dimethyl acetal	PCP	15-85	-	0.60	-	-	0.60
Monoethyl phthalate	Phthalate	1.4-9.2	37.5	0.57	0.00	0.00	0.57
1-Ethenylazepan-2-one	Dyes	0.8-8.4	157	0.53	0.00	0.00	0.53
Tetradecane-7-sulfonic acid	Surfactant	2.8-27	189	0.53	0.00	0.00	0.53
3-Pyridinol	PPP	1.8-12	135	0.27	0.27	0.00	0.53
9,1N.D.-Phenanthrenedione	Dyes	0.1-0.9	119	0.40	0.00	0.00	0.40
Tris(2-ethylhexyl) phosphate	Phosphate	0.01-25	24.3	0.27	0.03	0.10	0.40
Camphor	Pharmaceutical	29-164	339	0.20	0.20	0.00	0.40
TP1/2,4,6-Trimethylbenzaldehyde	Ind. chemical	2.9-7.5	61.9	0.20	0.20	0.00	0.40
Tris(4-methylphenyl) Phosphate	Phosphate	3.4-15	11.7	0.20	0.00	0.10	0.30
Acetyl tributyl citrate	PCP	1.9-22	18.0	0.10	0.10	0.10	0.30
Stearic acid, monoester with glycerol	Surfactant	17-43	43.0	0.10	0.10	0.10	0.30
Bis(2-ethylhexyl) decanedioate	Plasticizer	3.5-4.3	10.4	0.30	0.00	0.00	0.30
Pentaethylene glycol	Surfactant	19-925	2352	0.30	0.00	0.00	0.30
Stearic acid, compound with 2,2',2''-nitrilotriethanol (1:1)	Surfactant	1.2-2.1	39.2	0.30	0.00	0.00	0.30
N,N-Diethylaniline	Dyes	0.2-1.1	37.4	0.13	0.13	0.00	0.27
Amines, C1N.D.-16-alkyldimethyl, N-oxides	Surfactant	0.7-2	-	0.23	-	-	0.23
Benzoic acid, 4-methoxy-	Ind. chemical	59-140	362	0.23	0.00	0.00	0.23
1,3-Benzenedimethanamine	Ind. chemical	0.6-1.3	95.5	0.23	0.00	0.00	0.23
TP1/Isophorone	Ind. chemical	0.9-15	-	0.23	-	-	0.23
Decanedioic acid	Plasticizer	3.3-83	1181	0.20	0.00	0.00	0.20
1,3-Dioxolane, 2,4-dimethyl-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-	PCP	11-19	19.9	0.10	0.10	0.00	0.20
N,N-Bis(2-hydroxyethyl)dodecanamide	Surfactant	2.7-12	65.0	0.20	0.00	0.00	0.20
Naphthalene-1-sulfonic acid	Surfactant	0.1-7.9	964	0.20	0.00	0.00	0.20
N,N-Diethyldodecanamide	Surfactant	5.9-34	12.9	0.10	0.00	0.10	0.20
Telbivudine	Pharmaceutical	7-67	95.5	0.20	0.00	0.00	0.20
Glycine, N-(1-oxooctyl)-	Ind. chemical	3-5.7	190	0.10	0.10	0.00	0.20
1-(2-Hydroxyethyl)-2,2,6,6-tetramethyl-4-piperidinol	Ind. chemical	0.4-8.1	259	0.20	0.00	0.00	0.20
Glycerol monomyristate	PCP	7.5-23	80.3	0.17	0.00	0.00	0.17
Tetradecylamine	Surfactant	1-12	15.2	0.17	0.00	0.00	0.17
N-Dodecyl-4-methoxybenzamide	Surfactant	5.6-16	-	0.17	-	-	0.17
Octanedioic acid	Plasticizer	13-50	515	0.07	0.07	0.00	0.13
Isobutyl hydrogen Phthalate	Phthalate	3.1-4.1	24.0	0.07	0.07	0.00	0.13
Succinic acid, sodium adduct	PCP	3.6-3.8	83.3	0.07	0.07	0.00	0.13
2,3-Dihydroxypropyl pentadecanoate	Surfactant	1.3-4.7	106	0.13	0.00	0.00	0.13
1-Butanol, 3-methoxy-3-methyl-, acetate	Ind. chemical	37-47	101	0.07	0.07	0.00	0.13

Contaminant	Classification	Detection Range	PNEC	FoA	FoE	EoE	Risk
Bis-(2-ethylhexyl) Phthalate	Phthalate	4.9-7.8	-	0.10	-	-	0.10
Octylphenol diethoxylates (OP2EO)	Surfactant	1N.D.-14	36.9	0.07	0.03	0.00	0.10
TP1/Phosphoric acid, trihexyl ester	Phosphate	113-113	529	0.03	0.03	0.00	0.07
Dodecanedioic acid	Surfactant	1N.D.-10	464	0.03	0.03	0.00	0.07
Bethanidine	Pharmaceutical	1.5-1.5	27.6	0.03	0.03	0.00	0.07
Ethyl 3-(N-butylacetamido)propionate	PPP	0.4-2.1	248	0.07	0.00	0.00	0.07
Benzenesulfonamide, N,4-dimethyl-N-nitroso-	Ind. chemical	3.6-4	47.0	0.07	0.00	0.00	0.07
(3S-trans)-Hexahydro-3-isobutylpyrrolo[1,2-a]pyrazine-1,4-dione	Ind. chemical	88-190	207	0.07	0.00	0.00	0.07
TP1/1,4-Bis[(ethenyloxy)methyl]cyclohexane	Ind. chemical	9.1-15	-	0.07	-	-	0.07
TP1/Tert-butyl phenyl glycidyl ether	Dyes	18-18	-	0.03	-	-	0.03
Bis(2-ethylhexyl) Phosphate	Phosphate	31-31	43.7	0.03	0.00	0.00	0.03
GLYCERYL LINOLENATE	PCP	7.2-7.2	120	0.03	0.00	0.00	0.03
TP1/1-(2-Aminoethyl)piperazine	Ind. chemical	16-16	294	0.03	0.00	0.00	0.03
2-Propanol, 1,1'-[[3-(dimethylamino)propyl]imino]bis-	Ind. chemical	0.09-0.09	259	0.03	0.00	0.00	0.03
1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl-	Ind. chemical	1.3-1.3	38.0	0.03	0.00	0.00	0.03
reaction mass of isomers of: C7-9-alkyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	Ind. chemical	7.9-7.9	23.0	0.03	0.00	0.00	0.03
TP2/1-Propanamine, 3,3'-[1,4-butanediylbis(oxy)]bis-	Ind. chemical	0.04-0.04	-	0.03	-	-	0.03
isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	Dyes	-	188	0.00	0.00	0.00	0.00
Hexa(methoxymethyl)melamine	Plasticizer	-	0.84	0.00	0.00	0.00	0.00
Diethylene glycol monoisobutyl ether	Surfactant	-	2148	0.00	0.00	0.00	0.00
1-Eicosanol, Phosphate, compd. with 2,2'-iminobis[ethanol]	Surfactant	-	85.4	0.00	0.00	0.00	0.00
N,N-Dimethyldecylamine oxide	Surfactant	-	1046	0.00	0.00	0.00	0.00
3,6,9,12-Tetraoxatricosan-1-ol	Surfactant	-	6664	0.00	0.00	0.00	0.00
2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol	Surfactant	-	194	0.00	0.00	0.00	0.00
C14 Alkyl amine oxide	Surfactant	-	-	0.00	-	-	0.00
PEG Diethylhexanoate n10	Surfactant	-	-	0.00	-	-	0.00
Nonanedioic acid	Pharmaceutical	-	862	0.00	0.00	0.00	0.00
Tolazoline	Pharmaceutical	-	70.8	0.00	0.00	0.00	0.00
Ornithine	Pharmaceutical	-	274	0.00	0.00	0.00	0.00
Misoprostol	Pharmaceutical	-	923	0.00	0.00	0.00	0.00
PEMA (2-Phenyl-2-ethylmalonamid)	Pharmaceutical	-	71.9	0.00	0.00	0.00	0.00
Vernakalant	Pharmaceutical	-	439	0.00	0.00	0.00	0.00
Iloprost	Pharmaceutical	-	3351	0.00	0.00	0.00	0.00
Methyldopa	Pharmaceutical	-	405	0.00	0.00	0.00	0.00
isoprolol TP M1	Pharmaceutical	-	-	0.00	-	-	0.00
Hymexazol	PPP	-	71.7	0.00	0.00	0.00	0.00
RP 12913 (TP of Carbetamide)	PPP	-	21.6	0.00	0.00	0.00	0.00

Contaminant	Classification	Detection Range	PNEC	FoA	FoE	EoE	Risk
N-Butyl-1-butanamine	PPP	-	20.3	0.00	0.00	0.00	0.00
(Z)-1,1,1,4,4,4-Hexafluoro-2-butene	PFAS	-	103	0.00	0.00	0.00	0.00
N,N-Diethylethanolamine	Ind. chemical	-	229	0.00	0.00	0.00	0.00
Butyl acrylate	Ind. chemical	-	11.0	0.00	0.00	0.00	0.00
1-(2-Aminoethyl)piperazine	Ind. chemical	-	58.3	0.00	0.00	0.00	0.00
1H-Indole-3-methanamine, N,N-dimethyl-	Ind. chemical	-	30.9	0.00	0.00	0.00	0.00
2-Butenedioic acid (2Z)-, monobutyl ester	Ind. chemical	-	13.8	0.00	0.00	0.00	0.00
Diethylmethylbenzenediamine	Ind. chemical	-	-	0.00	-	-	0.00
TP1/2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	Ind. chemical	-	-	0.00	-	-	0.00

The detected compounds belong to the class of Industrial chemicals with a wide number of uses (n=26), surfactants (n=17), plasticizers (n=13), chemicals used in cosmetic products (PCPs; n=12), Pharmaceuticals (n=8), PPPs (n=8), dyes (n=7), phosphate esters (n=4) and phthalate esters (n=3). Compounds that were detected in all samples were the PCP 3a,4,5,6,7,7a-Hexahydro-4,7-methano-1H-inden-5-yl propionate and Pharmaceuticals Dacarbazine and 5'-Methylthioadenosine. High FoA (>90%) was observed for the PPPs 4,4-Dimethyl oxazolidine, CGA 353042, for the Industrial chemicals Trimethylolpropane trimethacrylate, Sodium hydroxy-methane sulfonate and 4-Morpholinecarboxaldehyde, for the plasticizers N-Methyl-2-pyrrolidone, 2-[2-(Dimethylamino)ethoxy]ethanol and Methacrylamide, for the PPP Musk and for the surfactant Pentanedioic acid, bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] ester. 44 compounds were detected in more than half of the samples, whereas rest of the compounds were detected sporadically.

The least contaminated samples were HELCOM PreEMPT 90 and 92 with cumulative concentrations of 3.26 and 2.76 µg/kg d.w., respectively. The sample with the highest number of detected individual compounds was HELCOM PreEMPT 83 (80 out of 99 suspect compounds detected in all samples). The most contaminated samples were HELCOM PreEMPT 76 and 67 with cumulative concentrations 422 and 289 µg/kg d.w., respectively.

Analysis of the 30 sediment samples revealed the presence of 44 compounds, which exceeded their ecotoxicological threshold value in at least one sample (**Table 33**).

The PCP 3a,4,5,6,7,7a-Hexahydro-4,7-methano-1H-inden-5-yl propionate exceeded its PNEC in all samples. High FoE (>0.97) was observed for the Industrial chemical 4-Morpholinecarboxaldehyde and the PPP 4,4-Dimethyl oxazolidine. 19 compounds exceeded their PNEC in ca. half of the samples. However, high EoE (≥0.5) was observed only for the plasticizer Bis(2-chloro-1-methylethyl) 2-

chloropropyl phosphate. A careful scrutiny of the ecotoxicological threshold values and further experimental toxicity evidence is suggested to support the outcomes of this risk assessment.

8.3.2 Suspect screening results of biota samples and risk assessment

123 contaminants were determined in the 64 tested biota samples (33 fish and 31 mussel samples). Detailed results are provided in the separately submitted DCTs. Data on the frequency of appearance and concentration ranges are included in **Table 34**. Risk assessment results are summarized in **Tables 35** and **36** for fish and mussels samples, respectively. Based on the available information about substances' main use, chemical class or application, their main use category was proposed, although some compounds may have multiple uses. For example, plasticizers and surfactants can be a subcategory of Industrial chemicals. However, in this report, we use the term Industrial chemicals to describe chemicals with possibly many uses and no clear main application. It might be worth noting that 76 out of 123 detected contaminants are registered in the ECHA database, which means that they are produced in or imported into EU in amounts of more than 1 ton per year. Some of the detected compounds are produced at very high tonnage band. For example, Isobutyric acid, monoester,2,2,4-, Trimethylpentane-1,3-diol and 1,3-Diphenylguanidine are produced in high annual tonnage (1,000-100,000 t/a). The risk associated with the exceedance of toxicity threshold values has been assessed by comparing the measured concentrations with the PNEC values from the NORMAN Ecotoxicology Database (https://www.norman-network.com/nds/ecotox/lowestPnecsIndex.php). For some compounds, PNECs were not available and, consequently, no risk assessment could be carried out for these compounds.

Table 34. Summary results of suspect screening analyses of the 33 fish and 31 mussels HELCOM PreEMPT samples. Concentrations are expressed in µg/kg wet weight.

