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Research Article

# Occurrence and intake risk assessment of high production volume chemicals in highly consumed seafood species

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ABSTRACT

High production volume chemicals (HPVCs) found in the environment and fish may pose health risks through dietary intake. This study measured the levels of 30 HPVCs in the ten most consumed fish species in Spain over one year. The compounds with the highest average concentrations were di-(2-ethylhexyl) phthalate (740.8 ng/g dw (dry weight)), di-(2-ethylhexyl)-adipate (675.8 ng/g dw), and galaxolidone (579.0 ng/g dw). The highest intake values were recorded in Atlantic tuna, with 51.0 ng/(kg bw·day) in the high-consumption scenario. Non-carcinogenic risks were greatest for benzosulfonamides, particularly in sardine and Atlantic tuna. Carcinogenic risk factors were highest for Atlantic mackerel and tuna but remained below European Food Safety Authority safety limits, suggesting low concern for public health. Long-term monitoring provided a more accurate estimate of dietary exposure and associated health risks.

## 1. Introduction

The Organization for Economic Co-operation and Development (OECD) and the Environmental Protection Agency (EPA) play key roles in international economic and environmental policymaking. In 2004 the OECD published a list of High Production Volume Chemicals (HPVC) (OECD, 2004) with many of the compounds also classified by the EPA (EPA, 2004). This list contains all chemicals that are produced at levels above 1000 tons per year in at least one member country of the OECD. Due to their high production, many of these compounds have toxicological characteristics for humans and the ecosystem (OECD, 2004). The presence of HPVC has been reported in different environmental compartments (Estévez-Danta et al., 2021; He et al., 2019; Shi et al., 2019), including the marine environment (Hou et al., 2024; Yang et al., 2023; Xie et al., 2024) and fish (Aminot et al., 2023; Castro et al., 2023a; Sala et al., 2022). Due to all these routes of exposure, these chemicals can be incorporated into the human diet and can cause health problems for the population (Hou et al., 2024; Pantelaki and Voutsa, 2020; Pardo et al., 2014; Trabalón et al., 2015).

HPVC encompass a wide range of families but in this study, we focus on those considered to be of greatest interest. One of these families is synthetic musk fragrances, which are used in the production of most detergents, fabric softeners, cleaning products and cosmetic products (Duedahl-Olesen et al., 2005). Although their effects on the population and their toxicity have not yet been confirmed, musk fragrances are believed to act as endocrine disruptors (Ros et al., 2015). Galaxolide (HHCB) and tonalide (AHTN) are the two predominant compounds in polycyclic musks. The European Union has regulated the use of AHTN in the cosmetic industries (Directive 2008/42/EC) (Trabalón et al., 2015) and macrocyclic musks have emerged as an alternative. However, macrocyclic musks are very costly to synthesize (Vallecillos et al., 2015) and therefore polycyclic musks are still produced.

Another family is organophosphate esters, which are used as flame retardants and plasticizers in a wide range of household products such as furniture, plastic materials, electronic materials, etc. Organophosphate esters emerged as an alternative to brominated flame retardants (BFRs), which are widely used along with hexabromocyclododecane (HBCD) and polybrominated diphenyl esters (PBDE). The ban on the use of BFRs exponentially increased the use of organophosphate flame retardants and they are now ubiquitous in our environment (Castro et al., 2020; García-Garcinuño et al., 2024; Giulivo et al., 2017; Pantelaki and Voutsa, 2020). Furthermore, it is known that high concentrations of organophosphate esters (OPEs) can cause adverse health effects such as neurotoxicity and reproductive toxicity, and they have carcinogenic, mutagenic, and even endocrine disrupting effects (Xu et al., 2015).

Benzothiazoles are another family. They are used in the production of rubber as vulcanization accelerators, in the manufacture of paper and leather as biocides, in the manufacture of antifreezes as inhibitors of corrosion, as fungicides and herbicides and as stabilizers of ultraviolet light in plastics and textiles (Trabalón et al., 2017). To date, some studies have shown that benzothiazole and its derivatives exhibit dermal sensitizers and respiratory tract irritants (Asimakopoulos et al., 2013).

