

## ELECTRONIC SUPPLEMENTARY MATERIAL TO:

### “Screening of organic micropollutants in mollusc and fish samples from the Portuguese coast by combining liquid and gas chromatography with high resolution mass spectrometry”

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**Table S1. Chemical formula, supplier information and concentration of standards used as internal standards in the two different chromatographic systems (CS), liquid chromatograph (LC) and gas chromatograph (GC).**

Name	Formula	Supplier	CS
<i>Internal standards</i>			
Acesulfame-d4 potassium salt	C4D4KNO4S	TRC	LC
Atenolol-d7	C14D7H15N2O3	Sigma Aldrich	LC
Benzoylecgonine-d3	C16D3H16NO4	Cerilliant	LC
Bisphenol-S-d8	C12D8H2O4S	LGC standards	LC
<sup>13</sup> C3-caffeine	<sup>13</sup> C3C5H10N4O2	Sigma Aldrich	LC
Cocaine-d3	C17D3H18NO4	Cerilliant	LC
Dibutylphthalate-d4	C16D4H18O4	Cerilliant	LC
<sup>13</sup> C6-diclofenac	<sup>13</sup> C6C8H11Cl2NO2	LGC standards	LC
Diethylhexylphthalate-d4	C24D4H34O4	Sigma Aldrich	LC
Dimethylphthalate-d4	C10D4H6O4	Sigma Aldrich	LC
Irbesartan-d4	C25D4H24N6O	TRC	LC
Metformin-d6	C4D6H5N5	Biozol	LC
Methyl-4-hydroxybenzoate-d4	C8D4H4O3	LGC standards	LC
O-desmethylvenlafaxine-d6	C16D6H19NO2	Cerilliant	LC
<sup>13</sup> C4-perfluorooctanoic acid	<sup>13</sup> C4C4HF15O2	Wellington Laboratories	LC
<sup>13</sup> C4-sodium perfluorooctanesulfonate	<sup>13</sup> C4C4F17O3SNa	Wellington Laboratories	LC
Tramadol-d3	C16D3H22NO2	Cerilliant	LC
Tris(1-chloro-2-propyl) phosphate-d18	C9D18Cl3O4P	LGC standards	LC
Tri-n-butyl phosphate-d27	C12D27O4P	Wellington Laboratories	LC
Venlafaxine-d6	C17D6H21NO2	Cerilliant	LC
<sup>13</sup> C6-triclosan	<sup>13</sup> C6C6H7Cl3O2	LGC standards	GC
α-HCH-d6	C6D6Cl6	LGC standards	GC
Naphthalene-d8	C10D8	Sigma Aldrich	GC
Phenanthrene-d10	C14D10	Sigma Aldrich	GC
PCB -30	C12H7Cl3	LGC Standards	GC

**Table S2. PFCAs and PFSA s considered in the study. Chemical formula, acronyms and standards supplier information.**

<b>Name</b>	<b>Acronym</b>	<b>Formula</b>	<b>Supplier</b>
<i>Analytes</i>			
Perfluoro-n-butanoic acid	PFBA	C4HF7O2	Wellington Laboratories
Perfluoro-n-hexanoic acid	PFHxA	C6HF11O2	Wellington Laboratories
Perfluoro-n-octanoic acid	PFOA	C8HF15O2	Wellington Laboratories
Perfluoro-n-nonanoic acid	PFNA	C9HF17O2	Wellington Laboratories
Perfluoro-n-decanoic acid	PFDeA	C10HF19O2	Wellington Laboratories
Perfluoro-n-undecanoic acid	PFUnA	C11HF21O2	Wellington Laboratories
Perfluoro-n-dodecanoic acid	PFDoA	C12HF23O2	Wellington Laboratories
Perfluorohexane sulfonic acid	PFHxS	C6HF13O3S	Wellington Laboratories
Perfluorooctane sulfonic acid	PFOS	C8HF17O3S	Wellington Laboratories
<i>Internal standards</i>			
Perfluoro-n-( <sup>13</sup> C <sub>4</sub> ) butanoic acid	<sup>13</sup> C <sub>4</sub> PFBA	<sup>13</sup> C <sub>4</sub> HF7O2	Wellington Laboratories
Perfluoro-n-(1,2,3,4,6- <sup>13</sup> C <sub>5</sub> ) hexanoic acid	<sup>13</sup> C <sub>5</sub> PFHxA	<sup>13</sup> C <sub>5</sub> CHF11O2	Wellington Laboratories
Perfluoro-n-( <sup>13</sup> C <sub>8</sub> ) octanoic acid	<sup>13</sup> C <sub>8</sub> PFOA	<sup>13</sup> C <sub>8</sub> HF15O2	Wellington Laboratories
Perfluoro-n-( <sup>13</sup> C <sub>9</sub> ) nonanoic acid	<sup>13</sup> C <sub>9</sub> PFNA	<sup>13</sup> C <sub>9</sub> HF17O2	Wellington Laboratories
Perfluoro-n-(1,2,3,4,5,6- <sup>13</sup> C <sub>6</sub> ) decanoic acid	<sup>13</sup> C <sub>6</sub> PFDeA	<sup>13</sup> C <sub>6</sub> C4HF19O2	Wellington Laboratories
Perfluoro-n-(1,2,3,4,5,6,7- <sup>13</sup> C <sub>7</sub> ) undecanoic acid	<sup>13</sup> C <sub>7</sub> PFUnA	<sup>13</sup> C <sub>7</sub> C4HF21O2	Wellington Laboratories
Perfluoro-n-(1,2- <sup>13</sup> C <sub>2</sub> ) dodecanoic acid	<sup>13</sup> C <sub>2</sub> PFDoA	<sup>13</sup> C <sub>2</sub> C10HF23O2	Wellington Laboratories
Sodium perfluoro-1-(2,3,4- <sup>13</sup> C <sub>3</sub> ) hexane sulfonate	<sup>13</sup> C <sub>3</sub> PFHxS	<sup>13</sup> C <sub>3</sub> C3HF13O3SNa	Wellington Laboratories
Sodium perfluoro-1-( <sup>13</sup> C <sub>8</sub> ) octanesulfonate	<sup>13</sup> C <sub>8</sub> PFOS	<sup>13</sup> C <sub>8</sub> HF17O3SNa	Wellington Laboratories