NORMAN ID	Compound	Class	*Fish (n=33)*		*Mussels (n=31)*	
			Conc. Range	*%FoA*	*Conc. Range*	*%FoA*
NS00020126	2-Naphthylamine	Dyes	2-78	63.6	1.9-54	83.9
NS00014430	2H-1-Benzopyran-2-one, 7-amino-4-methyl-	Dyes	0.4-1.6	6.1	0.2-4	90.3
NS00014591	9,1N.D.-Phenanthrenedione	Dyes	0.01-0.08	51.5	0.001-0.02	6.5
NS00008484	Isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	Dyes	1.9-8.1	30.3	0.9-71	80.6
NS00004049	1-Ethenylazepan-2-one	Dyes	0.3-0.9	12.1	0.3-3.2	35.5
NS00003372	N,N-Diethylaniline	Dyes	0.1-0.1	3.0	0.01-12	64.5
NS00102069	TP1/tert-Butyl phenyl glycidyl ether	Dyes	7.5-29	93.9	2.1-42	96.8
NS00102071	TP3/tert-Butyl phenyl glycidyl ether	Dyes	-	0.0	4.5-18	22.6
NS00010726	Erucamide	Plasticizer	0.5-20	21.2	0.001-7.8	35.5
NS00009178	N-Methyl-2-pyrrolidone	Plasticizer	3.4-224	93.9	9.8-97	96.8
NS00011501	Decanedioic acid	Plasticizer	0.1-3.3	21.2	0.8-83	71.0
NS00003892	Methacrylamide	Plasticizer	33-34	6.1	15-250	93.5
NS00015186	Octanedioic acid	Plasticizer	0.5-25	48.5	0.7-205	96.8
NS00021348	Bis(2-chloro-1-methylethyl) 2-chloropropyl Phosphate	Plasticizer	0.1-18	42.4	0.2-0.7	35.5
NS00013580	Bis(2-ethylhexyl) decanedioate	Plasticizer	0.5-0.8	15.2	0.1-0.3	48.4
NS00011462	1,3-Diphenylguanidine	Plasticizer	1-12	18.2	0.7-1.6	6.5
NS00042428	2-Allyloxymethyl-2-ethylpropanediol	Plasticizer	0.007-7	75.8	0.8-12	96.8
NS00001756	2-[2-(Dimethylamino)ethoxy]ethanol	Plasticizer	0.4-12	36.4	0.5-1.7	16.1
NS00003249	Octadecanamide	Plasticizer	16-69	15.2	4.1-4.1	3.2
NS00002538	N-Vinyl-2-pyrrolidone	Plasticizer	0.2-2.1	57.6	0.1-7.8	51.6
NS00009863	Methylhexahydrophthalic anhydride	Plasticizer	0.3-1.9	36.4	0.06-4.6	87.1

NORMAN ID	Compound	Class	*Fish (n=33)*		*Mussels (n=31)*	
			Conc. Range	*%FoA*	*Conc. Range*	*%FoA*
NS00010296	Hexa(methoxymethyl)melamine	Plasticizer	-	0.0	0.2-1.7	6.5
NS00010915	Isobutyl hydrogen phthalate	Phthalate	0.7-23	24.2	0.3-158	61.3
NS00010914	Monoethyl phthalate	Phthalate	0.2-0.3	9.1	0.2-0.2	3.2
NS00010309	Bis-(2-ethylhexyl) phthalate	Phthalate	0.1-3.1	6.1	0.02-0.4	38.7
NS00002729	Tris(2-ethylhexyl) phosphate	Phosphate	0.4-65	18.2	0.2-15	51.6
NS00005874	Bis(2-ethylhexyl) phosphate	Phosphate	209-249	6.1	1N.D.-167	38.7
NS00103490	TP1/Phosphoric acid, trihexyl ester	Phosphate	5.8-22	18.2	3.1-14	12.9
NS00008724	Tris(4-methylphenyl) phosphate	Phosphate	-	0.0	-	0.0
NS00012545	3a,4,5,6,7,7a-Hexahydro-4,7-methano-1H-inden-5-yl propionate	PCP	1.2-1.7	6.1	0.4-10	100.0
NS00049705	Glycerol monomyristate	PCP	1.1-24	69.7	1.2-4.8	38.7
NS00011940	2-Propen-1-yl 2-(cyclohexyloxy)acetate	PCP	3.1-134	97.0	3.9-249	100.0
NS00024174	1,3-Dioxolane, 2,4-dimethyl-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-	PCP	1.3-4.4	45.5	0.05-7.7	93.5
NS00013704	Glyceryl linolenate	PCP	1.4-7.1	15.2	0.8-7.6	38.7
NS00001785	Tricyclodecanedimethanol	PCP	-	0.0	0.5-9.1	67.7
NS00010307	Acetyl tributyl citrate	PCP	0.2-0.2	3.0	0.1-1.2	54.8
NS00085085	Succinic acid, sodium adduct	PCP	0.03-0.4	9.1	0.1-1.7	61.3
NS00102046	Sodium levulinate	PCP	4.2-62	60.6	1.2-59	45.2
NS00012531	Musk	PCP	7.5-119	84.8	1.2-172	93.5
NS00103822	TP1/Hydroxycitronellal dimethyl acetal	PCP	5.5-8.3	15.2	1.7-43	38.7
NS00004841	Octinoxate	PCP	1.1-1.1	3.0	0.2-17	38.7
NS00010591	N,N-Bis(2-hydroxyethyl)dodecanamide	Surfactant	1.3-28	30.3	0.1-8.3	38.7
NS00001002	Pentaethylene glycol	Surfactant	28-29	6.1	27-27	3.2
NS00010129	Dodecanedioic acid	Surfactant	0.6-13	90.9	0.7-28	100.0
NS00021795	Diethylene glycol monoisobutyl ether	Surfactant	0.2-13	15.2	1-2.6	16.1

NORMAN ID	Compound	Class	*Fish (n=33)*		*Mussels (n=31)*	
			Conc. Range	*%FoA*	*Conc. Range*	*%FoA*
NS00014521	Tetradecane-7-sulfonic acid	Surfactant	1.4-22	27.3	0.08-2.5	22.6
NS00006554	Naphthalene-1-sulfonic acid	Surfactant	0.2-9.2	54.5	0.1-4.1	58.1
NS00082957	Stearic acid, compound with 2,2',2''-nitrilotriethanol (1:1)	Surfactant	-	0.0	0.06-0.06	3.2
NS00093005	1-Eicosanol, phosphate, compd. with 2,2'-iminobis[ethanol]	Surfactant	0.2-97	90.9	9-84	74.2
NS00101016	Octylphenol diethoxylates (OP2EO)	Surfactant	5.8-335	93.9	3.7-460	100.0
NS00005741	Miristalkonium	Surfactant	0.1-1.3	12.1	0.03-0.9	61.3
NS00006048	Cetylpyridinium	Surfactant	3.3-4	9.1	0.3-2.4	51.6
NS00102595	TP2/Pentanedioic acid, bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] ester	Surfactant	0.4-18	93.9	0.4-13	90.3
NS00000395	N,N-Dimethyldecylamine oxide	Surfactant	0.1-28	27.3	0.01-5.3	51.6
NS00076622	3,6,9,12-Tetraoxatricosan-1-ol	Surfactant	0.1-6.1	21.2	1.1-1.1	3.2
NS00009560	Tetradecylamine	Surfactant	0.04-16	39.4	0.5-39	22.6
NS00013706	2,3-Dihydroxypropyl pentadecanoate	Surfactant	0.5-3.2	69.7	0.2-0.8	22.6
NS00029504	N,N-Diethyldodecanamide	Surfactant	-	0.0	-	0.0
NS00076681	2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol	Surfactant	6.9-381	100.0	6.4-33	35.5
NS00006688	Stearic acid, monoester with glycerol	Surfactant	0.2-36	39.4	0.02-1.2	25.8
NS00095734	C14 Alkyl amine oxide	Surfactant	0.01-44	36.4	0.009-31	80.6
NS00076962	N-Hexyl-N-(3-phenylpropyl)hexan-1-amine	Surfactant	3.3-4	9.1	0.3-2.4	51.6
NS00007831	N-Dodecyl-4-methoxybenzamide	Surfactant	5.5-58	100.0	1-16	100.0
NS00017693	PEG Diethylhexanoate n10	Surfactant	0.1-0.1	3.0	0.06-0.06	3.2
NS00014247	Amines, C1N.D.-16-alkyldimethyl, N-oxides	Surfactant	0.6-0.6	3.0	0.2-0.9	58.1
NS00014568	5'-Methylthioadenosine	Pharmaceutical	4.3-123	97.0	0.3-48	77.4
NS00015142	Threonate	Pharmaceutical	16-391	100.0	2.1-183	100.0
NS00003762	Camphor	Pharmaceutical	13-54	24.2	1.8-81	83.9
NS00011498	Nonanedioic acid	Pharmaceutical	1.6-6.2	54.5	0.6-49	90.3

NORMAN ID	Compound	Class	*Fish (n=33)*		*Mussels (n=31)*	
			Conc. Range	*%FoA*	*Conc. Range*	*%FoA*
NS00003680	Tolazoline	Pharmaceutical	0.1-7	72.7	0.6-13	90.3
NS00013927	Ornithine	Pharmaceutical	-	0.0	0.1-1.3	58.1
NS00005889	Bethanidine	Pharmaceutical	4.1-53	45.5	1.2-6.4	32.3
NS00005831	Misoprostol	Pharmaceutical	2-386	100.0	7.8-123	100.0
NS00001939	Telbivudine	Pharmaceutical	0.08-5.1	81.8	0.6-194	100.0
NS00009497	PEMA (2-Phenyl-2-ethylmalonamid)	Pharmaceutical	1.3-40	90.9	0.7-11	45.2
NS00038039	Vernakalant	Pharmaceutical	-	0.0	12-248	64.5
NS00003686	Iloprost	Pharmaceutical	0.8-10	72.7	0.6-20	96.8
NS00009014	Dacarbazine	Pharmaceutical	0.6-0.8	6.1	0.08-1.1	58.1
NS00007484	Methyldopa	Pharmaceutical	8.7-8.7	3.0	2.3-81	48.4
NS00018321	Penicillic acid	Pharmaceutical	4-22	9.1	2.3-2.3	3.2
NS00050500	Hexaprofen	Pharmaceutical	-	0.0	0.03-0.2	22.6
NS00008248	Bisoprolol TP M1	Pharmaceutical	0.5-0.5	3.0	0.1-2.1	19.4
NS00000458	N-(2,4-Dimethylphenyl)formamide	PPP	1.9-190	12.1	0.3-47	71.0
NS00014858	Jasmonic acid	PPP	0.4-1.6	27.3	0.6-4.8	67.7
NS00000983	3-Pyridinol	PPP	0.8-2.4	39.4	0.5-36	90.3
NS00004518	Hymexazol	PPP	0.001-0.001	3.0	0.03-0.09	16.1
NS00008005	Ethyl 3-(N-butylacetamido)propionate	PPP	0.8-343	81.8	0.88-219	93.5
NS00010285	4,4-Dimethyl oxazolidine	PPP	2.5-100	97.0	3.1-96	100.0
NS00002145	Hexa-2,4-dienoic acid	PPP	18-45	30.3	9.2-156	77.4
NS00001813	Piperonal	PPP	0.01-0.7	9.1	0.01-4.5	90.3
NS00067187	RP 12913 (TP of Carbetamide)	PPP	-	0.0	0.1-3.6	64.5
NS00014277	CGA 353042	PPP	-	0.0	-	0.0
NS00004620	N-Butyl-1-butanamine	PPP	3.7-97	57.6	1.1-33	22.6

NORMAN ID	Compound	Class	*Fish (n=33)*		*Mussels (n=31)*	
			Conc. Range	*%FoA*	*Conc. Range*	*%FoA*
NS00006736	4-tert-Butylbenzoic acid	Ind. chemical	16-86	27.3	5.6-125	87.1
NS00036313	Benzoic acid, 4-(1,1-dimethylethyl)-, 1-methylethyl ester	Ind. chemical	2-2.5	6.1	0.5-3.4	74.2
NS00009029	3-Methylbenzoic acid	Ind. chemical	3.3-9.9	15.2	0.01-30	96.8
NS00013936	Benzoic acid, 4-methoxy-	Ind. chemical	25-25	3.0	1N.D.-46	32.3
NS00000641	Benzenesulfonamide, N,4-dimethyl-N-nitroso-	Ind. chemical	-	0.0	0.02-0.9	22.6
NS00009350	(Z)-1,1,1,4,4,4-Hexafluoro-2-butene	PFAS	0.002-0.09	54.5	0.003-0.03	12.9
NS00005138	N,N-Dimethylformamide	Ind. chemical	1.9-11	39.4	0.1-1.5	38.7
NS00006944	4-Morpholinecarboxaldehyde	Ind. chemical	0.1-3.6	42.4	0.3-6	48.4
NS00005690	1-Butanol, 3-methoxy-3-methyl-, acetate	Ind. chemical	7.4-21	100.0	1.9-80	100.0
NS00001272	Cyclohexylamine	Ind. chemical	0.9-0.9	3.0	0.08-2.4	41.9
NS00006343	N,N-Diethylethanolamine	Ind. chemical	4.3-36	36.4	0.4-18	35.5
NS00001643	1,3-Benzenedimethanamine	Ind. chemical	0.6-29	97.0	0.3-17	96.8
NS00102251	TP3/Trimethylolpropane trimethacrylate	Ind. chemical	0.3-61	45.5	0.4-157	71.0
NS00007563	Butyl acrylate	Ind. chemical	13-131	100.0	5-38	93.5
NS00002293	Glycine, N-(1-oxooctyl)-	Ind. chemical	0.4-13	12.1	0.2-1.5	80.6
NS00014059	Sodium hydroxy- methane sulfonate	Ind. chemical	-	0.0	-	0.0
NS00004675	1-(2-Aminoethyl)piperazine	Ind. chemical	2.2-7.3	6.1	1.1-3.3	51.6
NS00102783	TP1/1-(2-Aminoethyl)piperazine	Ind. chemical	4.7-20	30.3	2.7-10	25.8
NS00009588	2-Propanol, 1,1'-[[3-(dimethylamino)propyl]imino]bis-	Ind. chemical	0.007-0.04	51.5	0.1-0.1	6.5
NS00103201	TP1/2,4,6-Trimethylbenzaldehyde	Ind. chemical	0.9-3.4	18.2	0.2-3.8	96.8
NS00036915	1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl-	Ind. chemical	0.5-116	90.9	0.4-51	90.3
NS00049404	(3S-trans)-Hexahydro-3-isobutylpyrrolo[1,2-a]pyrazine-1,4-dione	Ind. chemical	3.6-51	60.6	3.4-78	48.4
NS00002849	reaction mass of isomers of: C7-9-alkyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	Ind. chemical	0.9-6.1	18.2	-	0.0