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Benzothiazole (BT) has a food limit of 0.05 mg/kg according to the European Food Safety Authority (EFSA, 2016).

HPVC also include benzosulfonamides, which are used in various industrial applications. Examples of these compounds are para-toluesulfonamide (p-TSA), used as a plasticizer and in the manufacture of pharmaceuticals and pesticides, and it is the main byproducts of chloramine-T (a disinfectant used in the food industry); and ortho-toluesulfonamide (o-TSA), which is primarily used in the production of an artificial sweetener (e.g., saccharin) and benzosulfonamide (BSA), which is used in synthetics dyes, phytochemicals and disinfectants (Castro et al., 2023b; Richter et al., 2008a). There are very few studies on the toxicity of benzosulfonamides, despite their widespread use in industry.

Phthalic acid esters (PAEs) are used as plasticizers in the plastic industry and some are also used as solvents and fragrance fixatives. To date, many studies have shown that PAEs are of particular concern to humans since they are considered to have endocrine-disrupting and carcinogenic effects (Paluselli et al., 2018). The EFSA technical committee established tolerable dietary intake limits (TDI) for certain phthalates in 2007 (EU, 2007). Currently, plastic materials used in relation to food that is marketed in the European Union must comply with Regulation (EU) no 10/2022 (EU, 2012) and Framework Regulation 1935/2004 (EU, 2004) on plastic materials and objects in contact with foods.

However, despite these regulations, most of these HPVC continue to be found in marine species. In a recent study, musk fragrances were detected in 87 % of all the analyzed fish samples (including mackerel, pomfret, halibut and hairtail) with concentrations ranging from 0.15 to 85.2 ng/g ww (wet weight) (Tran-Lam et al., 2024). These fragrances are extensively studied in fish samples due to their high presence, as in the case of HHCB and AHTN, which were found up to concentrations of 2619 ng/g ww and 349 ng/g ww in species such as tilapia, carp and sea bream (Yao et al., 2018). OPEs haven been detected in numerous fish samples, as their high toxicity increases the concern about the presence in food products. Li et al. (2022) analyzed OPEs in fish muscle samples with a range of 2.04 to 22.94 ng/g ww. OPEs have been found in different fish species such as cod, hake, mackerel and salmon with a mean concentration of 5.3 ng/g ww, with tributyl phosphate (TBP), tri-isobutyl phosphate (TiBP) and tris (2-chloroisopropyl) phosphate (TCPP) as the main contaminants (Castro et al., 2020). There are few studies on the concentration of benzothiazoles and benzosulfonamides in fish. Their presence was confirmed by studies such as Chen et al. (2020) in which mackerel samples were analyzed, finding BT concentrations between 15.4 and 26.1 ng/g (dw). Phthalates are present in many environments and have been determined in fish samples, such as in Sambolino et al. (2022), which found maximum concentrations of DEHP (44.1 ± 2.1 ng/g ww) and DiBP (10.2 ± 3.4 ng/g ww). DEHP has also been found to have a high mean concentration of 83.3 ng/g dw) in fish species such as crab and sea bass (Lee et al., 2019).

Due to increasing consumer awareness and expectations about food safety, a wide range of analytical methods have been developed for determining specific families of HPVC in fish samples. However, few methods include a wild range of HPVC. These procedures include many extraction techniques, ranging from Soxhlet extraction (He et al., 2019), solid-liquid extraction (SLE) (Lorenzo et al., 2018; Poma et al., 2018), microwave-assisted extraction (MAE) (Navarro et al., 2010), ultrasound-assisted extraction (USAE) (Kowalski and Płaszczyk, 2017; Malarvannan et al., 2015; Santín et al., 2016), pressurized liquid extraction (PLE) (Brandsma et al., 2015; Gao et al., 2014; Kim et al., 2011; Mcgoldrick et al., 2014; Giulivo et al., 2017) and QuEChERS extraction (Castro et al., 2023a; Hidalgo-Serrano et al., 2021; Sambolino et al., 2022). After extraction, many of the methods include a clean-up step, such as gel permeation chromatography (GPC) (Giulivo et al., 2017), and solid phase extraction (SPE) (Kowalski and Płaszczyk, 2017). Another cleaning technique used is the LipiFiltr® cartridge from United Chemical (UCT) (Castro et al., 2020; Hidalgo-Serrano et al., 2021). The most commonly used analysis techniques are liquid (Chen et al., 2020; Hidalgo-Serrano et al., 2020; Panio et al., 2020) and gas chromatographic techniques (Castro et al., 2023b, 2020; Sambolino et al., 2022).