**Table S3. Information of the analysed samples. N.B. location was codified as N (North), C (Center), A (Algarve) and L (Lisbon).**

Sample type	Number of pooled individuals	Scientific name	Code	Matrix type	Location
Fish	50	<i>Trachurus trachurus</i>	HOM_MUSCLE_N	Muscle	N
Fish	10	<i>Trachurus trachurus</i>	HOM_MUSCLE_L	Muscle	L
Fish	40	<i>Trachurus trachurus</i>	HOM_MUSCLE_C	Muscle	C
Fish	50	<i>Trachurus trachurus</i>	HOM_LIVER_N	Liver	N
Fish	10	<i>Trachurus trachurus</i>	HOM_LIVER_L	Liver	L
Fish	40	<i>Trachurus trachurus</i>	HOM_LIVER_C	Liver	C
Fish	3	<i>Solea solea</i>	LING_MUSCLE_L	Muscle	L
Fish	6	<i>Solea solea</i>	LING_LIVER_L	Liver	L
Fish	6	<i>Microchirus azevia</i>	AZ_MUSCLE_L	Muscle	L
Fish	6	<i>Microchirus variegatus</i>	AZR_LIVER_L	Liver	L
Fish	5	<i>Trisopterus luscus</i>	BIB_LIVER_N	Liver	N
Clam <sup>1</sup>	36	<i>Spisula solida</i>	SSOL_N1_A	Whole body	N
Clam <sup>1</sup>	36	<i>Spisula solida</i>	SSOL_N2_A	Whole body	N
Clam <sup>2</sup>	8	<i>Spisula solida</i>	SSOL_N2_B	Whole body	N
Clam <sup>1</sup>	16	<i>Spisula solida</i>	SSOL_C_A	Whole body	C
Clam <sup>1</sup>	16	<i>Spisula solida</i>	SSOL_A_A	Whole body	A
Clam <sup>2</sup>	8	<i>Spisula solida</i>	SSOL_C_B	Whole body	C
Clam <sup>2</sup>	8	<i>Spisula solida</i>	SSOL_A_B	Whole body	A

<sup>1</sup>Campaign A: September 2020. <sup>2</sup>Campaign B: June 2022.

**Table S4. Instrumental parameters and transitions used for quantification (Q1) and confirmation (Q2), optimal collision energy (CE) and cone voltage (CV) values, deuterated compounds used as surrogate or internal standards (IS) and retention time (RT) for every analyte.**