NORMAN ID	Compound	Class	*Fish (n=33)*		*Mussels (n=31)*	
			Conc. Range	*%FoA*	*Conc. Range*	*%FoA*
NS00039200	1H-Indole-3-methanamine, N,N-dimethyl-	Ind. chemical	0.3-5.7	33.3	1.2-1.2	3.2
NS00011457	1-(2-Hydroxyethyl)-2,2,6,6-tetramethyl-4-piperidinol	Ind. chemical	0.02-0.7	12.1	0.02-0.5	6.5
NS00102695	TP1/Dimethyl succinate	Ind. chemical	3.2-135	93.9	0.7-179	93.5
NS00009935	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	Ind. chemical	1.8-171	72.7	0.81-180	93.5
NS00002295	2-Butenedioic acid (2Z)-, monobutyl ester	Ind. chemical	-	0.0	5.4-61	54.8
NS00048813	2,2,6,6-Tetramethyl-4-oxopiperidinooxy	Ind. chemical	-	0.0	-	0.0
NS00102776	TP2/1-Propanamine, 3,3'-[1,4-butanediylbis(oxy)]bis-	Ind. chemical	0.003-0.06	57.6	0.002-1	100.0
NS00102956	TP1/1,4-Bis[(ethenyloxy)methyl]cyclohexane	Ind. chemical	2.6-67	87.9	2.5-278	96.8
NS00061419	Diethylmethylbenzenediamine	Ind. chemical	1.5-4.2	36.4	0.8-10	74.2
NS00104163	TP1/2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	Ind. chemical	0.5-30	48.5	0.2-0.4	9.7
NS00103199	TP1/Isophorone	Ind. chemical	2.9-9.2	54.5	1.1-26	87.1

112 compounds were determined by the suspect screening in the 33 tested fish samples. Most of the detected compounds (29 out of 112) belonged to the class of Industrial chemicals, which are compounds with a wide variety of applications. Other important categories were surfactants (22 out of 112), Pharmaceuticals (14 out 112 compounds), plasticizers (13 out of 112 compounds), PCPs (11 out of 112 compounds), PPPs (9 out of 112 compounds), dyes (7 out of 112 compounds) phosphate esters (3 out of 112 compounds), phthalate esters (3 out of 112 compounds) and PFAS (1 out of 112 compounds). The following compounds were detected in all fish samples: Industrial chemicals Butyl acrylate and 1-Butanol, 3-methoxy-3-methyl-, acetate, surfactants N-Dodecyl-4-methoxybenzamide and 2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol and the Pharmaceuticals Misoprostol and Threonate. Regarding FoE, the Industrial chemical Butyl acrylate and the surfactant 2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol exceeded their PNECs in all samples. Pharmaceuticals Misoprostol and 5'-Methylthioadenosine exceeded PNEC in 97% of the samples. The analysis of 33 fish samples revealed the presence of 57 compounds, which exceeded their ecotoxicological threshold value in at least one sample (**Table 35**).; 16 of them exceeded the PNEC in more than half of the samples.

Table 35. Ranking of the detected contaminants in fish samples based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in μg/kg wet weight.

Contaminant	Classification	PNEC	FoA	FoE	EoE	Risk
5'-Methylthioadenosine	Pharmaceutical	0.07	0.97	0.97	1.00	2.94
Butyl acrylate	Ind. chemical	0.98	1.00	1.00	0.50	2.50
1-Eicosanol, phosphate, compd. with 2,2'-iminobis[ethanol]	Surfactant	0.21	0.91	0.88	0.50	2.29
2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol	Surfactant	6.27	1.00	1.00	0.20	2.20
Misoprostol	Pharmaceutical	5.61	1.00	0.97	0.20	2.17
Octylphenol diethoxylates (OP2EO)	Surfactant	8.36	0.94	0.88	0.20	2.02
PEMA (2-Phenyl-2-ethylmalonamid)	Pharmaceutical	1.38	0.91	0.88	0.20	1.99
N-Methyl-2-pyrrolidone	Plasticizer	11.5	0.94	0.82	0.20	1.96
1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl-	Ind. chemical	1.32	0.91	0.79	0.20	1.90
1-Butanol, 3-methoxy-3-methyl-, acetate	Ind. chemical	9.78	1.00	0.76	0.10	1.86
Threonate	Pharmaceutical	97.1	1.00	0.70	0.10	1.80
2-Propen-1-yl 2-(cyclohexyloxy)acetate	PCP	7.34	0.97	0.58	0.20	1.75
4,4-Dimethyl oxazolidine	PPP	18.3	0.97	0.48	0.10	1.55
1,3-Benzenedimethanamine	Ind. chemical	6.59	0.97	0.45	0.10	1.52
Ethyl 3-(N-butylacetamido)propionate	PPP	10.2	0.82	0.48	0.20	1.50
2-Naphthylamine	Dyes	2.49	0.64	0.58	0.20	1.41
Musk	PCP	15.5	0.85	0.45	0.10	1.40

Contaminant	Classification	PNEC	FoA	FoE	EoE	Risk
3,5-Di-tert-butyl-4-hydroxybenzaldehyde	Ind. chemical	27.9	0.73	0.55	0.10	1.37
Bis(2-chloro-1-methylethyl) 2-chloropropyl phosphate	Plasticizer	0.02	0.42	0.42	0.50	1.35
N-Butyl-1-butanamine	PPP	8.36	0.58	0.55	0.20	1.32
Telbivudine	Pharmaceutical	1.79	0.82	0.39	0.10	1.31
(3S-trans)-Hexahydro-3-isobutylpyrrolo[1,2-a]pyrazine-1,4-dione	Ind. chemical	5.72	0.61	0.58	0.10	1.28
Dodecanedioic acid	Surfactant	6.49	0.91	0.27	0.10	1.28
Glycerol monomyristate	PCP	4.67	0.70	0.42	0.10	1.22
TP1/Dimethyl succinate	Ind. chemical	15.4	0.94	0.18	0.10	1.22
Tolazoline	Pharmaceutical	4.19	0.73	0.30	0.10	1.13
Bis(2-ethylhexyl) phosphate	Phosphate	0.23	0.06	0.06	1.00	1.12
Bethanidine	Pharmaceutical	4.79	0.45	0.36	0.20	1.02
N-Dodecyl-4-methoxybenzamide	Surfactant	-	1.00	-	-	1.00
Iloprost	Pharmaceutical	5.12	0.73	0.15	0.10	0.98
TP1/tert-Butyl phenyl glycidyl ether	Dyes	-	0.94	-	-	0.94
TP2/Pentanedioic acid, bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] ester	Surfactant	36.4	0.94	0.00	0.00	0.94
Erucamide	Plasticizer	0.11	0.21	0.21	0.50	0.92
TP1/1,4-Bis[(ethenyloxy)methyl]cyclohexane	Ind. chemical	-	0.88	-	-	0.88
Stearic acid, monoester with glycerol	Surfactant	1.22	0.39	0.27	0.20	0.87
Tris(2-ethylhexyl) phosphate	Phosphate	0.19	0.18	0.18	0.50	0.86
Hexa-2,4-dienoic acid	PPP	2.70	0.30	0.30	0.20	0.81
Octadecanamide	Plasticizer	0.57	0.15	0.15	0.50	0.80
2-Allyloxymethyl-2-ethylpropanediol	Plasticizer	35.1	0.76	0.00	0.00	0.76
4-tert-Butylbenzoic acid	Ind. chemical	2.49	0.27	0.27	0.20	0.75
Tetradecane-7-sulfonic acid	Surfactant	2.04	0.27	0.24	0.20	0.72
2,3-Dihydroxypropyl pentadecanoate	Surfactant	7.69	0.70	0.00	0.00	0.70
Octanedioic acid	Plasticizer	22.6	0.48	0.06	0.10	0.65
Isobutyl hydrogen phthalate	Phthalate	0.92	0.24	0.18	0.20	0.62
Sodium levulinate	PCP	75.7	0.61	0.00	0.00	0.61
N,N-Diethylethanolamine	Ind. chemical	14.4	0.36	0.12	0.10	0.58
N-Vinyl-2-pyrrolidone	Plasticizer	12.9	0.58	0.00	0.00	0.58
TP2/1-Propanamine, 3,3'-[1,4-butanediylbis(oxy)]bis-	Ind. chemical	-	0.58	-	-	0.58
Camphor	Pharmaceutical	13.4	0.24	0.21	0.10	0.55
Naphthalene-1-sulfonic acid	Surfactant	16.2	0.55	0.00	0.00	0.55
Nonanedioic acid	Pharmaceutical	13.6	0.55	0.00	0.00	0.55
(Z)-1,1,1,4,4,4-Hexafluoro-2-butene	PFAS	23.6	0.55	0.00	0.00	0.55
TP1/Isophorone	Ind. chemical	-	0.55	-	-	0.55
N,N-Bis(2-hydroxyethyl)dodecanamide	Surfactant	3.43	0.30	0.12	0.10	0.52
Tetradecylamine	Surfactant	7.57	0.39	0.03	0.10	0.52
9,1N.D.-Phenanthrenedione	Dyes	2.48	0.52	0.00	0.00	0.52
2-Propanol, 1,1'-[[3-(dimethylamino)propyl]imino]bis-	Ind. chemical	15.3	0.52	0.00	0.00	0.52

Contaminant	Classification	PNEC	FoA	FoE	EoE	Risk
1H-Indole-3-methanamine, N,N-dimethyl-	Ind. chemical	3.81	0.33	0.06	0.10	0.49
TP1/2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	Ind. chemical	-	0.48	-	-	0.48
1,3-Dioxolane, 2,4-dimethyl-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-	PCP	25.5	0.45	0.00	0.00	0.45
TP3/Trimethylolpropane trimethacrylate	Ind. chemical	110.06	0.45	0.00	0.00	0.45
reaction mass of isomers of: C7-9-alkyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	Ind. chemical	0.99	0.18	0.15	0.10	0.43
4-Morpholinecarboxaldehyde	Ind. chemical	4.72	0.42	0.00	0.00	0.42
Bis(2-ethylhexyl) decanedioate	Plasticizer	0.11	0.15	0.15	0.10	0.40
1,3-Diphenylguanidine	Plasticizer	2.09	0.18	0.12	0.10	0.40
N,N-Dimethyldecylamine oxide	Surfactant	17.6	0.27	0.03	0.10	0.40
3-Pyridinol	PPP	21.2	0.39	0.00	0.00	0.39
N,N-Dimethylformamide	Ind. chemical	18111	0.39	0.00	0.00	0.39
2-[2-(Dimethylamino)ethoxy]ethanol	Plasticizer	26.7	0.36	0.00	0.00	0.36
Methylhexahydrophthalic anhydride	Plasticizer	31.0	0.36	0.00	0.00	0.36
C14 Alkyl amine oxide	Surfactant	-	0.36	-	-	0.36
Diethylmethylbenzenediamine	Ind. chemical	-	0.36	-	-	0.36
N-(2,4-Dimethylphenyl)formamide	PPP	8.09	0.12	0.03	0.20	0.35
TP1/Phosphoric acid, trihexyl ester	Phosphate	17.6	0.18	0.03	0.10	0.31
isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	Dyes	61.3	0.30	0.00	0.00	0.30
TP1/1-(2-Aminoethyl)piperazine	Ind. chemical	26.0	0.30	0.00	0.00	0.30
Cetylpyridinium	Surfactant	1.19	0.09	0.09	0.10	0.28
Penicillic acid	Pharmaceutical	2.26	0.09	0.09	0.10	0.28
Jasmonic acid	PPP	4.03	0.27	0.00	0.00	0.27
Glycine, N-(1-oxooctyl)-	Ind. chemical	3.39	0.12	0.03	0.10	0.25
Methacrylamide	Plasticizer	15.4	0.06	0.06	0.10	0.22
Pentaethylene glycol	Surfactant	21.1	0.06	0.06	0.10	0.22
Dacarbazine	Pharmaceutical	0.51	0.06	0.06	0.10	0.22
Decanedioic acid	Plasticizer	13.2	0.21	0.00	0.00	0.21
3,6,9,12-Tetraoxatricosan-1-ol	Surfactant	34.6	0.21	0.00	0.00	0.21
1-(2-Aminoethyl)piperazine	Ind. chemical	2.94	0.06	0.03	0.10	0.19
TP1/2,4,6-Trimethylbenzaldehyde	Ind. chemical	4.50	0.18	0.00	0.00	0.18
Benzoic acid, 4-methoxy-	Ind. chemical	21.3	0.03	0.03	0.10	0.16
Glyceryl linolenate	PCP	7.46	0.15	0.00	0.00	0.15
TP1/Hydroxycitronellal dimethyl acetal	PCP	-	0.15	-	-	0.15
Diethylene glycol monoisobutyl ether	Surfactant	240	0.15	0.00	0.00	0.15
3-Methylbenzoic acid	Ind. chemical	12.9	0.15	0.00	0.00	0.15
1-Ethenylazepan-2-one	Dyes	18.7	0.12	0.00	0.00	0.12
Miristalkonium	Surfactant	2.17	0.12	0.00	0.00	0.12
1-(2-Hydroxyethyl)-2,2,6,6-tetramethyl-4-piperidinol	Ind. chemical	16.4	0.12	0.00	0.00	0.12
Monoethyl phthalate	Phthalate	1.33	0.09	0.00	0.00	0.09
Succinic acid, sodium adduct	PCP	12.7	0.09	0.00	0.00	0.09

Contaminant	Classification	PNEC	FoA	FoE	EoE	Risk
N-Hexyl-N-(3-phenylpropyl)hexan-1-amine	Surfactant	-	0.09	-	-	0.09
Piperonal	PPP	7.67	0.09	0.00	0.00	0.09
2H-1-Benzopyran-2-one, 7-amino-4-methyl-	Dyes	9.05	0.06	0.00	0.00	0.06
Bis-(2-ethylhexyl) phthalate	Phthalate	-	0.06	-	-	0.06
3a,4,5,6,7,7a-Hexahydro-4,7-methano-1H-inden-5-yl propionate	PCP	38.1	0.06	0.00	0.00	0.06
Benzoic acid, 4-(1,1-dimethylethyl)-, 1-methylethyl ester	Ind. chemical	16.3	0.06	0.00	0.00	0.06
N,N-Diethylaniline	Dyes	50.8	0.03	0.00	0.00	0.03
Acetyl tributyl citrate	PCP	2.24	0.03	0.00	0.00	0.03
Octinoxate	PCP	295	0.03	0.00	0.00	0.03
PEG Diethylhexanoate n10	Surfactant	-	0.03	-	-	0.03
Amines, C1N.D.-16-alkyldimethyl, N-oxides	Surfactant	1362	0.03	0.00	0.00	0.03
Methyldopa	Pharmaceutical	18.4	0.03	0.00	0.00	0.03
Bisoprolol TP M1	Pharmaceutical	-	0.03	-	-	0.03
Hymexazol	PPP	5.00	0.03	0.00	0.00	0.03
Cyclohexylamine	Ind. chemical	15.5	0.03	0.00	0.00	0.03
TP3/tert-Butyl phenyl glycidyl ether	Dyes	-	0.00	-	-	0.00
Hexa(methoxymethyl)melamine	Plasticizer	0.02	0.00	0.00	0.00	0.00
Tris(4-methylphenyl) phosphate	Phosphate	3.56	0.00	0.00	0.00	0.00
Tricyclodecanedimethanol	PCP	62.8	0.00	0.00	0.00	0.00
Stearic acid, compound with 2,2',2''-nitrilotriethanol (1:1)	Surfactant	5.31	0.00	0.00	0.00	0.00
N,N-Diethyldodecanamide	Surfactant	6.89	0.00	0.00	0.00	0.00
Ornithine	Pharmaceutical	36.6	0.00	0.00	0.00	0.00
Vernakalant	Pharmaceutical	10.5	0.00	0.00	0.00	0.00
Hexaprofen	Pharmaceutical	-	0.00	-	-	0.00
RP 12913 (TP of Carbetamide)	PPP	1.41	0.00	0.00	0.00	0.00
CGA 353042	PPP	-	0.00	-	-	0.00
Benzenesulfonamide, N,4-dimethyl-N-nitroso-	Ind. chemical	8.67	0.00	0.00	0.00	0.00
Sodium hydroxy- methane sulfonate	Ind. chemical	52.9	0.00	0.00	0.00	0.00
2-Butenedioic acid (2Z)-, monobutyl ester	Ind. chemical	2.11	0.00	0.00	0.00	0.00
2,2,6,6-Tetramethyl-4-oxopiperidinooxy	Ind. chemical	111	0.00	0.00	0.00	0.00

Regarding the mussels samples, 121 compounds were detected by the suspect screening. The most populous category of compounds was Industrial chemicals (30 out of 121 compounds) followed by surfactants (23 out of 121 compounds). Other important categories of compounds were Pharmaceuticals (17 out of 121 compounds), plasticizers (14 out of 121 compounds), PCPs (12 out of 121 compounds) and PPPs (10 out of 121 compounds. The remaining categories of compounds were dyes (8 out of 121 compounds), phthalates (3 out of 121 compounds) and PFAS (1 out of 121 compounds).