The aim of this study is to monitor, over the course of one year, the concentration of thirty high-production-volume chemicals from five compounds families (benzothiazoles, benzosulfonamides, organophosphate esters, phthalates acid esters and synthetic musk fragrances) found in ten of the most consumed fish species in Spain. These data will be used to determine dietary intake and characterize the health risk for the population. An analytical method will be developed to determine these contaminants in the muscle part of the fish, based on gas chromatography coupled with mass spectrometry.

## 2. Materials and methods

### 2.1. Reagents and standards

Dr. Ehrenstorfer™ (Augsburg, Germany) provided four polycyclic musks (MUSKs) for the study: 7-acetyl-1,1,3,4,4,6-hexamethyl-1,2,3,4-tetrahydronaphtalene (Tonalide, AHTN), 5-acetyl-1,1,2,6-tetramethyl-3-isopropylindane (Traseolide, ATII), 6,7-dihydro-1,1,2,3,3-pentamethyl-4-(5H)indanone (Cashmeran, DPMI), and 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylcyclopenta-[g]−2-benzopyran (Galaxolide, HHCB). Toronto Research Chemicals (Toronto, Canada) provided 4,6,7,8-Tetrahydro-4,6,6,7,8,8-hexamethyl-cyclopenta[g]−2-benzopyran-1(3H)-one (Galaxolidone, HHCB-lactone). The internal standard, $d_{15}$-musk xylene ($d_{15}$−MX), was also supplied by Dr. Ehrenstorfer™. Sigma Aldrich (St. Louis, USA) provided nine OPEs for the study: tri-isobutyl phosphate (TiBP), tris (2-ethylhexyl)-phosphate (TEHP), tris (2-chloroethyl)-phosphate (TCEP), tris (2-chloroisopropyl) phosphate (TCPP), triethyl phosphate (TEP), triphenyl phosphate (TPP), 2-ethylhexyl-diphenyl-phosphate (EHDPP), tributyl phosphate (TBP), and tritolyl phosphate (TTP). The internal standard, tributyl phosphate deuterated (TBP-$d_{27}$), was supplied by Sigma Aldrich, which also provided five benzothiazoles (BTs) for the study: 2-aminobenzothiazole ($NH_2$BT), benzothiazole (BT), 2-(methylthio)-benzothiazole (MeSBT), 5-chloro-1-benzothiazole (ClBT), and 2-hydroxybenzothiazole (OHBT). The internal standard, benzothiazole deuterate (BT-$d_{27}$), was supplied by the same company. Sigma Aldrich also supplied five benzosulfonamides (BSAs): ortho-toluesulfonamide (o-TSA), N-ethyl-para-toluesulfonamide (Et-p-TSA), N-methyl-para-toluesulfonamide (Me-p-TSA), para-toluesulfonamide (p-TSA) and benzosulfonamide (BSA). Ortho-toluesulfonamide deuterated (TSA-p-$d_4$) was the internal standard supplied by Sigma Aldrich. In addition, Sigma Aldrich supplied six standards of PAEs for the study: diethyl phthalate (DEP), dimethyl phthalate (DMP), di-(2-ethylhexyl)-adipate (DEHA), isobutyl phthalate (DiBP), di-(2-ethylhexyl)-phthalate (DEHP) and di-n-octyl phthalate (DnOP). Di-(2-ethylhexyl)phthalate deuterated (DEHP-d4) was used as the internal standard and was supplied by Sigma Aldrich.

We used ethyl acetate and acetonitrile gas chromatography (GC) grade with purity > 99.9 % from JT Baker (Deventer, The Netherlands). Helium and nitrogen gas with 99.999 % purity from Carburos Metálicos were used for the chromatographic analysis (Tarragona, Spain). We used ultrapure water acquired through a Millipore purification system (Massachusetts, USA).