<b>Compound</b>	<b>Q1</b>	<b>CE</b>	<b>Q2</b>	<b>CE</b>	<b>CV</b>	<b>IS</b>	<b>RT</b>
	m/z	(V)	m/z	(V)	(V)		(min)
<i>Analytes</i>							
PFBA	213 >169	10			20	<sup>13</sup> C <sub>4</sub> PFBA	4.6
PFHxA	313 >269	10	313 >119	28	18	<sup>3</sup> C <sub>2</sub> PFHxA	6.0
PFOA	413 > 369	20	413 >169	14	20	<sup>13</sup> C <sub>4</sub> PFOA	7.0
PFNA	463 >419	14	463 >219	22	22	<sup>13</sup> C <sub>5</sub> PFNA	7.3
PFDeA	513 > 469	14	513 >269	24	22	<sup>13</sup> C <sub>2</sub> PFDeA	7.6
PFUnA	563 >519	14	563 >169	32	22	<sup>13</sup> C <sub>2</sub> PFUnA	7.9
PFDoA	613 >569	16	613 >169	36	24	<sup>13</sup> C <sub>2</sub> PFDoA	8.1
PFHxS	399 >80	42	399 >99	35	67	<sup>13</sup> C <sub>3</sub> PFHxS	6.6
PFOS	499 >80	50	499 >99	40	78	<sup>13</sup> C <sub>8</sub> PFOS	7.1
<i>Internal standards</i>							
<sup>13</sup> C <sub>4</sub> PFBA	217 >172	10	-	-	20	-	4.6
<sup>13</sup> C <sub>5</sub> PFHxA	318 >273	10	-	-	18	-	6.0
<sup>13</sup> C <sub>8</sub> PFOA	421 >376	14	-	-	20	-	7.0
<sup>13</sup> C <sub>9</sub> PFNA	472 >427	14	-	-	22	-	7.3
<sup>13</sup> C <sub>6</sub> PFDeA	519 >274	24	-	-	22	-	7.6
<sup>13</sup> C <sub>7</sub> PFUnA	570 >525	14	-	-	22	-	7.9
<sup>13</sup> C <sub>2</sub> PFDoA	615 >169	36	-	-	24	-	8.1
<sup>13</sup> C <sub>3</sub> PFHxS	402 >80	42	-	-	67	-	6.6
<sup>13</sup> C <sub>8</sub> PFOS	507 >80	50	-	-	78	-	7.1

**Table S5. PFAS methodology performance parameters: linearity, instrumental precision, quantification limits (IQL), trueness and method precision.**

Compound	Linear range (ng/mL)	Determination coefficient (R <sup>2</sup> )	RSD (%)		IQL (ng/mL)	Trueness and precision (% R and %RSD)	MQL (ng/g)		
			1 ng/mL	100 ng/mL			25 ng/mL	Clam	Fish muscle
<b>PFBA</b>	0.5-100	0.9962	2	1	0.5	97 (10)	0.02	0.02	0.05
<b>PFHxA</b>	0.05-100	0.9995	7	9	0.05	82 (10)	0.002	0.002	0.004
<b>PFOA</b>	0.5-100	0.9941	10	11	0.5	66 (9)	0.01	0.01	0.03
<b>PFNA</b>	0.1-100	0.9977	9	10	0.1	110 (3)	0.004	0.005	0.01
<b>PFDeA</b>	0.1-100	0.9902	12	13	0.1	121 (25)	0.005	0.005	0.01
<b>PFOUnA</b>	0.5-100	0.9926	11	9	0.5	102 (23)	0.02	0.02	0.05
<b>PFDoA</b>	0.5-100	0.9919	14	10	0.5	132 (9)	0.03	0.03	0.07
<b>PFHxS</b>	0.1-100	0.9965	7	2	0.1	100 (1)	0.004	0.004	0.01
<b>PFOS</b>	0.05-100	0.9956	12	8	0.05	100 (6)	0.002	0.002	0.01

**Table S6. Compounds identified by LC-QTOF.**

Compound	CAS	No. clam samples detections (n=7)	No. fish tissue sample detections (n=11)	% Detection	ID Level	Uses
2,4-Dinitrophenol	51-28-5	0	1	6	1	Industrial chemical
2-hydroxy-hydroquinone	123-31-9	2	0	11	2a	Industrial chemical
3,4,5,6-Tetrahydrophthalic acid anhydride	2426-02-0	2	0	11	2a	Pesticide
3,5-di-tert-butylsalicylic acid	19715-19-6	0	6	33	1	Industrial chemical
3-Hydroxyphenylacetic acid	621-37-4	3	1	22	2a	Industrial chemical
4-Chlorophenol	106-48-9	2	8	56	2a	Industrial chemical
4-Hydroxybenzoic acid	99-96-7	4	11	83	1	Industrial chemical
4-Nitrophenol	100-02-7	7	8	83	1	Industrial chemical
4-Phenolsulfonic acid	98-67-9	0	4	22	2a	Industrial chemical
Aceclidine	827-61-2	2	0	11	2a	Pharmaceutical
Acesulfame	55589-62-3	1	0	6	1	Food additive
Acetanilide	103-84-4	7	11	100	2a	Industrial chemical
Adenosine / Vidarabin	58-61-7/ 24356-66-9	3	0	17	2a	Pharmaceutical
Allethrin	584-79-2	7	0	39	2a	Pesticide
Anhydroecgonine	127379-23-1	3	0	17	2a	Pharmaceutical
Anhydroecgonine methylester	43021-26-7	3	0	17	2a	Pharmaceutical
$\alpha$ -PBP / $\alpha$ -Pyrrolidinobutiophenone	13415-54-8	2	0	11	2a	Pharmaceutical
Benzododecinium	139-07-1	0	1	6	2a	Pharmaceutical
Bicalutamide	90357-06-5	0	2	11	2a	Pharmaceutical
Bisphenol S	80-09-1	0	1	6	1	Industrial chemical
2,4-dimethylformanilide	60397-77-5	2	2	22	2a	Pesticide
Canrenoic acid	2181-04-6	2	0	11	2a	Pharmaceutical
Caproylresorcinol	3144-54-5	1	2	17	2a	Industrial chemical
Carbamazepine	298-46-4	2	1	17	1	Pharmaceutical
Carbamazepine 10,11-epoxide	36507-30-9	2	1	17	1	Pharmaceutical
Diethyltoluamide	134-62-3	5	2	39	1	Pesticide
Denatonium	3734-33-6	3	2	28	2a	Industrial chemical
Diethyl phthalate	84-66-2	3	0	17	1	Industrial chemical