The analysis of 31 blue mussel samples revealed the presence of 83 compounds, which exceeded their ecotoxicological threshold value in at least one sample (**Table 36**). The following compounds exceeded PNEC in all samples: PCP 2-Propen-1-yl 2-(cyclohexyloxy)acetate, surfactant Octylphenol diethoxylates (OP2EO) and Pharmaceuticals Misoprostol and Telbivudine. All of them with the exception of Misoprostol had the value of EoE 0.5. The highest EoE (EoE: 1.0) was observed for the Pharmaceutical 5'-Methylthioadenosine, surfactant 1-Eicosanol, phosphate (compound with 2,2'-iminobis[ethanol]) and the phosphate Bis(2-ethylhexyl) phosphate. A careful scrutiny of the ecotoxicological threshold values and further experimental toxicity evidence is suggested to support the outcomes of this risk assessment.

Table 36. Ranking of the detected contaminants in mussels samples based on their final score (Sum of FoA+EoE+FoE). Concentrations are expressed in μg/kg wet weight.

Contaminant	Classification	PNEC	FoA	FoE	EoE	Risk
5'-Methylthioadenosine	Pharmaceutical	0.02	0.77	0.77	1.00	2.55
2-Propen-1-yl 2-(cyclohexyloxy)acetate	PCP	1.84	1.00	1.00	0.50	2.50
Octylphenol diethoxylates (OP2EO)	Surfactant	2.09	1.00	1.00	0.50	2.50
Telbivudine	Pharmaceutical	0.45	1.00	1.00	0.50	2.50
1-Eicosanol, phosphate, compd. with 2,2'-iminobis[ethanol]	Surfactant	0.05	0.74	0.74	1.00	2.48
Butyl acrylate	Ind. chemical	0.25	0.94	0.94	0.50	2.37
1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl-	Ind. chemical	0.33	0.90	0.90	0.50	2.31
4-tert-Butylbenzoic acid	Ind. chemical	0.62	0.87	0.87	0.50	2.24
Misoprostol	Pharmaceutical	1.40	1.00	1.00	0.20	2.20
4,4-Dimethyl oxazolidine	PPP	4.58	1.00	0.97	0.20	2.17
N-Methyl-2-pyrrolidone	Plasticizer	2.87	0.97	0.97	0.20	2.14
1-Butanol, 3-methoxy-3-methyl-, acetate	Ind. chemical	2.45	1.00	0.94	0.20	2.14
Methacrylamide	Plasticizer	3.85	0.94	0.94	0.20	2.07
Hexa-2,4-dienoic acid	PPP	0.67	0.77	0.77	0.50	2.05
Tolazoline	Pharmaceutical	1.05	0.90	0.87	0.20	1.97
Dodecanedioic acid	Surfactant	1.62	1.00	0.74	0.20	1.94

Iloprost	Pharmaceutical	1.28	0.97	0.77	0.20	1.94
3,5-Di-tert-butyl-4-hydroxybenzaldehyde	Ind. chemical	6.97	0.94	0.81	0.20	1.94
Octanedioic acid	Plasticizer	5.65	0.97	0.74	0.20	1.91
Musk	PCP	3.88	0.94	0.77	0.20	1.91
Ethyl 3-(N-butylacetamido)propionate	PPP	2.56	0.94	0.77	0.20	1.91
2-Naphthylamine	Dyes	0.62	0.84	0.84	0.20	1.88
1,3-Benzenedimethanamine	Ind. chemical	1.65	0.97	0.71	0.20	1.88
TP1/Dimethyl succinate	Ind. chemical	3.85	0.94	0.74	0.20	1.88
Threonate	Pharmaceutical	24.3	1.00	0.74	0.10	1.84
3-Methylbenzoic acid	Ind. chemical	3.24	0.97	0.77	0.10	1.84
Camphor	Pharmaceutical	3.36	0.84	0.77	0.20	1.81
Bis(2-ethylhexyl) Phosphate	Phosphate	0.06	0.39	0.39	1.00	1.77
Isobutyl hydrogen phthalate	Phthalate	0.23	0.61	0.61	0.50	1.73
TP1/2,4,6-Trimethylbenzaldehyde	Ind. chemical	1.13	0.97	0.65	0.10	1.71
Nonanedioic acid	Pharmaceutical	3.39	0.90	0.58	0.20	1.68
2-Butenedioic acid (2Z)-, monobutyl ester	Ind. chemical	0.53	0.55	0.55	0.50	1.60
Tris(2-ethylhexyl) phosphate	Phosphate	0.05	0.52	0.52	0.50	1.53
Vernakalant	Pharmaceutical	2.62	0.65	0.65	0.20	1.49
N-(2,4-Dimethylphenyl)formamide	PPP	2.02	0.71	0.52	0.20	1.43
Decanedioic acid	Plasticizer	3.29	0.71	0.48	0.20	1.39
3-Pyridinol	PPP	5.30	0.90	0.39	0.10	1.39
RP 12913 (TP of Carbetamide)	PPP	0.35	0.65	0.45	0.20	1.30
2-Allyloxymethyl-2-ethylpropanediol	Plasticizer	8.77	0.97	0.23	0.10	1.29
Dacarbazine	Pharmaceutical	0.13	0.58	0.55	0.10	1.23
Bis(2-chloro-1-methylethyl) 2-chloropropyl phosphate	Plasticizer	0.01	0.35	0.35	0.50	1.21
2H-1-Benzopyran-2-one, 7-amino-4-methyl-	Dyes	2.26	0.90	0.19	0.10	1.20
Bis(2-ethylhexyl) decanedioate	Plasticizer	0.03	0.48	0.48	0.20	1.17
(3S-trans)-Hexahydro-3-isobutylpyrrolo[1,2-a]pyrazine-1,4-dione	Ind. chemical	1.43	0.48	0.48	0.20	1.17
TP2/Pentanedioic acid, bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] ester	Surfactant	9.10	0.90	0.16	0.10	1.16
Jasmonic acid	PPP	1.01	0.68	0.39	0.10	1.16
Piperonal	PPP	1.92	0.90	0.16	0.10	1.16
Glycine, N-(1-oxooctyl)-	Ind. chemical	0.85	0.81	0.26	0.10	1.16
Erucamide	Plasticizer	0.03	0.35	0.29	0.50	1.15
Methyldopa	Pharmaceutical	4.61	0.48	0.45	0.20	1.14
3a,4,5,6,7,7a-Hexahydro-4,7-methano-1H-inden-5-yl propionate	PCP	9.54	1.00	0.03	0.10	1.13
Cetylpyridinium	Surfactant	0.30	0.52	0.52	0.10	1.13
1-(2-Aminoethyl)piperazine	Ind. chemical	0.73	0.52	0.52	0.10	1.13
PEMA (2-Phenyl-2-ethylmalonamid)	Pharmaceutical	0.34	0.45	0.45	0.20	1.10
1,3-Dioxolane, 2,4-dimethyl-2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-	PCP	6.39	0.94	0.03	0.10	1.07
isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	Dyes	15.3	0.81	0.13	0.10	1.04

N-Dodecyl-4-methoxybenzamide	Surfactant	-	1.00	-	-	1.00
TP2/1-Propanamine, 3,3'-[1,4-butanediylbis(oxy)]bis-	Ind. chemical	-	1.00	-	-	1.00
TP1/tert-Butyl phenyl glycidyl ether	Dyes	-	0.97	-	-	0.97
TP1/1,4-Bis[(ethenyloxy)methyl]cyclohexane	Ind. chemical	-	0.97	-	-	0.97
2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol	Surfactant	1.57	0.35	0.35	0.20	0.91
TP3/Trimethylolpropane trimethacrylate	Ind. chemical	27.5	0.71	0.10	0.10	0.91
Glycerol monomyristate	PCP	1.17	0.39	0.39	0.10	0.87
Acetyl tributyl citrate	PCP	0.56	0.55	0.23	0.10	0.87
Methylhexahydrophthalic anhydride	Plasticizer	7.75	0.87	0.00	0.00	0.87
TP1/Isophorone	Ind. chemical	-	0.87	-	-	0.87
N,N-Bis(2-hydroxyethyl)dodecanamide	Surfactant	0.86	0.39	0.32	0.10	0.81
C14 Alkyl amine oxide	Surfactant	-	0.81	-	-	0.81
Glyceryl linolenate	PCP	1.87	0.39	0.29	0.10	0.78
N-Vinyl-2-pyrrolidone	Plasticizer	3.22	0.52	0.13	0.10	0.75
Miristalkonium	Surfactant	0.54	0.61	0.03	0.10	0.75
Bethanidine	Pharmaceutical	1.20	0.32	0.32	0.10	0.75
Benzoic acid, 4-methoxy-	Ind. chemical	5.32	0.32	0.32	0.10	0.75
4-Morpholinecarboxaldehyde	Ind. chemical	1.18	0.48	0.16	0.10	0.75
Benzoic acid, 4-(1,1-dimethylethyl)-, 1-methylethyl ester	Ind. chemical	4.08	0.74	0.00	0.00	0.74
Diethylmethylbenzenediamine	Ind. chemical	-	0.74	-	-	0.74
Naphthalene-1-sulfonic acid	Surfactant	4.06	0.58	0.03	0.10	0.71
Tricyclodecanedimethanol	PCP	15.7	0.68	0.00	0.00	0.68
Sodium levulinate	PCP	18.9	0.45	0.10	0.10	0.65
N,N-Dimethyldecylamine oxide	Surfactant	4.39	0.52	0.03	0.10	0.65
N,N-Diethylaniline	Dyes	12.7	0.65	0.00	0.00	0.65
Hexa(methoxymethyl)melamine	Plasticizer	0.00	0.06	0.06	0.50	0.63
Tetradecylamine	Surfactant	1.89	0.23	0.19	0.20	0.62
N-Butyl-1-butanamine	PPP	2.09	0.23	0.19	0.20	0.62
N,N-Diethylethanolamine	Ind. chemical	3.60	0.35	0.16	0.10	0.62
Succinic acid, sodium adduct	PCP	3.17	0.61	0.00	0.00	0.61
Amines, C1N.D.-16-alkyldimethyl, N-oxides	Surfactant	341	0.58	0.00	0.00	0.58
Ornithine	Pharmaceutical	9.16	0.58	0.00	0.00	0.58
Tetradecane-7-sulfonic acid	Surfactant	0.51	0.23	0.19	0.10	0.52
N-Hexyl-N-(3-phenylpropyl)hexan-1-amine	Surfactant	-	0.52	-	-	0.52
Stearic acid, monoester with glycerol	Surfactant	0.30	0.26	0.10	0.10	0.45
TP1/1-(2-Aminoethyl)piperazine	Ind. chemical	6.49	0.26	0.10	0.10	0.45
Cyclohexylamine	Ind. chemical	3.88	0.42	0.00	0.00	0.42
Bis-(2-ethylhexyl) Phthalate	Phthalate	-	0.39	-	-	0.39
TP1/Hydroxycitronellal dimethyl acetal	PCP	-	0.39	-	-	0.39
Octinoxate	PCP	73.7	0.39	0.00	0.00	0.39
N,N-Dimethylformamide	Ind. chemical	4528	0.39	0.00	0.00	0.39
1-Ethenylazepan-2-one	Dyes	4.68	0.35	0.00	0.00	0.35