A working mixture solution of 100 µg/mL was prepared in ethyl acetate, containing all the compounds except for the internal standards and HHCB-lactone. For the internal standards a working mixture solution of 100 µg/mL in ethyl acetate was also prepared. An individual working solution for HHCB-lactone was prepared at the same concentration with the same solvent.

### 2.2. Sampling and sample pre-treatment

A total of forty samples of the ten species most consumed by the Spanish population were collected every four months over the course of one year. The species were purchased in October 2022, February 2023,

June 2023, and October 2023. All samples were acquired from a central market in Tarragona, Spain, and all sample characteristics are summarized in **Appendix A Table S1**.

The selected species were divided into two groups: species with a high lipid content and species with a low lipid content. The high lipid content species selected were Atlantic bluefin tuna (*Thunnus thynnus*), Atlantic mackerel (*Scomber scombrus*), swordfish (*Xiphias gladius*), sardine (*Sardina pilchardus*) and rooved carpet shell or palourde clam (*Ruditapes decussatus*). The low lipid content species selected were European hake (*merluccius*), blue whiting (*Micromesistius poutassou*), sea bream (*Sparus aurata*), sea bass (*Dicentrarchus labrax*) and European squid (*Loligo vulgaris*). After collecting the samples, the fish were dissected, and the clams were taken out of their shells. All the samples were stored in a freezer at −17 °C for one day and then lyophilized using a miVac Duo system from Genevac (Ipswich, United Kingdom). Once lyophilized, the samples were stored in a dry place at 20 °C.

### 2.3. Analytical methods

The extraction method was based on a previous study (Castro et al., 2020). A total of 0.1 g of lyophilized sample was weighed into a 50 mL centrifuge tube, 10 mL of acetonitrile and 10 mL of ultrapure water were added, and the tube was shaken for 1 min. A QuEChERS extraction salt pack containing 4 g of magnesium sulphate and 1 g of sodium chloride was then added. The QuEChERS salt packet was supplied by Scharlab (Barcelona, Spain). The mixture was mixed with a vortex during 3 min then centrifuged for 5 min at 4000 r/min in a Hettich Universal 32R (Tuttlingen, Germany). The supernatant was removed and transferred into a 20 mL vial with the aid of a syringe connected to a LipiFiltr cartridge for lipid clean-up, supplied by United Chemical Technologies (Bristol, PA). Once transferred, the solution was evaporated under a gentle stream of nitrogen gas to approximately 1 mL. The solution was filtered with a 0.22 μm PTFE syringe filter (Biosigma, Cona, Venice, Italia). Subsequently, 100 μL of 1 ppm internal standard solution was added to obtain a final concentration of 50 μg/L. Finally, the solution was reconstituted to a volume of 2 mL with ethyl acetate.

We used an Agilent 7890A GC system coupled to a triple quadrupole mass spectrometer (Agilent Technologies, Palo Alto, California, USA). The column used was a ZB-50 (30 m × 0.25 mm × 0.25 μm film thickness) from Phenomenex (Torrance, California, USA). The oven temperature gradient was: 75 °C (for 2.87 min) and then 300 °C at 15 °C/min (maintained 10 min). An Agilent multimode input (MMI) large volume injector was used to inject 25 μL. A solvent ventilation mode was employed with a temperature gradient, beginning at an initial temperature of 75 °C (for 0.37 min) and then at 325 to 600 °C/min (maintained for 5 min). Helium was used at a constant flow of 1.2 mL/min as a carrier gas. The total time was 27.87 min with a solvent delay of 3 min. We used a triple quadrupole mass spectrometer with the electron ionization mode at 70 eV. The temperatures were 280 °C for the ionization source, 150 °C for the first quadrupole and 150 °C for the second quadrupole. An multiple reaction monitoring (MRM) mode was used with one quantifier ion and two qualifier ions for the confirmation of each compound. The GC Mass Hunter software acquisition program was used and the collision energies for each transition were optimized with the GC–MS Optimizer program. All transitions are summarized in **Appendix A Table S2**.