Compound	CAS	No. clam samples detections (n=7)	No. fish tissue sample detections (n=11)	% Detection	ID Level	Uses
Diprostene	81703-55-1	0	2	11	2a	Pharmaceutical
Dexpanthenol	81-13-0	4	0	22	2a	Cosmetic
Dimetridazole	551-92-8	0	2	11	2a	Pharmaceutical
Empenthrin	54406-48-3	3	2	28	2a	Pesticide
Ethinodiol diacetate	297-76-7	3	0	17	2a	Pharmaceutical
Ethyl 4-hydroxybenzoate	35285-68-8	3	0	17	1	Cosmetic
Etonogestrel	54048-10-1	1	2	17	2a	Pharmaceutical
Gepefrine	18840-47-6	2	2	22	2a	Pharmaceutical
Gestonorone	1253-28-7	0	1	6	2a	Pharmaceutical
Guazatine	108173-90-6	1	0	6	2a	Pesticide
Hydroxyethyl tetramethylpiperidinol	52722-86-8	1	0	6	2a	Industrial chemical
Hydroxyprogesterone acetate	302-23-8	0	2	11	2a	Pharmaceutical
Isoprocarb	2631-40-5	0	1	6	2a	Pesticide
Isopropyl 4-hydroxybenzoate	4191-73-5	2	0	11	2a	Cosmetic
Medrysone	2668-66-8	2	1	17	2a	Pharmaceutical
Mesterolone	1424-00-6	2	0	11	2a	Pharmaceutical
Metalaxyl	57837-19-1	4	6	56	1	Pesticide
Metamfepramone	15351-09-4	3	0	17	2a	Pharmaceutical
Metformin	657-24-9	3	0	17	1	Pharmaceutical
Methenolone acetate	434-05-9	2	0	11	2a	Pharmaceutical
Methoprene	40596-69-8	1	1	11	2a	Pharmaceutical
Methylsalicylate	119-36-8	4	2	33	1	Cosmetic
Morpholine	147-90-0	4	2	33	2a	Industrial chemical
Naphtalene sulfonic acid	85-47-2	1	5	33	1	Industrial chemical
Norethisterone	51-98-9	6	5	61	2a	Pharmaceutical
Norethynodrel	68-23-5	0	1	6	2a	Pharmaceutical
Phenylpiperazine	92-54-6	3	0	17	2a	Pharmaceutical
O-1918	536697-79-7	0	1	6	2a	Pharmaceutical
Octhilinone	26530-20-1	0	2	11	2a	Industrial chemical
p-(Aminomethyl)benzoic acid	56-91-7	4	4	44	2a	Pharmaceutical
Perfluoro-n-butanoic acid	375-22-4	2	2	22	1	Industrial chemical
Perfluoro-n-decanoic acid	335-76-2	4	8	67	1	Industrial chemical
Perfluoro-n-dodecanoic acid	307-55-1	2	2	22	1	Industrial chemical
Perfluoro-n-hexanoic acid	307-24-4	0	2	11	1	Industrial chemical
Perfluoro-n-nonanoic acid	375-95-1	0	2	11	1	Industrial chemical

Compound	CAS	No. clam samples detections (n=7)	No. fish tissue sample detections (n=11)	% Detection	ID Level	Uses
Perfluoro-n-octanoic acid	335-67-1	3	5	44	1	Industrial chemical
Perfluoro-n-undecanoic acid	2058-94-8	0	1	6	1	Industrial chemical
Perfluorooctane sulfonic acid	1763-23-1	0	6	33	1	Industrial chemical
Phenmetrazine	1707-14-8	3	0	17	2a	Pharmaceutical
Phenylephrine	61-76-7	3	3	33	2a	Pharmaceutica
Phenylpyruvic acid	156-06-9	2	0	11	2a	Industrial chemical
p-Phenetidine	156-43-4	7	3	56	2a	Industrial chemical
Saccharin	82385-42-0	1	0	6	1	Food additive
Salicylic acid	69-72-7	1	0	6	2a	Pharmaceutical
Sulpiride	15676-16-1	2	0	11	1	Pharmaceutical
Tapentadol	175591-09-0	0	1	6	2a	Pharmaceutical
Terbutryn	86-50-0	1	0	6	1	Pesticide
Thymotic acid	548-51-6	3	1	22	2a	Cosmetic
Tridemorph	24602-86-6	2	6	44	2a	Pesticide
Trifluoromethanesulfonic acid	1493-13-6	6	1	39	1	Industrial chemical
Tri-isobutyl phosphate	126-71-6	3	0	17	1	Industrial chemical
Tris(1-chloro-2-propyl) phosphate	13674-84-5	3	0	17	1	Industrial chemical
Valpromide	2430-27-5	2	1	17	2a	Pharmaceutical
Vigabatrin	60643-86-9	5	4	50	2a	Pharmaceutical