Octadecanamide	Plasticizer	0.14	0.03	0.03	0.20	0.26
TP1/Phosphoric acid, trihexyl ester	Phosphate	4.41	0.13	0.03	0.10	0.26
1,3-Diphenylguanidine	Plasticizer	0.52	0.06	0.06	0.10	0.23
TP3/tert-Butyl phenyl glycidyl ether	Dyes	-	0.23	-	-	0.23
2,3-Dihydroxypropyl pentadecanoate	Surfactant	1.92	0.23	0.00	0.00	0.23
Hexaprofen	Pharmaceutical	-	0.23	-	-	0.23
Benzenesulfonamide, N,4-dimethyl-N-nitroso-	Ind. chemical	2.17	0.23	0.00	0.00	0.23
Bisoprolol TP M1	Pharmaceutical	-	0.19	-	-	0.19
Pentaethylene glycol	Surfactant	5.26	0.03	0.03	0.10	0.16
Penicillic acid	Pharmaceutical	0.56	0.03	0.03	0.10	0.16
1H-Indole-3-methanamine, N,N-dimethyl-	Ind. chemical	0.95	0.03	0.03	0.10	0.16
2-[2-(Dimethylamino)ethoxy]ethanol	Plasticizer	6.68	0.16	0.00	0.00	0.16
Diethylene glycol monoisobutyl ether	Surfactant	60.0	0.16	0.00	0.00	0.16
Hymexazol	PPP	1.25	0.16	0.00	0.00	0.16
(Z)-1,1,1,4,4,4-Hexafluoro-2-butene	PFAS	5.90	0.13	0.00	0.00	0.13
TP1/2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	Ind. chemical	-	0.10	-	-	0.10
9,1N.D.-Phenanthrenedione	Dyes	0.62	0.06	0.00	0.00	0.06
2-Propanol, 1,1'-[[3-(dimethylamino)propyl]imino]bis-	Ind. chemical	3.83	0.06	0.00	0.00	0.06
1-(2-Hydroxyethyl)-2,2,6,6-tetramethyl-4-piperidinol	Ind. chemical	4.10	0.06	0.00	0.00	0.06
Monoethyl Phthalate	Phthalate	0.33	0.03	0.00	0.00	0.03
Stearic acid, compound with 2,2',2''-nitrilotriethanol (1:1)	Surfactant	1.33	0.03	0.00	0.00	0.03
3,6,9,12-Tetraoxatricosan-1-ol	Surfactant	8.64	0.03	0.00	0.00	0.03
PEG Diethylhexanoate n10	Surfactant	-	0.03	-	-	0.03
Tris(4-methylphenyl) Phosphate	Phosphate	0.89	0.00	0.00	0.00	0.00
N,N-Diethyldodecanamide	Surfactant	1.72	0.00	0.00	0.00	0.00
CGA 353042	PPP	-	0.00	-	-	0.00
Sodium hydroxy- methane sulfonate	Ind. chemical	13.2	0.00	0.00	0.00	0.00
reaction mass of isomers of: C7-9-alkyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	Ind. chemical	0.25	0.00	0.00	0.00	0.00
2,2,6,6-Tetramethyl-4-oxopiperidinooxy	Ind. chemical	27.9	0.00	0.00	0.00	0.00

The results of target and suspect screening and their spatial distribution can be visualized within the application (https://norman-data.eu/HELCOM%20pre-EMPT ; screenshot as shown in **Figure 14**).

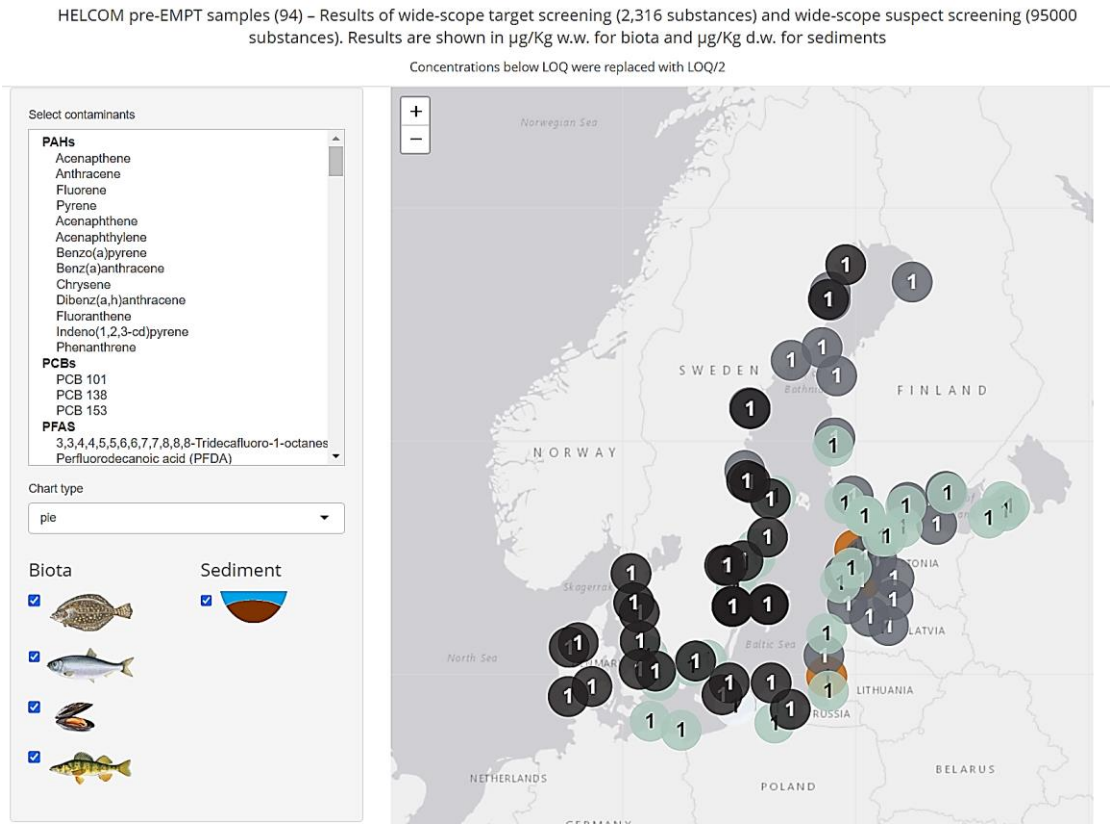

Figure 14. Spatial distribution of compounds detected in the HELCOM PreEMPT biota and sediment samples by wide-scope target and suspect screening analysis.

8.4 Suspect screening results and risk assessment by sample provider

8.4.1 Swedish Agency for Marine and Water Management

86 compounds were detected in sediment samples provided by the Swedish Agency for Marine and Water Management (HELCOM PreEMPT 63-84). Compounds with the highest concentrations were Pentaethylene glycol (N.D.-925 µg/kg d.w.), Hexa-2,4-dienoic acid (N.D.-471 µg/kg d.w.), Musk (N.D.-416 µg/kg d.w.), TP3/tert-Butyl phenyl glycidyl ether (N.D.-251 µg/kg d.w.) and 4-tert-Butylbenzoic acid (N.D.-271 µg/kg d.w.). All other substances were detected at concentration ranges below 200 µg/kg d.w. Three compounds were detected in all sediment samples but at lower concentration levels; 5'-Methylthioadenosine (1.5-16 µg/kg d.w.), Dacarbazine (1.0-14 µg/kg d.w.), and 3a,4,5,6,7,7a-Hexahydro-4,7-methano-1H-inden-5-yl propionate (2.9-135 µg/kg d.w.).

Prioritization algorithm was applied only to samples HELCOM PreEMPT 63-84 and the result of the ranking process is presented in **Table 37** (risk score >1.0). Altogether, 27 compounds were prioritized. The compounds with the highest risk

were: 5'-Methylthioadenosine, Dacarbazine, 3a,4,5,6,7,7a-Hexahydro-4,7-methano-1H-inden-5-yl propionate, and Musk.

Table 37. Prioritised substances in sediment samples HELCOM PreEMPT 63-84 based on their risk. The table presents the concentration range in µg/kg d.w., Frequency of Appearance (FoA), Frequency of PNEC Exceedance (FoE Score), Extent of PNEC Exceedance (EoE Score) and the total risk (sum of the FoA + FoE + EoE).

NORMAN ID	Compound name	Concentration range sediments	FoA	FoE	EoE	Risk
NS00014568	5'-Methylthioadenosine	1.5-16	1.00	1.00	0.20	2.20
NS00009014	Dacarbazine	1-14	1.00	1.00	0.10	2.10
NS00012545	3a,4,5,6,7,7a-Hexahydro-4,7-methano-1H-inden-5-yl propionate	2.9-135	1.00	1.00	0.00	2.00
NS00012531	Musk	N.D.-416	0.86	0.86	0.20	1.93
NS00011462	1,3-Diphenylguanidine	N.D.-41	0.91	0.91	0.10	1.92
NS00010285	4,4-Dimethyl oxazolidine	N.D.-47	0.95	0.91	0.00	1.86
NS00020126	2-Naphthylamine	N.D.-196	0.82	0.82	0.20	1.84
NS00006736	4-tert-Butylbenzoic acid	N.D.-271	0.82	0.82	0.20	1.84
NS00006048	Cetylpyridinium	N.D.-22	0.86	0.86	0.10	1.83
NS00006944	4-Morpholinecarboxaldehyde	N.D.-12	0.95	0.82	0.00	1.77
NS00003892	Methacrylamide	N.D.-125	0.91	0.86	0.00	1.77
NS00009935	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	N.D.-406	0.82	0.82	0.10	1.74
NS00009178	N-Methyl-2-pyrrolidone	N.D.-113	0.95	0.77	0.00	1.73
NS00036313	Benzoic acid, 4-(1,1-dimethylethyl)-, 1-methylethyl ester	N.D.-14	0.77	0.77	0.10	1.65
NS00014059	Sodium hydroxy- methane sulfonate	N.D.-159	0.91	0.68	0.00	1.59
NS00014430	2H-1-Benzopyran-2-one, 7-amino-4-methyl-	N.D.-115	0.73	0.73	0.10	1.55
NS00005741	Miristalkonium	N.D.-4.2	0.77	0.77	0.00	1.55
NS00002145	Hexa-2,4-dienoic acid	N.D.-471	0.59	0.59	0.20	1.38
NS00004841	Octinoxate	N.D.-24	0.68	0.68	0.00	1.36
NS00001813	Piperonal	N.D.-4.8	0.73	0.59	0.00	1.32
NS00018321	Penicillic acid	N.D.-142	0.59	0.59	0.10	1.28
NS00014858	Jasmonic acid	N.D.-15	0.64	0.64	0.00	1.27
NS00011940	2-Propen-1-yl 2-(cyclohexyloxy)acetate	N.D.-9.2	0.64	0.59	0.00	1.23
NS00003249	Octadecanamide	N.D.-46	0.50	0.50	0.20	1.20
NS00048813	2,2,6,6-Tetramethyl-4-oxopiperidinooxy	N.D.-151	0.50	0.50	0.10	1.10
NS00010914	Monoethyl phthalate	N.D.-8.5	0.55	0.55	0.00	1.09
NS00001756	2-[2-(Dimethylamino)ethoxy]ethanol	N.D.-14	0.95	0.09	0.00	1.05

8.4.2 Swedish Museum of Natural History

107 compounds were detected in blue mussels (HELCOM PreEMPT 45-55) and European perch samples (HELCOM PreEMPT 56-61) provided by the Swedish

Museum of Natural History. Compounds with the highest concentrations were TP1/1,4-Bis[(ethenyloxy)methyl]cyclohexane (64-278 µg/kg w.w.) and Methacrylamide (0-250 µg/kg w.w.) in blue mussels samples. Compounds with the highest concentrations in European perch samples were 2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol (9.7-338 µg/kg w.w.) and 1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl- (1.2-116 µg/kg w.w.). Prioritization algorithm was applied only to samples HELCOM PreEMPT 45-61 and the result of the ranking process is presented in **Table 38** (risk score >1.0). Altogether, 46 compounds were prioritised. The compounds with the highest risk were: 5'-Methylthioadenosine, 2-Propen-1-yl 2-(cyclohexyloxy)acetate, N-Methyl-2-pyrrolidone, and Butyl acrylate.

Table 38. Prioritised substances based on their risk in biota samples HELCOM PreEMPT 45-61. The table presents the concentration range in µg/kg w.w., Frequency of Appearance (FoA), Frequency of PNEC Exceedance (FoE Score), Extent of PNEC Exceedance (EoE Score) and the total risk (sum of the FoA + FoE + EoE).

NORMAN ID	Compound name	Concentation range fish	Concentration range molluscs	FoA	FoE	EoE	Risk
NS00014568	5'-Methylthioadenosine	22-110	N.D.-1.5	0.94	0.94	1.00	2.88
NS00011940	2-Propen-1-yl 2-(cyclohexyloxy)acetate	6.6-12	69-217	1.00	0.76	0.50	2.26
NS00009178	N-Methyl-2-pyrrolidone	36-63	46-97	1.00	1.00	0.20	2.20
NS00007563	Butyl acrylate	22-67	9.1-18	1.00	1.00	0.20	2.20
NS00005831	Misoprostol	2-80	28-73	1.00	0.94	0.20	2.14
NS00036915	1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl-	1.2-116	0.4-2.3	1.00	0.94	0.20	2.14
NS00020126	2-Naphthylamine	N.D.-20	8.6-54	0.94	0.94	0.20	2.08
NS00101016	Octylphenol diethoxylates (OP2EO)	N.D.-34	20-172	0.94	0.94	0.20	2.08
NS00005690	1-Butanol, 3-methoxy-3-methyl-, acetate	7.4-16	8.8-31	1.00	0.88	0.20	2.08
NS00021348	Bis(2-chloro-1-methylethyl) 2-chloropropyl Phosphate	N.D.-18	N.D.-0.7	0.76	0.76	0.50	2.03
NS00001939	Telbivudine	N.D.-0.8	9.6-126	0.82	0.65	0.50	1.97
NS00010285	4,4-Dimethyl oxazolidine	2.5-40	33-96	1.00	0.76	0.20	1.96
NS00001643	1,3-Benzenedimethanamine	2.2-29	0.4-7.8	1.00	0.82	0.10	1.92
NS00002145	Hexa-2,4-dienoic acid	N.D.-22	N.D.-73	0.71	0.71	0.50	1.91
NS00002729	Tris(2-ethylhexyl) phosphate	N.D.-47	N.D.-1.1	0.65	0.65	0.50	1.79
NS00003686	Iloprost	N.D.-2.4	5.3-20	0.94	0.65	0.20	1.79
NS00010129	Dodecanedioic acid	N.D.-7.8	2.5-5.6	0.94	0.71	0.10	1.75
NS00015142	Threonate	16-41	64-183	1.00	0.65	0.10	1.75
NS00003680	Tolazoline	N.D.-4.6	1.6-7.7	0.94	0.71	0.10	1.75
NS00005874	Bis(2-ethylhexyl) phosphate	N.D.	N.D.-139	0.35	0.35	1.00	1.71
NS00000983	3-Pyridinol	N.D.-2	15-36	0.94	0.65	0.10	1.69
NS00008005	Ethyl 3-(N-butylacetamido)propionate	N.D.-42	1.5-203	0.94	0.53	0.20	1.67
NS00009935	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	N.D.-34	22-72	0.76	0.71	0.20	1.67