### 2.4. Exposure assessment and risk characterization

To evaluate the risk of these contaminants for human health, the calculations recommended by the European Food Safety Authority (EFSA, 2012a) and the Environmental Protection Agency (EPA, 2022) were conducted. It is essential to include consumption data studies in the characterization of the dietary exposure in the population. The dietary exposure of each contaminant $t$ (ng/(kg bw·day)) was calculated using Eq. (1) (EFSA, 2012a):

$$E_t = \sum_{f=1}^{p} C_f X_{t,f} \quad (1)$$

where, $C_f$ (g/(kg bw·day)) is the average consumption of each fish species $f$ according to the survey of the Ministry of Agriculture, Fisheries and Food (SG, 2023) and $X_{t,f}$ (ng/g) is the concentration of contaminant $t$ in the specie $f$. The calculations were performed taking into account two possible scenarios for the population: the low-bond scenario and the high-bond scenario. The low-bond scenario was performed with the geometric mean of the samples for each compound and the high-bond scenario was performed with the 95th percentile.

Characterizing the health risk involved separate calculations for non-carcinogenic and carcinogenic compounds. The health risk for non-carcinogenic compounds was calculated using Eq. (2) (EPA, 2022).

$$R_t = \left( \frac{E_t}{\mathrm{ADI}_t} \right) \times 100 \quad (2)$$

where, $R_t$ is the non-carcinogenic risk factor, $E_t$ is the dietary exposure of chemical $t$ (g/(kg bw·day)), and $\mathrm{ADI}_t$ is the acceptable dietary intake exposure for the given chemical $t$ (g/(kg bw·day)). The $\mathrm{ADI}_t$ values were calculated for each compound from the no-observed-adverse-effect-level (NOAEL) divided by a factor of 100 (EFSA, 2005). The NOAEL values can be found in supplementary **Appendix A Table S3**.

For carcinogenic compounds the risk was calculated with Eq. (3) (EPA, 2022).

$$\mathrm{MOE}_t = \frac{\mathrm{BMD}_t}{E_t} \quad (3)$$

where, $\mathrm{MOE}_t$ is the margin of exposure for compound $t$, $\mathrm{BMD_t}$ is the reference dose for compound $t$ (g/(kg bw·day)) and $E_t$ is the dietary exposure for compound $t$ (g/(kg bw·day)). The $\mathrm{BMD}_t$ values can be found in **Appendix A Table S3**. In the treatment of results, in cases where a certain value had a concentration below the method detection limit (MDL) and therefore had a non-detected concentration (n.d.), in order to perform the risk calculations it was assumed that the concentration was half of the MDL, according to World Health Organization recommendations (WHO, 2009).

## 3. Results and discussion

### 3.1. Validation of the analytical method

The analytical method used was based on the method developed in Castro et al. (2020). The method was tested for those compounds not previously analyzed, such as musk fragrances, and favorable extraction results were obtained.

Excellent linearity ($R^2 > 0.999$) was observed for all the compounds, with an instrumental range between 0.005 and 250 μg/L. Apparent recoveries ($R_{app}$) were calculated for high and low lipid content samples. The sardine species was used for the high lipid content samples, and sea bass was used for the low lipid content samples. The 0.1 g sample was spiked at a concentration of 2000 ng/g ($n$ = 5). The $R_{app}$ for the high lipid samples ranged from 37 % to 130 % (except for EHDTT and DnOP) and for the low lipid samples from 38 % to 128 % (except for DiBP). No difference was observed between high lipid and low lipid samples when the analytical method was carried out; therefore, the following parameters are shown those calculated using the sea bass sample matrix.

The method detection limits (MDLs) and the method qualification limits (MQLs) were estimated from the $R_{app}$ and the instrumental detection limit (0.001–0.01 ng/g dw) and the instrumental quantification limit (0.005–0.5 ng/g dw), respectively. The MDL ranged from 0.01 to 0.15 ng/g dw and the MQLs, ranged from 0.06 to 7.2 ng/g dw.