**Table S7. Compounds identified by GC-QTOF**

Compound	CAS	No. clam samples detections (n=7)	No. fish tissue sample detections (n=11)	% Detection	ID Level	Uses
1,1'-Biphenyl	92-52-4	6	5	61	1	Industrial chemical
1,2,3-Trichlorobenzene	87-61-6	0	3	17	1	Industrial chemical
1,2,4-Trichlorobenzene	120-82-1	4	3	39	1	Industrial chemical
1-Methylnaphthalene	90-12-0	1	4	28	1	Industrial chemical
2-(2-Chlorophenyl)-2-(4-chlorophenyl)-1,1-dichloroethene	3424-82-6	0	3	17	2a	Pesticide
2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3	1	3	22	1	Industrial chemical
2,2',3,4,4',5'-Hexachlorobiphenyl	35065-28-2	6	3	50	1	Industrial chemical
2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1	0	1	6	2a	Industrial chemical
2,2-Bis(4-chlorophenyl)-1,1-dichloroethylene	72-55-9	4	10	78	1	Industrial chemical
2,3,3',4,4',5-Hexachlorobiphenyl	38380-08-4	6	5	61	2a	Industrial chemical
2,3,3',4,4'-Pentachlorobiphenyl	32598-14-4	2	3	28	1	Industrial chemical
2,3',4,4',5-Pentachlorobiphenyl	31508-00-6	4	10	78	1	Industrial chemical
2,4,6-Tribromophenol	118-79-6	4	5	50	2a	Pesticide
2,6-Dibromophenol	608-33-3	4	0	22	1	Industrial chemical
2,6-Dichlorophenol	87-65-0	4	5	50	1	Industrial chemical
2,6-Diisopropylnaphthalene	24157-81-1	3	4	39	2a	Food additive
2,6-Di-tert-butyl-1,4-benzoquinone	719-22-2	0	5	28	1	Industrial chemical
2,6-Di-tert-butyl-4-methylphenol	128-37-0	0	4	22	1	Industrial chemical
2-Ethylhexyl 4-methoxycinnamate	5466-77-3	3	2	28	1	Cosmetic
2-Ethylhexyl salicylate	118-60-5	7	8	83	1	Cosmetic
2-Methylnaphthalene	91-57-6	3	2	28	2a	Industrial chemical
2-tert-Butyl-1,4-dihydroxybenzene	1948-33-0	3	5	44	1	Cosmetic
3,5-Di-tert-butyl-4-hydroxybenzaldehyde	1620-98-0	3	3	33	1	Cosmetic
4-Chlorophenol	106-48-9	0	8	44	1	Industrial chemical

Compound	CAS	No. clam samples detections (n=7)	No. fish tissue sample detections (n=11)	% Detection	ID Level	Uses
4-Formylaminoantipyrine	1672-58-8	0	2	11	2a	Pharmaceutical
4-Methylphenol	128-37-0	3	0	17	1	Industrial chemical
Acenaphthylene	208-96-8	2	0	11	1	Industrial chemical
Anthracene	120-12-7	3	0	17	1	Industrial chemical
Benzenesulfonamide	98-10-2	0	2	11	1	Pesticide
Benzyl butyl phthalate	85-68-7	4	5	50	1	Industrial chemical
Benzyl salicylate	118-58-1	3	2	28	1	Cosmetic
Bis(2-ethylhexyl) phthalate	117-81-7	1	0	6	1	Industrial chemical
Bisphenol A	80-05-7	3	5	44	1	Industrial chemical
Di-(2-ethylhexyl) terephthalate	6422-86-2	1	2	17	1	Industrial chemical
Dibenzyl phosphate	1623-08-1	1	0	6	1	Industrial chemical
Dibutyl phthalate	84-74-2	1	6	39	1	Industrial chemical
Diethyl phthalate	84-66-2	0	7	39	1	Industrial chemical
Diisobutyl phthalate	84-69-5	0	4	22	1	Industrial chemical
Diisodecyl phthalate	26761-40-0	0	3	17	1	Industrial chemical
Diphenyl ether	101-84-8	3	7	56	1	Industrial chemical
Diphenyl phosphate	838-85-7	0	4	22	1	Industrial chemical
Fluoranthene	206-44-0	6	8	78	2a	Industrial chemical
Fluorene	86-73-7	4	2	33	1	Industrial chemical
Galaxolide	1222-05-5	1	3	22	1	Cosmetic
Isobutyl 4-hydroxybenzoate	4247-02-3	3	0	17	1	Cosmetic
Naphthalene	91-20-3	3	9	67	1	Industrial chemical
N-Nitrosodiphenylamine	86-30-6	2	0	11	1	Industrial chemical
Oxybenzone (BP-3)	131-57-7	0	6	33	1	Cosmetic
Phenanthrene	85-01-8	5	5	56	1	Industrial chemical
Phenol	108-95-2	3	0	17	1	Industrial chemical
Pyrene	129-00-0	7	10	94	1	Industrial chemical