NS00093005	1-Eicosanol, phosphate, compd. with 2,2'-iminobis[ethanol]	N.D.-14	N.D.-51	0.59	0.53	0.50	1.62
NS00003762	Camphor	N.D.-28	N.D.-81	0.71	0.71	0.20	1.61
NS00006736	4-tert-Butylbenzoic acid	N.D.-22	13-54	0.71	0.71	0.20	1.61
NS00011498	Nonanedioic acid	N.D.-6.2	2.6-9.6	0.88	0.59	0.10	1.57
NS00103201	TP1/2,4,6-Trimethylbenzaldehyde	N.D.-1.3	1.3-3.4	0.76	0.65	0.10	1.51
NS00015186	Octanedioic acid	N.D.	13-62	0.65	0.65	0.20	1.49
NS00049705	Glycerol monomyristate	2.4-6.1	N.D.-2.4	0.76	0.59	0.10	1.45
NS00009029	3-Methylbenzoic acid	N.D.-3.3	6-14	0.71	0.65	0.10	1.45
NS00007484	Methyldopa	N.D.-8.7	N.D.-81	0.65	0.59	0.20	1.44
NS00000458	N-(2,4-Dimethylphenyl)formamide	N.D.	1.9-47	0.65	0.59	0.20	1.44
NS00012531	Musk	N.D.-15	1.8-7.9	0.82	0.47	0.10	1.39
NS00102695	TP1/Dimethyl succinate	N.D.-11	N.D.-14	0.82	0.47	0.10	1.39
NS00003892	Methacrylamide	N.D.	N.D.-250	0.59	0.59	0.20	1.38
NS00006048	Cetylpyridinium	N.D.	N.D.-2.4	0.59	0.59	0.10	1.28
NS00010726	Erucamide	N.D.-19	N.D.-0.1	0.41	0.35	0.50	1.26
NS00013580	Bis(2-ethylhexyl) decanedioate	N.D.	N.D.-0.3	0.53	0.53	0.20	1.26
NS00038039	Vernakalant	N.D.	N.D.-248	0.53	0.53	0.20	1.26
NS00042428	2-Allyloxymethyl-2-ethylpropanediol	N.D.-3.4	4.4-12	0.88	0.24	0.10	1.22
NS00006688	Stearic acid, monoester with glycerol	0.2-36	N.D.-0.9	0.71	0.29	0.20	1.20
NS00004675	1-(2-Aminoethyl)piperazine	N.D.	N.D.-3.3	0.53	0.53	0.10	1.16
NS00014430	2H-1-Benzopyran-2-one, 7-amino-4-methyl-	N.D.-0.4	N.D.-4	0.65	0.35	0.10	1.10
NS00010915	Isobutyl hydrogen phthalate	N.D.	N.D.-25	0.29	0.29	0.50	1.09
NS00002295	2-Butenedioic acid (2Z)-, monobutyl ester	N.D.	N.D.-51	0.41	0.41	0.20	1.02

8.4.3 Estonian Environmental Research Centre

103 compounds were detected in the European perch or flounder samples (HELCOM PreEMPT 19-23 and HELCOM PreEMPT 29-33) and the blue mussel samples (HELCOM PreEMPT 24-28) provided by the Estonian Environmental Research Centre. For blue mussels, the highest concentration was observed for Octylphenol diethoxylates (19-293 µg/kg w.w.) and Ethyl 3-(N-butylacetamido)propionate (1.2-219 µg/kg w.w.). All other compounds were detected at concentration lower than 100 µg/kg w.w. For fish samples, the highest concentration was observed for Threonate (82-391 µg/kg w.w.) and Misoprostol (34-193 µg/kg w.w.), whereas all other substances were detected at concentration level below 150 µg/kg w.w.

Prioritization algorithm was applied only to samples HELCOM PreEMPT 19-33 and the result of the ranking process is presented in **Table 39** (risk score >1.0). Altogether, 25 compounds were prioritised. The compounds with the highest risk were: 5'-Methylthioadenosine, 1-Eicosanol, phosphate (compound with 2,2'-iminobis[ethanol]) and Octylphenol diethoxylates (OP2EO).

Table 39. Prioritised substances based on their risk from samples HELCOM PreEMPT 19-33. The table presents the concentration range in µg/kg w.w., Frequency of Appearance (FoA), Frequency of PNEC Exceedance (FoE Score), Extent of PNEC Exceedance (EoE Score) and the total risk (sum of the FoA + FoE + EoE).

NORMAN ID	Compound name	Concentation range fish	Concentration range molluscs	FoA	FoE	EoE	Risk
NS00014568	5'-Methylthioadenosine	14-123	0.5-2	1.00	1.00	1.00	3.00
NS00093005	1-Eicosanol, phosphate, compd. with 2,2'-iminobis[ethanol]	0.8-97	17-50	1.00	1.00	0.50	2.50
NS00101016	Octylphenol diethoxylates (OP2EO)	N.D.-36	16-293	0.93	0.87	0.50	2.30
NS00005831	Misoprostol	34-193	7.9-38	1.00	1.00	0.20	2.20
NS00007563	Butyl acrylate	13-31	5-16	1.00	1.00	0.20	2.20
NS00036915	1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl-	1.5-14	0.6-8.1	1.00	1.00	0.20	2.20
NS00009497	PEMA (2-Phenyl-2-ethylmalonamid)	1.3-14	0.7-9.3	1.00	0.93	0.20	2.13
NS00009178	N-Methyl-2-pyrrolidone	3.4-130	9.8-39	1.00	0.80	0.20	2.00
NS00005690	1-Butanol, 3-methoxy-3-methyl-, acetate	8.5-18	1.9-9.8	1.00	0.73	0.10	1.83
NS00011940	2-Propen-1-yl 2-(cyclohexyloxy)acetate	N.D.-25	6-34	0.93	0.67	0.20	1.80
NS00008005	Ethyl 3-(N-butylacetamido)propionate	N.D.-134	1.2-219	0.93	0.67	0.20	1.80
NS00001939	Telbivudine	N.D.-4.5	0.6-6.4	0.93	0.60	0.20	1.73
NS00004620	N-Butyl-1-butanamine	3.7-41	N.D.-33	0.80	0.73	0.20	1.73
NS00015142	Threonate	82-391	2.1-14	1.00	0.60	0.10	1.70
NS00076681	2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol	11-137	N.D.-16	0.73	0.73	0.20	1.67
NS00009935	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	20-72	0.81-26	1.00	0.53	0.10	1.63
NS00049404	(3S-trans)-Hexahydro-3-isobutylpyrrolo[1,2-a]pyrazine-1,4-dione	N.D.-21	N.D.-36	0.73	0.67	0.20	1.60
NS00010285	4,4-Dimethyl oxazolidine	N.D.-44	3.1-78	0.93	0.47	0.20	1.60
NS00102695	TP1/Dimethyl succinate	N.D.-86	0.7-62	0.93	0.47	0.20	1.60
NS00010129	Dodecanedioic acid	N.D.-9.1	0.8-2.6	0.93	0.47	0.10	1.50
NS00003680	Tolazoline	N.D.-7	0.6-6.6	0.93	0.47	0.10	1.50
NS00012531	Musk	N.D.-27	N.D.-8.5	0.80	0.53	0.10	1.43
NS00020126	2-Naphthylamine	N.D.-5.7	2.1-9.9	0.53	0.53	0.20	1.27
NS00014521	Tetradecane-7-sulfonic acid	N.D.-22	N.D.-1.4	0.53	0.53	0.20	1.27
NS00005889	Bethanidine	N.D.-5.7	N.D.-3.4	0.53	0.40	0.10	1.03

8.4.4 Finnish Environment Institute

99 compounds were detected in the European perch samples (HELCOM PreEMPT 01-06) and the blue mussel samples (HELCOM PreEMPT 07-12) provided by the Finnish Environment Institute. For blue mussels, the highest concentration was observed for the surfactant Octylphenol diethoxylates (OP2EO) (175-460 µg/kg w.w.), and Industrial chemicals 2-Propen-1-yl 2-(cyclohexyloxy)acetate (91 -249 µg/kg w.w.) and Octanedioic acid (43-205 µg/kg w.w.). All other compounds were detected at concentration lower than 200 µg/kg w.w. For fish samples, the highest

concentration was observed for Misoprostol (92-386 µg/kg w.w.), 2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol (44-381 µg/kg w.w.) and Threonate (107-302 µg/kg w.w., whereas all other substances were detected at concentration levels below 150 µg/kg w.w.

Prioritisation algorithm was applied only to samples HELCOM PreEMPT 19-33 and the result of the ranking process is presented in **Table 40** (risk score >1.0). Altogether, 42 compounds were prioritised. The compounds with the highest risk score were: the surfactant 1-Eicosanol, phosphate (compd. with 2,2'-iminobis[ethanol]), surfactant Octylphenol diethoxylates (OP2EO), and the Industrial chemical Butyl acrylate. Butyl acrylate is known to be produced at very high tonnage in Europe (100,000-1,000,000 t/a).

Table 40. Prioritised substances based on their risk in samples HELCOM PreEMPT 19-33. The table presents the concentration range in µg/kg w.w., Frequency of Appearance (FoA), Frequency of PNEC Exceedance (FoE Score), Extent of PNEC Exceedance (EoE Score) and the total risk (sum of the FoA + FoE + EoE).

NORMAN ID	Compound name	Concentration range fish	Concentration range molluscs	FoA	FoE	EoE	Risk
NS00093005	1-Eicosanol, phosphate, compd. with 2,2'-iminobis[ethanol]	0.8-3.6	N.D.-84	0.83	0.83	1.00	2.67
NS00101016	Octylphenol diethoxylates (OP2EO)	16-146	175-460	1.00	1.00	0.50	2.50
NS00007563	Butyl acrylate	24-56	19-38	1.00	1.00	0.50	2.50
NS00010915	Isobutyl hydrogen phthalate	N.D.-23	17-158	0.92	0.92	0.50	2.33
NS00009178	N-Methyl-2-pyrrolidone	102-224	38-77	1.00	1.00	0.20	2.20
NS00005831	Misoprostol	92-386	26-99	1.00	1.00	0.20	2.20
NS00001939	Telbivudine	2.1-4.7	3.3-42	1.00	1.00	0.20	2.20
NS00005690	1-Butanol, 3-methoxy-3-methyl-, acetate	9.9-14	32-80	1.00	1.00	0.20	2.20
NS00036915	1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl-	4.2-11	0.6-2.6	1.00	1.00	0.10	2.10
NS00011940	2-Propen-1-yl 2-(cyclohexyloxy)acetate	3.3-12	91-249	1.00	0.58	0.50	2.08
NS00076681	2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol	44-381	N.D.-33	0.92	0.92	0.20	2.03
NS00010129	Dodecanedioic acid	1.7-13	4.9-28	1.00	0.83	0.20	2.03
NS00009935	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	21-43	49-180	1.00	0.83	0.20	2.03
NS00015142	Threonate	107-302	24-46	1.00	0.92	0.10	2.02
NS00010285	4,4-Dimethyl oxazolidine	5.8-25	7.6-87	1.00	0.67	0.20	1.87
NS00001643	1,3-Benzenedimethanamine	1.7-19	2.2-8.4	1.00	0.75	0.10	1.85
NS00006736	4-tert-Butylbenzoic acid	N.D.-20	55-125	0.67	0.67	0.50	1.83
NS00012531	Musk	10-20	23-172	1.00	0.58	0.20	1.78
NS00009497	PEMA (2-Phenyl-2-ethylmalonamid)	N.D.-21	N.D.-8.1	0.75	0.75	0.20	1.70
NS00102695	TP1/Dimethyl succinate	6.3-12	27-179	1.00	0.50	0.20	1.70
NS00015186	Octanedioic acid	N.D.-5.8	43-205	0.92	0.50	0.20	1.62
NS00011498	Nonanedioic acid	N.D.-5.2	9.4-49	0.92	0.50	0.20	1.62
NS00008005	Ethyl 3-(N-butylacetamido)propionate	N.D.-237	N.D.-7	0.83	0.58	0.20	1.62

NS00003680	Tolazoline	2.4-6.4	N.D.-12	0.83	0.50	0.20	1.53
NS00049404	(3S-trans)-Hexahydro-3-isobutylpyrrolo[1,2-a]pyrazine-1,4-dione	N.D.-14	N.D.-23	0.67	0.67	0.20	1.53
NS00014568	5'-Methylthioadenosine	9.5-53	N.D.	0.50	0.50	0.50	1.50
NS00002145	Hexa-2,4-dienoic acid	N.D.	46-92	0.50	0.50	0.50	1.50
NS00011501	Decanedioic acid	N.D.-1.8	24-83	0.75	0.50	0.20	1.45
NS00010591	N,N-Bis(2-hydroxyethyl)dodecanamide	N.D.-15	N.D.-8.3	0.75	0.58	0.10	1.43
NS00102595	TP2/Pentanedioic acid, bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] ester	1.2-5.9	8.2-13	1.00	0.33	0.10	1.43
NS00004620	N-Butyl-1-butanamine	39-97	N.D.-18	0.58	0.58	0.20	1.37
NS00042428	2-Allyloxymethyl-2-ethylpropanediol	3.3-4.8	3-11	1.00	0.17	0.10	1.27
NS00003686	Iloprost	N.D.-2.2	1.9-4	0.67	0.50	0.10	1.27
NS00003892	Methacrylamide	N.D.	24-137	0.50	0.50	0.20	1.20
NS00003762	Camphor	N.D.	15-75	0.50	0.50	0.20	1.20
NS00005889	Bethanidine	8.8-53	N.D.	0.50	0.50	0.20	1.20
NS00002295	2-Butenedioic acid (2Z)-, monobutyl ester	N.D.	11-27	0.50	0.50	0.20	1.20
NS00049705	Glycerol monomyristate	N.D.-8.6	N.D.-4.8	0.58	0.50	0.10	1.18
NS00006554	Naphthalene-1-sulfonic acid	0.2-1.5	0.1-4.1	1.00	0.08	0.10	1.18
NS00009029	3-Methylbenzoic acid	N.D.	4.2-18	0.50	0.50	0.10	1.10
NS00013704	Glyceryl linolenate	N.D.	1.5-7.6	0.50	0.42	0.10	1.02
NS00002293	Glycine, N-(1-oxooctyl)-	N.D.-1.3	0.7-1	0.67	0.25	0.10	1.02

8.4.5 Latvian Institute of Aquatic Ecology

96 compounds were detected in the fish samples (HELCOM PreEMPT 37-38 Atlantic herring and HELCOM PreEMPT 39-43 European perch) and the blue mussel sample (HELCOM PreEMPT 44) provided by the Latvian Institute of Aquatic Ecology. For the blue mussel sample, the highest concentration was observed for the surfactant Octylphenol diethoxylates (OP2EO) (254 µg/kg w.w.), Industrial chemical TP1/1,4-Bis[(ethenyloxy)methyl]cyclohexane (238 µg/kg w.w.) and the Pharmaceutical Telbivudine (194 µg/kg w.w.). All other compounds were determined at concentrations lower than 200 µg/kg w.w. For the fish samples (considering Atlantic herring and European perch samples together), the highest concentration was observed for the surfactant Octylphenol diethoxylates (OP2EO) (7.6-335 µg/kg w.w.), Threonate (75-213 µg/kg w.w.) and the PPP Ethyl 3-(N-butylacetamido)propionate (N.D.-202 µg/kg w.w.), whereas all other substances were detected at concentration levels below 200 µg/kg w.w.