The repeatability (intra-day precision) values (%RSD, $n$ = 5, 2000 ng/g dw) of the method were below 25 % (except for BSA and

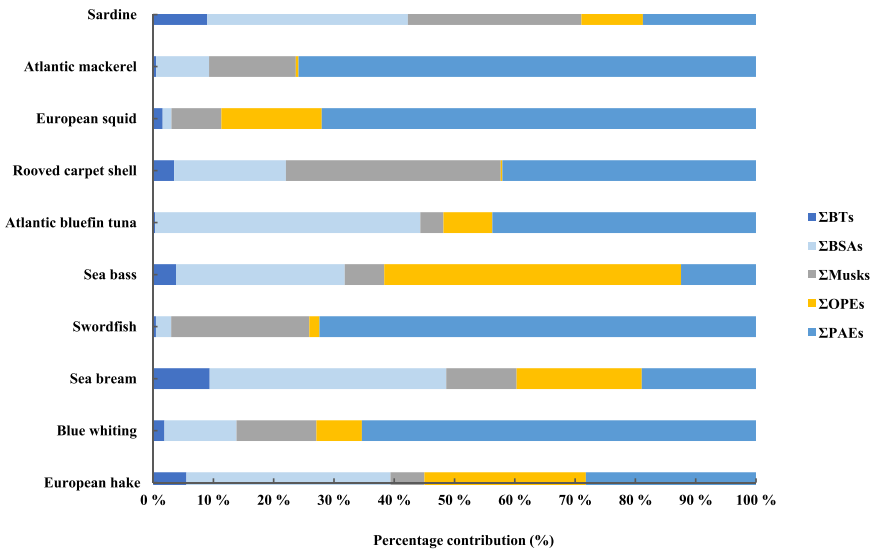


**Fig. 1 –** Total contribution (%) of each family of contaminants for each species analyzed. BTs: benzothiazoles; BSAs: benzosulphonamides; Musks: musk fragrances; OPEs: organophosphates esters; PAEs: phthalates.

DEHA, which were 27 %). The reproducibility (inter-day precision) between days values (%RSD, $n = 5$, 2000 ng/g dw) of the method was below 25 %, except for five compounds, which were mainly PAEs. Therefore, the method obtained a satisfactory validation and all the parameters are listed in **Appendix A Table S4**.

### 3.2. Occurrence of HPVC in seafood

The method was applied to samples of the ten most consumed fish for the Spanish population, according to the report of the Ministry of Agricultura, Fisheries and Food (SG, 2023), because the objective was to determine the compounds found in the fish consumed by the population in the area. For musk fragrances, HHCB-lactone was also determined as a degradation product of HHCB, one of the most used fragrances (Trabalón et al., 2015). In total, thirty compounds were determined in forty samples. Tables 1 and 2 contain the geometric mean (ng/g dw), the minimum and maximum concentrations (ng/g dw) and the detection frequency (%) for each fish species.

The results showed significant differences among the specimens of the same species. This may be due to the different origin of the specimens even though they all were purchased in the Tarragona central market. It has to be highlighted that our aim was to evaluate the health risk for the population through consumption.

The mean concentration of BTs, BSAs, MUSKs, OPEs and PAEs were 19.0, 123.3, 91.9, 72.2 and 283.3, respectively, which demonstrates that there is a high concentration of PAEs. We found predominant compounds within the families. For PAEs a maximum concentration of DEHP (5530.1 ng/g dw) was found in the blue whiting species. For musk fragrances, the maximum was found in HCCB-lactone, with a concentration of 2441.0 ng/g dw in the squid species. In the benzothiazoles, $NH_2BT$ was found with a maximum concentration of 911.8 ng/g dw in sea bream, and in the benzosulfonamides, o-TSA with a value of 3227.8 ng/g dw in Atlantic tuna. Finally, in the OPEs, TPP was found with a value of 7480.3 ng/g dw in sea bass. Regarding the detection frequencies of the different compounds, Me-p-TSA and DMP were detected in 78 % of the samples, followed by TTP in 60 %. TCEP was the only compound not detected in any sample, and BT, ClBT, OHBT, BSA and TBP were only detected in a few samples (DF < 15 %).