Compound	CAS	No. clam samples detections (n=7)	No. fish tissue sample detections (n=11)	% Detection	ID Level	Uses
Styrene	100-42-5	3	2	28	1	Industrial chemical
Tolyltriazole	29385-43-1	0	1	6	1	Industrial chemical
Tri-n-butyl phosphate	126-73-8	0	1	6	1	Industrial chemical
Triphenyl phosphate	115-86-6	0	4	22	1	Industrial chemical
Tris(1-chloro-2-propyl) phosphate	13674-84-5	0	3	17	1	Industrial chemical

**Table S8. Compounds identified by GC-QTOF (NIST.17).**

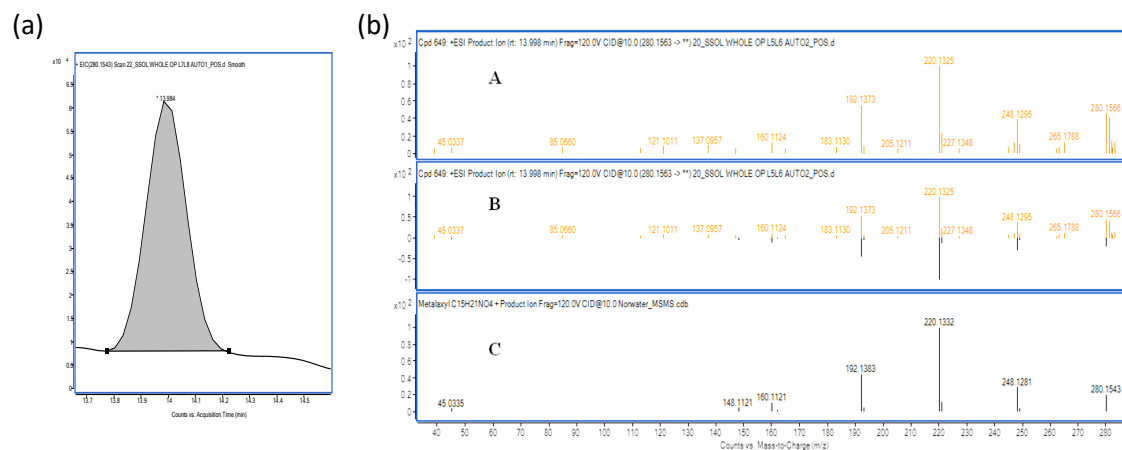
Compound	No. Clam samples detections (n=7)	No. Fish samples detections (n=11)	% Detection	ID Level	Uses
1,1'-Biphenyl, 2,2',3,3',4,4'-hexachloro-	1	1	11	3	Industrial chemical
1,1'-Biphenyl, 2,2',3,4,4',5',6-heptachloro-	1	3	22	3	Industrial chemical
1,1'-Biphenyl, 2,2',3,4,5,6'-Hexachloro-	1	1	11	3	Industrial chemical
1,1'-Biphenyl, 2,3,6-trichloro-	5	2	39	3	Industrial chemical
1,2-Benzenediol, O-dichloroacetyl-O'-(3-methylbut-2-enoyl)-	1	2	17	3	Industrial chemical
2,3,3',4,4',5,5'-Heptachloro-1'-methyl-1,2'-bipyrrole	0	1	6	3	Industrial chemical
2,4',6-Trichloro-1,1'-biphenyl	1	2	17	3	Industrial chemical
2,6-Dibromohydroquinone	1	2	17	3	Industrial chemical
2-Bromo dodecane	1	2	17	3	Industrial chemical
2-Bromotetradecane	0	1	6	3	Industrial chemical
2-Methyl-2-bromohept-6-en-3-one	1	3	22	3	Industrial chemical
2-Methyl-3-(2-chloro-5-hydroxyphenyl)-4(3H)-quinazolinone	1	0	6	3	Industrial chemical
2-Piperidinone, N-[4-bromo-n-butyl]-	0	1	6	3	Industrial chemical
2-Propanol, 1-chloro-, phosphate	2	1	17	3	Industrial chemical
3-Chlorophenol, trimethylsilyl ether	1	1	11	3	Industrial chemical
3-Chloropropionic acid, heptadecyl ester	1	2	17	3	Industrial chemical
3-Methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	1	2	17	3	Industrial chemical
4-Chlorobenzoic acid, 4-nitrophenyl ester	2	1	17	3	Industrial chemical
4-Ethylbenzoic acid, 2,3-dichlorophenyl ester	0	1	6	3	Industrial chemical
9,12-Octadecadienoyl chloride, (Z,Z)-	1	5	33	3	Industrial chemical
Benzaldehyde, 2-chloro-	1	0	6	3	Industrial chemical
Benzene, 1,2,3-trichloro-	1	1	11	3	Industrial chemical
Cyclohexane, 1-bromo-4-methyl-	1	2	17	3	Industrial chemical
Cyclohexene, 3-bromo-	1	0	6	3	Industrial chemical