Prioritisation algorithm was applied only to samples HELCOM PreEMPT 37-44 and the result of the ranking process is presented in **Table 41** (risk score >1.0). Altogether, 31 compounds were prioritised. Compounds with the highest risk were: Pharmaceutical Methylthioadenosine, surfactant 1-Eicosanol, phosphate () and Industrial chemical Butyl acrylate.

Table 41. Prioritised substances based on their risk in samples HELCOM PreEMPT 37-44. The table presents the concentration range in µg/kg w.w., Frequency of Appearance (FoA), Frequency of PNEC Exceedance (FoE Score), Extent of PNEC Exceedance (EoE Score) and the total risk (sum of the FoA + FoE + EoE).

NORMAN ID	Compound name	Concentration range fish	Concentration molluscs	FoA	FoE	EoE	Risk
NS00014568	5'-Methylthioadenosine	4.3-116	1.1	1.00	1.00	1.00	3.00
NS00093005	1-Eicosanol, phosphate, compd. with 2,2'-iminobis[ethanol]	N.D.-22	75	0.88	0.88	1.00	2.75
NS00007563	Butyl acrylate	35-97	33	1.00	1.00	0.50	2.50
NS00101016	Octylphenol diethoxylates (OP2EO)	7.6-335	254	1.00	0.88	0.50	2.38
NS00011940	2-Propen-1-yl 2-(cyclohexyloxy)acetate	8.7-134	141	1.00	1.00	0.20	2.20
NS00005831	Misoprostol	9-76	123	1.00	1.00	0.20	2.20
NS00009497	PEMA (2-Phenyl-2-ethylmalonamid)	3.7-34	2	1.00	1.00	0.20	2.20
NS00010285	4,4-Dimethyl oxazolidine	28-68	77	1.00	1.00	0.20	2.20
NS00020126	2-Naphthylamine	18-33	53	1.00	1.00	0.20	2.20
NS00012531	Musk	12-119	56	1.00	0.88	0.20	2.08
NS00002145	Hexa-2,4-dienoic acid	N.D.-39	74	0.75	0.75	0.50	2.00
NS00049705	Glycerol monomyristate	2.4-24	2.7	1.00	0.88	0.10	1.98
NS00001643	1,3-Benzenedimethanamine	5.3-19	4.2	1.00	0.88	0.10	1.98
NS00076681	2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol	6.9-190	N.D.	0.88	0.88	0.20	1.95
NS00005690	1-Butanol, 3-methoxy-3-methyl-, acetate	7.9-18	29	1.00	0.75	0.20	1.95
NS00049404	(3S-trans)-hexahydro-3-isobutylpyrrolo[1,2-a]pyrazine-1,4-dione	N.D.-51	32	0.88	0.88	0.20	1.95
NS00015142	Threonate	75-213	178	1.00	0.75	0.10	1.85
NS00006688	Stearic acid, monoester with glycerol	0.3-28	N.D.	0.88	0.75	0.20	1.83
NS00021348	Bis(2-chloro-1-methylethyl) 2-chloropropyl phosphate	N.D.-3.9	N.D.	0.63	0.63	0.50	1.75
NS00001939	Telbivudine	N.D.-5.1	194	0.88	0.38	0.50	1.75
NS00009178	N-Methyl-2-pyrrolidone	N.D.-166	74	0.75	0.75	0.20	1.70
NS00008005	Ethyl 3-(N-butylacetamido)propionate	N.D.-202	12	0.75	0.75	0.20	1.70
NS00003686	Iloprost	1.2-8.8	N.D.	1.00	0.50	0.10	1.60
NS00036915	1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl-	0.5-72	N.D.	0.88	0.50	0.20	1.58
NS00009935	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	N.D.-171	97	0.63	0.63	0.20	1.45
NS00013580	Bis(2-ethylhexyl) decanedioate	N.D.-0.8	N.D.	0.63	0.63	0.10	1.35
NS00011462	1,3-Diphenylguanidine	N.D.-12	N.D.	0.75	0.50	0.10	1.35
NS00102695	TP1/Dimethyl succinate	5.9-12	N.D.	1.00	0.13	0.20	1.33
NS00006736	4-tert-Butylbenzoic acid	N.D.-86	N.D.	0.38	0.38	0.50	1.25
NS00010129	Dodecanedioic acid	N.D.-5	5.7	0.88	0.13	0.10	1.10
NS00102595	TP2/Pentanedioic acid, bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] ester	N.D.-5.2	N.D.	0.88	0.13	0.10	1.10

8.4.6 Institute of Meteorology and Water Management (IMGW-PIB)

96 compounds were detected in the Altantic herring samples (HELCOM PreEMPT 16-17), top-layer sediment (HELCOM PreEMPT 13-15) and the blue mussel sample (HELCOM PreEMPT 18) provided by the Institute of Meteorology and Water Management (IMGW-PIB).

In the blue mussel sample, the highest concentration was observed for the Pharmaceutical Threonate (61 µg/kg w.w.), whereas all other substances were detected at concentration level below 50 µg/kg w.w. In the Atlantic herring samples, the highest concentration was observed for the Pharmaceutical Threonate (90-350 µg/kg w.w.), PPP N-(2,4-Dimethylphenyl)formamide (N.D.-190 µg/kg w.w.), Industrial chemical Butyl acrylate (66-131 µg/kg w.w.) and surfactant Octylphenol diethoxylates (OP2EO) (25-104 µg/kg w.w.). All other substances were detected at concentration level below 100 µg/kg w.w. For the top-layer sediment samples, the highest concentration was observed for TP3/tert-Butyl phenyl glycidyl ether (191-531 µg/kg d.w.), Musk (79-193 µg/kg d.w.) and PPP Hexa-2,4-dienoic acid (144-179 µg/kg d.w.). All other compounds were detected at concentration levels below 160 µg/kg w.w.

Prioritisation algorithm was applied only to samples HELCOM PreEMPT 13-18 and the result of the ranking process is presented in **Table 42** (risk score >1.0). Altogether, 17 compounds were prioritised. Compounds with the highest risk were: Industrial chemicals 4-tert-Butylbenzoic acid, 2-Propen-1-yl 2-(cyclohexyloxy)acetate and Butyl acrylate.

Table 42. Prioritised substances based on their risk for samples HELCOM PreEMPT 13-18. The table presents the concentration range in µg/kg w.w. for biota and µg/kg d.w. for sediment, Frequency of Appearance (FoA), Frequency of PNEC Exceedance (FoE Score), Extent of PNEC Exceedance (EoE Score) and the total risk (sum of the FoA + FoE + EoE).

NORMAN ID	Compound name	Concentration range fish	Concentration range molluscs	Concentration range sediment	FoA	FoE	EoE	Risk
NS00006736	4-tert-Butylbenzoic acid	24-30	26-26	111-160	1.00	1.00	0.20	2.20
NS00011940	2-Propen-1-yl 2-(cyclohexyloxy)acetate	26-27	3.9-3.9	0.01-6.9	1.00	0.50	0.10	1.60
NS00007563	Butyl acrylate	66-131	8.6-8.6	N.D.	0.50	0.50	0.50	1.50
NS00009178	N-Methyl-2-pyrrolidone	9.3-47	23-23	16-38	1.00	0.33	0.10	1.43
NS00093005	1-Eicosanol, phosphate, compd. with 2,2'-iminobis[ethanol]	4.5-16	9-9	N.D.	0.50	0.50	0.50	1.50
NS00014568	5'-Methylthioadenosine	N.D.-5.9	0.7-0.7	8.6-11	0.83	0.83	0.20	1.87
NS00020126	2-Naphthylamine	3.6-78	N.D.	13-20	0.83	0.83	0.20	1.87
NS00010285	4,4-Dimethyl oxazolidine	7.3-14	11-11	36-69	1.00	0.17	0.10	1.27
NS00015142	Threonate	90-350	61-61	N.D.-5.4	0.83	0.33	0.10	1.27
NS00005690	1-Butanol, 3-methoxy-3-methyl-, acetate	16-21	2.1-2.1	N.D.-47	0.83	0.33	0.10	1.27
NS00101016	Octylphenol diethoxylates (OP2EO)	25-104	3.7-3.7	N.D.	0.50	0.50	0.20	1.20
NS00009497	PEMA (2-Phenyl-2-ethylmalonamid)	6.2-13	3.5-3.5	N.D.	0.50	0.50	0.20	1.20
NS00012531	Musk	N.D.-22	2.6-2.6	79-193	0.83	0.67	0.20	1.70
NS00003680	Tolazoline	4.5-5.2	1.8-1.8	N.D.	0.50	0.50	0.10	1.10

NS00005831	Misoprostol	48-54	7.8-7.8	N.D.	0.50	0.50	0.10	1.10
NS00004620	N-Butyl-1-butanamine	9-29	7.7-7.7	N.D.	0.50	0.50	0.10	1.10
NS00102695	TP1/Dimethyl succinate	12-64	1.8-1.8	N.D.-25	0.83	0.17	0.10	1.10

8.4.7 Aarhus University

69 compounds were detected in the sediment samples (HELCOM PreEMPT 90-94) provided by the Aarhus University. The highest concentration was observed for Pharmaceutical 3,5-Di-tert-butyl-4-hydroxybenzaldehyde (77-504 µg/kg d.w.), 2-Naphthylamine (34-384 µg/kg d.w.) and TP3/tert-Butyl phenyl glycidyl ether (169-362 µg/kg d.w.). All other chemicals were detected at concentration below 270 µg/kg d.w.

The prioritisation algorithm was applied only to samples HELCOM PreEMPT 90-94 and the result of the ranking process is presented in **Table 43** (risk score >1.0). Altogether, 12 compounds were prioritised. Compounds with the highest risk were: Industrial chemical 2-Naphthylamine, PCPMusk and the Pharmaceutical 5'-Methylthioadenosine.

Table 43. Prioritised substances based on their risk for samples HELCOM PreEMPT 90-94. The table presents the concentration range in µg/kg w.w. for biota and µg/kg d.w. for sediment, Frequency of Appearance (FoA), Frequency of PNEC Exceedance (FoE Score), Extent of PNEC Exceedance (EoE Score) and the total risk (sum of the FoA + FoE + EoE).

NORMAN ID	Compound name	Concentration range sediment	FoA	FoE	EoE	Risk
NS00020126	2-Naphthylamine	34-384	1.00	1.00	0.20	2.20
NS00012531	Musk	89-265	1.00	1.00	0.20	2.20
NS00014568	5'-Methylthioadenosine	10-23	1.00	1.00	0.20	2.20
NS00018321	Penicillic acid	57-87	1.00	1.00	0.10	2.10
NS00002145	Hexa-2,4-dienoic acid	83-135	1.00	1.00	0.10	2.10
NS00009935	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	77-504	1.00	1.00	0.10	2.10
NS00003892	Methacrylamide	131-252	1.00	0.80	0.10	1.90
NS00009014	Dacarbazine	9.5-17	1.00	0.80	0.10	1.90
NS00036313	Benzoic acid, 4-(1,1-dimethylethyl)-, 1-methylethyl ester	8.2-18	1.00	0.80	0.10	1.90
NS00003249	Octadecanamide	N.D.-148	0.80	0.80	0.20	1.80
NS00048813	2,2,6,6-Tetramethyl-4-oxopiperidinooxy	N.D.-124	0.80	0.40	0.10	1.30
NS00006736	4-tert-Butylbenzoic acid	N.D.-191	0.60	0.60	0.10	1.30

8.4.8 Lithuanian Environmental Protection Agency

90 compounds were detected in the zebra mussel sample (HELCOM PreEMPT 36), Atlantic herring (HELCOM PreEMPT 35) and the European flounder (HELCOM PreEMPT 34) provided by the Lithuanian Environmental Protection Agency. In the zebra mussel sample, the highest concentration was observed for the surfactant Octylphenol diethoxylates (OP2EO) (208 µg/kg w.w.), phosphate Bis(2-ethylhexyl) phosphate (133 µg/kg w.w.) and Industrial chemical 1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl- (51 µg/kg w.w.). All other chemicals were detected at concentration below 50 µg/kg w.w. Higher concentration levels were observed in the fish samples. Considering the Atlantic herring and the European flounder samples together, the highest concentration was determined for Threonate (192-387 µg/kg w.w.), Ethyl 3-(N-butylacetamido)propionate (19-343 µg/kg w.w.), and Bis(2-ethylhexyl) phosphate (209-249 µg/kg w.w.). All other chemicals were detected in the samples at concentration levels below 250 µg/kg w.w.

The prioritisation algorithm was applied only to samples HELCOM PreEMPT 34-36 and the result of the ranking process is presented in **Table 44** (risk score >1.0). Altogether, 52 compounds were prioritised. The compounds with the highest risk were: 5'-Methylthioadenosine, 1-Eicosanol, phosphate (compd. with 2,2'-iminobis[ethanol]) and N-Methyl-2-pyrrolidone.

Table 44. Prioritised substances based on their risk in samples HELCOM PreEMPT 34-36. The table presents the concentration range in µg/kg w.w. for biota, Frequency of Appearance (FoA), Frequency of PNEC Exceedance (FoE Score), Extent of PNEC Exceedance (EoE Score) and the total risk (sum of the FoA + FoE + EoE).