Compound	No. Clam samples detections (n=7)	No. Fish samples detections (n=11)	% Detection	ID Level	Uses
Decane, 1-bromo-2-methyl-	0	4	22	3	Industrial chemical
Methane, dibromo-	2	0	11	3	Industrial chemical
p,p'-DDE	1	0	6	3	Industrial chemical
Palmitoyl chloride	2	0	11	3	Industrial chemical
Pentane, 3-bromo-	1	0	6	3	Industrial chemical
Phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-	1	0	6	3	Industrial chemical
Phenol, 2,4-dibromo-	2	0	11	3	Industrial chemical
Phenol, 2,6-dibromo-	1	0	6	3	Industrial chemical
Phenol, 4-chloro-	4	0	22	3	Industrial chemical
Phosphoric acid, 2-chloroethenyl dimethyl ester	1	0	6	3	Industrial chemical
Phthalic acid, 8-chlorooctyl ethyl ester	1	0	6	3	Industrial chemical
Propanoic acid, 3-chloro-, 4-formylphenyl ester	1	0	6	3	Industrial chemical
Terephthalic acid, 2-bromo-4-fluorophenyl octyl ester	1	0	6	3	Industrial chemical
Terephthalic acid, 3-chlorophenyl octyl ester	2	0	11	3	Industrial chemical

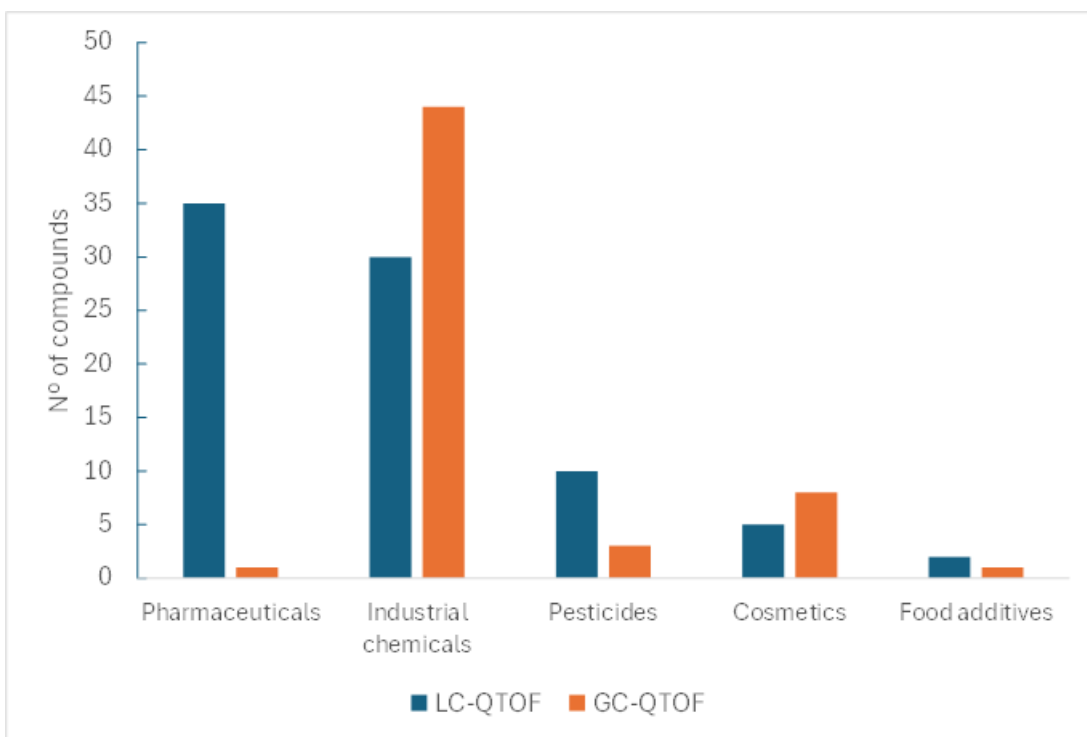
**Table S9. Permitted levels (ng/g) of  $\Sigma$ PFAS, PFOA, PFOS, PFNA and PFHxS in bivalve mollusc, fish muscle and HOM muscle.**

	<b>Bivalve mollusc</b>	<b>Fish muscle (general)</b>	<b>HOM muscle not intended for infant feed</b>
Permitted level $\Sigma$ PFAS (ng/g) ww (1)	5	2	8
Permitted level PFOA (ng/g) ww (1)	0,7	0,2	1
Permitted level PFOS (ng/g) ww (1)	3	2	7
Permitted level PFNA (ng/g) ww (1)	1	0,5	2,5
Permitted level PFHxS (ng/g) ww (1)	1,5	0,2	0,2

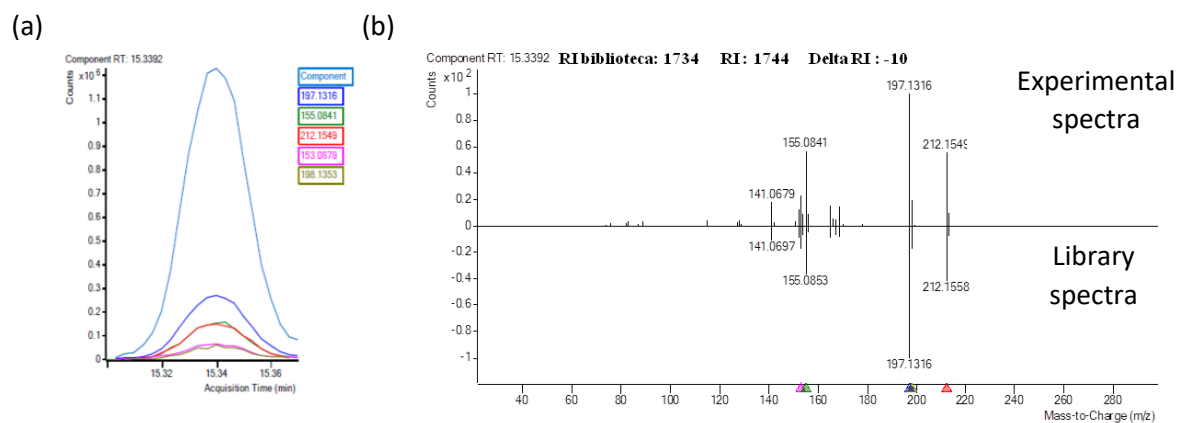
(1) Established in the Regulation 2023/915 section 4.2



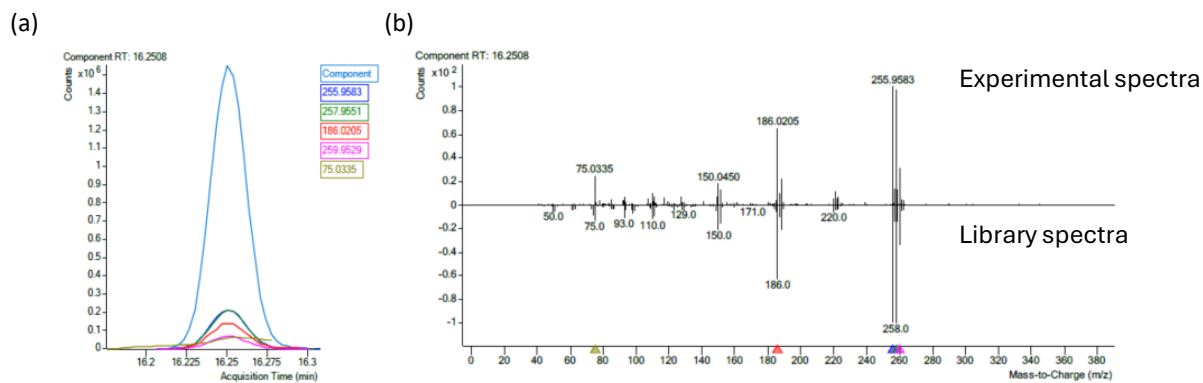
**Figure S1. Chromatogram and comparison of experimental spectrum obtained at 10V collision energy (A) and spectrum contained in library (C) for metalaxyl. (B) shows the comparison of both spectra.**



**Figure S2. Number of compounds identified by LC-QTOF (blue) and GC-QTOF (orange) according to their usage.**



**Figure S3. Chromatogram (a) and comparative of sample spectra (liver of pout sample) and library spectra (b) for 2,6-diisopropyl-naphthalene.**



**Figure S4. Chromatogram and comparative of sample spectra (clam sample) and library spectra for the 2,3,6-trichloro-1,1'-biphenyl (PCB 24).**