NORMAN ID	Compound name	Concentration range fish	Concentration range moluscs	FoA	FoE	EoE	Risk
NS00005874	Bis(2-ethylhexyl) phosphate	209-249	133	1.00	1.00	1.00	3.00
NS00093005	1-Eicosanol, phosphate, compd. with 2,2'-iminobis[ethanol]	23-48	30	1.00	1.00	0.50	2.50
NS00014568	5'-Methylthioadenosine	8.1-16	2.7	1.00	1.00	0.50	2.50
NS00011940	2-Propen-1-yl 2-(cyclohexyloxy)acetate	25-47	29	1.00	1.00	0.20	2.20
NS00101016	Octylphenol diethoxylates (OP2EO)	30-210	208	1.00	1.00	0.20	2.20
NS00076681	2-(2-(2-(4-Nonylphenoxy)ethoxy)ethoxy)ethanol	35-104	11	1.00	1.00	0.20	2.20
NS00005831	Misoprostol	101-239	23	1.00	1.00	0.20	2.20
NS00008005	Ethyl 3-(N-butylacetamido)propionate	19-343	40	1.00	1.00	0.20	2.20
NS00020126	2-Naphthylamine	18-29	2.2	1.00	1.00	0.20	2.20
NS00009178	N-Methyl-2-pyrrolidone	24-28	22	1.00	1.00	0.10	2.10
NS00003892	Methacrylamide	33-34	27	1.00	1.00	0.10	2.10
NS00001002	Pentaethylene glycol	28-29	27	1.00	1.00	0.10	2.10
NS00006048	Cetylpyridinium	3.3-4	1.3	1.00	1.00	0.10	2.10
NS00003762	Camphor	24-54	13	1.00	1.00	0.10	2.10
NS00010285	4,4-Dimethyl oxazolidine	39-100	19	1.00	1.00	0.10	2.10

NS00039200	1H-Indole-3-methanamine, N,N-dimethyl-	5.7-5.7	1.2	1.00	1.00	0.10	2.10
NS00102695	TP1/Dimethyl succinate	80-135	4.4	1.00	1.00	0.10	2.10
NS00010726	Erucamide	N.D.-0.5	7.8	0.67	0.67	0.50	1.83
NS00036915	1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl-	N.D.-13	51	0.67	0.67	0.50	1.83
NS00012531	Musk	7.5-23	4.7	1.00	0.67	0.10	1.77
NS00015142	Threonate	192-387	13	1.00	0.67	0.10	1.77
NS00001939	Telbivudine	1.3-3.9	0.8	1.00	0.67	0.10	1.77
NS00005690	1-Butanol, 3-methoxy-3-methyl-, acetate	9.5-17	5.8	1.00	0.67	0.10	1.77
NS00006343	N,N-Diethylethanolamine	13-16	4	1.00	0.67	0.10	1.77
NS00009497	PEMA (2-Phenyl-2-ethylmalonamid)	N.D.-40	2.1	0.67	0.67	0.20	1.53
NS00007563	Butyl acrylate	N.D.-64	N.D.	0.67	0.67	0.20	1.53
NS00010915	Isobutyl hydrogen Phthalate	0.7-0.7	1.5	1.00	0.33	0.10	1.43
NS00003680	Tolazoline	N.D.-4.7	3.8	0.67	0.67	0.10	1.43
NS00005889	Bethanidine	5.9-7.1	N.D.	0.67	0.67	0.10	1.43
NS00003686	Iloprost	5.3-10	N.D.	0.67	0.67	0.10	1.43
NS00002849	reaction mass of isomers of: C7-9-alkyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	5.5-6.1	N.D.	0.67	0.67	0.10	1.43
NS00010296	Hexa(methoxymethyl)melamine	N.D.	1.7	0.33	0.33	0.50	1.17
NS00002729	Tris(2-ethylhexyl) phosphate	N.D.	15	0.33	0.33	0.50	1.17
NS00014521	Tetradecane-7-sulfonic acid	1.4-2.9	N.D.	0.67	0.33	0.10	1.10
NS00005741	Miristalkonium	N.D.-1	0.9	0.67	0.33	0.10	1.10
NS00004675	1-(2-Aminoethyl)piperazine	N.D.-2.2	1.7	0.67	0.33	0.10	1.10

8.4.9 German Environmental Specimen Bank and Landesamt für Umwelt, Naturschutz und Geologie Mecklenburg-Vorpommern

92 compounds were detected in the blue mussel samples (HELCOM PreEMPT 62 and 85) provided by the Germany Environmental Specimen Bank and the State Office for the Environment, Nature Conservation and Geology. The highest concentration was observed for Bis(2-ethylhexyl) phosphate (137-167 µg/kg w.w.), Methacrylamide (60-158 µg/kg w.w.) and Threonate (5-92 µg/kg w.w.). All other chemicals were detected at concentrations below 90 µg/kg w.w. The prioritisation algorithm was applied only to samples HELCOM PreEMPT 62 and 85 and the result of the ranking process is presented in **Table 45** (risk score >1.0). Altogether, 50 compounds were prioritised. The compounds with the highest risk were: Bis(2-ethylhexyl) phosphate, 5'-Methylthioadenosine and Telbivudine.

Table 45. Prioritised substances based on their risk for samples HELCOM PreEMPT 34-36. The table presents the concentration range in µg/kg w.w. for biota and µg/kg d.w. for sediment, Frequency of Appearance (FoA), Frequency of PNEC Exceedance (FoE Score), Extent of PNEC Exceedance (EoE Score) and the total risk (sum of the FoA + FoE + EoE).

NORMAN ID	Compound name	Concentration range molluscs	FoA	FoE	EoE	Risk

NS00005874	Bis(2-ethylhexyl) phosphate	134-167	1.00	1.00	1.00	3.00
NS00014568	5'-Methylthioadenosine	0.9-2.6	1.00	1.00	0.50	2.50
NS00001939	Telbivudine	1.5-86	1.00	1.00	0.50	2.50
NS00003892	Methacrylamide	6N.D.-158	1.00	1.00	0.20	2.20
NS00011940	2-Propen-1-yl 2-(cyclohexyloxy)acetate	21-41	1.00	1.00	0.20	2.20
NS00101016	Octylphenol diethoxylates (OP2EO)	2N.D.-29	1.00	1.00	0.20	2.20
NS00005831	Misoprostol	9.6-22	1.00	1.00	0.20	2.20
NS00002145	Hexa-2,4-dienoic acid	11-22	1.00	1.00	0.20	2.20
NS00020126	2-Naphthylamine	8-53	1.00	1.00	0.20	2.20
NS00006736	4-tert-Butylbenzoic acid	15-27	1.00	1.00	0.20	2.20
NS00013580	Bis(2-ethylhexyl) decanedioate	0.1-0.2	1.00	1.00	0.10	2.10
NS00010915	Isobutyl hydrogen phthalate	0.3-0.4	1.00	1.00	0.10	2.10
NS00002729	Tris(2-ethylhexyl) hosphate	0.2-0.3	1.00	1.00	0.10	2.10
NS00012531	Musk	5-6.2	1.00	1.00	0.10	2.10
NS00006048	Cetylpyridinium	0.4-2.2	1.00	1.00	0.10	2.10
NS00003762	Camphor	5.8-27	1.00	1.00	0.10	2.10
NS00003680	Tolazoline	1.2-4.5	1.00	1.00	0.10	2.10
NS00005889	Bethanidine	1.2-4.4	1.00	1.00	0.10	2.10
NS00009014	Dacarbazine	0.6-0.6	1.00	1.00	0.10	2.10
NS00000458	N-(2,4-Dimethylphenyl)formamide	4.1-6.7	1.00	1.00	0.10	2.10
NS00008005	Ethyl 3-(N-butylacetamido)propionate	17-17	1.00	1.00	0.10	2.10
NS00010285	4,4-Dimethyl oxazolidine	8.7-45	1.00	1.00	0.10	2.10
NS00009029	3-Methylbenzoic acid	3.7-14	1.00	1.00	0.10	2.10
NS00005690	1-Butanol, 3-methoxy-3-methyl-, acetate	5.2-8.2	1.00	1.00	0.10	2.10
NS00001643	1,3-Benzenedimethanamine	2.9-3	1.00	1.00	0.10	2.10
NS00009935	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	17-23	1.00	1.00	0.10	2.10
NS00008484	Isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	0.9-17	1.00	0.50	0.10	1.60
NS00015186	Octanedioic acid	3.6-9.3	1.00	0.50	0.10	1.60
NS00010307	Acetyl tributyl citrate	0.5-1	1.00	0.50	0.10	1.60
NS00010129	Dodecanedioic acid	1.3-3	1.00	0.50	0.10	1.60
NS00006688	Stearic acid, monoester with glycerol	0.2-1.2	1.00	0.50	0.10	1.60
NS00015142	Threonate	5.5-92	1.00	0.50	0.10	1.60
NS00003686	Iloprost	1.1-6.2	1.00	0.50	0.10	1.60
NS00001813	Piperonal	0.6-2.7	1.00	0.50	0.10	1.60
NS00103201	TP1/2,4,6-Trimethylbenzaldehyde	1-1.4	1.00	0.50	0.10	1.60
NS00102695	TP1/Dimethyl succinate	2.2-22	1.00	0.50	0.10	1.60
NS00021348	Bis(2-chloro-1-methylethyl) 2-chloropropyl phosphate	N.D.-0.6	0.50	0.50	0.50	1.50
NS00093005	1-Eicosanol, phosphate, compd. with 2,2'-iminobis[ethanol]	N.D.-12	0.50	0.50	0.50	1.50
NS00009178	N-Methyl-2-pyrrolidone	N.D.-57	0.50	0.50	0.20	1.20
NS00038039	Vernakalant	N.D.-78	0.50	0.50	0.20	1.20
NS00007563	Butyl acrylate	N.D.-19	0.50	0.50	0.20	1.20
NS00002295	2-Butenedioic acid (2Z)-, monobutyl ester	N.D.-21	0.50	0.50	0.20	1.20

NS00049705	Glycerol monomyristate	N.D.-1.7	0.50	0.50	0.10	1.10
NS00009560	Tetradecylamine	N.D.-6.1	0.50	0.50	0.10	1.10
NS00007484	Methyldopa	N.D.-9.7	0.50	0.50	0.10	1.10
NS00067187	RP 12913 (TP of Carbetamide)	N.D.-0.5	0.50	0.50	0.10	1.10
NS00004620	N-Butyl-1-butanamine	N.D.-3	0.50	0.50	0.10	1.10
NS00013936	Benzoic acid, 4-methoxy-	N.D.-10	0.50	0.50	0.10	1.10
NS00004675	1-(2-Aminoethyl)piperazine	N.D.-2.7	0.50	0.50	0.10	1.10
NS00036915	1-Propanone, 1-(4-dodecylphenyl)-2-hydroxy-2-methyl-	N.D.-0.8	0.50	0.50	0.10	1.10

9. Conclusions and recommendations

A wide-scope target and suspect screening of 94 marine biota and sediment samples obtained from nine HELCOM countries within the HELCOM PreEMPT project was carried out using LC-ESI-HRMS and GC-APCI-HRMS techniques. The wide-scope target analysis comprised screening and quantification of 2,528 substances in each sample, whereas suspect screening provided information on presence/absence of 95,739 substances and semi-quantitative estimate of detected substances in each sample.

A risk assessment/prioritisation has been performed for all identified/determined substances using Frequency of Appearance (FoA), Frequency of Exceedance (FoE) and Extent of Exceendance (EoE) of ecotoxicity threshold values. In cases when no EU environmental quality standard was available for a detected/determined substance, ecotoxicity threshold (PNEC) values for biota and sediment from the NORMAN Ecotoxicology Database were used for the risk assessment.

Overall, 52 and 75 contaminants were determined in the 30 sediment and 64 biota (33 fish and 31 mussels) samples by the wide-scope target screening. Out of these, 22 and 23 compounds exceeded their ecotoxicological threshold value in at least one sediment or biota sample, respectively.

The suspect screening resulted in tentative identification of additional (to those determined by target screening) 98 contaminants in the sediment samples and 123 contaminants in the biota samples. Suspect screening provides only semi-quantitative estimation of the concentrations of the detected substances, however, there is a strong indication that 44 compounds exceeded their ecotoxicological threshold value in at least one sediment sample and 57 compounds exceeded their ecotoxicological threshold value in at least one fish sample, while 16 of them exceeded the PNEC in more than half of the fish samples. The analysis of 31 blue mussel samples revealed the presence of 83 compounds, which exceeded their ecotoxicological threshold value in at least one sample.

Results obtained by wide-scope target screening were uploaded into the LIFE APEX Database System - Chemical Occurrence Data (analyses of biota samples; https://www.norman-network.com/apex/lacod/) and NORMAN Database System - EMPODAT Database - Chemical Occurrence Data (all samples; https://www.norman-network.com/nds/empodat/), used for the collection and assessment of data on the presence of chemicals in the environment. Concentration results of all target and suspect substances detected in the

PreEMPT samples can be visualised at **https://norman-data.eu/HELCOM%20pre-EMPT**. All NORMAN network data, including those in the LIFE APEX Database System, are shared with the Information Platform on Chemical Monitoring (IPCHEM) of the European Commission on an annual basis.

High resolution mass spectrometry data used for suspect screening were stored in the NORMAN Database System – Digital Sample Freezing Platform (DSFP). This data are available for future retrospective screening of even wider range of chemical contaminants, including those which were not on the suspect list during the PreEMPT project.

An access to both the wide-scope target and suspect screening data is at present restricted only to the experts identified as eligible by the Baltic Marine Environment Protection Commission.

It is recommended to store systematically data from further screening campaigns of HELCOM countries in the NORMAN Database System (https://www.norman-network.com/nds/), which would allow for their review in comparison with data from other European countries, North America and globally. **Also, it is recommended to encourage HELCOM Contracting Parties to provide NORMAN Association with commonly agreed marine sediment, water and biota ecotoxicity threshold values (PNECs) for as many substances as possible. This is to facilitate more accurate prioritisation of the contaminants detected in environmental samples in the Baltic Sea based on the exceedance of these values.**
Additional efforts are taking place within NORMAN to develop a specific prioritisation scheme taking into account model-predicted PBT (persistence, bioaccumulation, toxicity) values for all substances listed in the Substance Database (https://www.norman-network.com/nds/susdat/). Once ready, they can be re-applied on the substances identified in the analyzed samples in the current screening/monitoring programmes. Also, there is an on-going discussion with European Chemicals Agency (ECHA) to increase the importance of environmental occurrence data in the substance evaluation scheme and receiving feedback which of the REACH substances (including their transformation products) might be preferably targeted in the updated EU Water Framework Directive (WFD) and The Marine Strategy Framework Directive (MSFD) monitoring schemes.

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