Phthalates represents the major contribution of contaminants in most species, followed by MUSKs and BSAs, as illustrated in Fig. 1. However, OPEs and BTs are observed to have a minor contribution in most species. Regarding the highest presence of contaminants within species, we found that sardines and sea breams are the species with the highest contribution of BTs. BSAs are found in the Atlantic tuna and sardine species. For the MUSK fragrances the Rooved carpet shell and sardine stand out, and for the OPEs the sea bass and European squid species stands out with a higher percentage of contaminants. Finally, the highest contribution of PAEs was found in the Atlantic mackerel and European squid species.

The BTs are the compounds with the lowest mean concentration as they were only detected in a few samples and at low concentrations. Regarding the distribution of the detected compound in the same family group in terms of concentrations, BTs showed a trend of $NH_2BT$ > MeSBT > ClBT > BT > OHBT, with a different mean concentration between 2.27 ng/g dw (OHBT) and 62.9 ng/g dw ($NH_2BT$). These compounds have been determined in other studies, such as Trabalón et al. (2017), who found similar concentrations to those of our study. Their concentrations vary between 6 and 82 ng/g dw for four benzothiazoles in commonly consumed marine species, such as cod, hake and salmon, with BT being present at the highest concentration (82 ng/g dw), followed by $NH_2BT$, ClBT and MeSBT.

The BSA concentrations showed the following pattern: o-TSA > Me-p-TSA > p-TSA > Et-p-TSA > BSA. The mean concentrations were between 5.4 ng/g dw for BSA and 206.0 ng/g dw for o-TSA. Although there is little available information, a few authors suggest that wastewater treatment facilities are capable of inducing the bioconversion/biodegradation of high-molecular-weight benzosulfonamides (Ajibola et al., 2015; Richter et al., 2008b). Despite this, some studies, such as Castro et al. (2023a), have found two compounds of the benzosulfonamide family, Et-p-TSA and BSA, with maximum concentrations of 165.7 and 138.76 ng/g ww, respectively, in mackerel species.

The following trend in concentrations is observed in the occurrence of musk fragrances within the same family group: HHCB-lactone > ATII > DPMI > AHTN > HHCB. Notably, there was a significant difference in the mean concentration between HHCB (6.47 ng/g dw) and HHCB-lactone (578.9 ng/g dw). The primary metabolite of HHCB, HHCB-lactone, was detected in high concentrations and with a high frequency. In contrast, HHCB was detected at low concentrations, possibly due to its rapid degradation. In Cunha et al. (2018), a maximum concentration of 414.4 ng/g dw for HHCB was reported in plaice and sole, while for HHCB-lactone the maximum concentration was 228.5 ng/g dw in mackerel. Other authors, such as Vallecillos et al. (2015), also detected HHCB and HHCB-lactone in fish samples (red mullet, sea bream, turbot, perch, sheatfish and carp) with a concentration between 2.9-18.4 ng/g dw and n.d.-15.9 ng/g dw, respectively. In the same study, the compounds DPMI and AHTN were determined in concentrations ranging from 12.8 to 33.5 ng/g dw and 1.1 to 8.4 ng/g dw, respectively.

**Table 1 –** Mean and range of concentrations in ng/g (dw) and percentage of detection frequency (%DF) of benzothiazoles, benzosulfonamides and musk fragrances.

| | | *Benzothiazoles* | | | | | *Benzosulfonamides* | | | | | *Musk fragrances* | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | BT | ClBT | MeSBT | OHBT | NH2BT | BSA | o-TSA | Me-p-TSA | p-TSA | Et-p-TSA | ATII | DPMI | HHCB | AHTN | HHCB-lactone |
| European hake | Mean | n.d | n.d | n.d | n.d | 41.9 | 7.8 | 20.8 | 207.1 | 1.7 | 0.7 | 0.01 | 1.9 | 8.4 | 10.8 | 21.5 |
| *Merluccius merluccius* | range | n.d | n.d | n.d | n.d | n.d - 167.4 | n.d - 31.0 | n.d - 81.2 | 5.5 - 783.6 | n.d - 3.5 | n.d - 2.6 | n.d | n.d - 7.4 | n.d - 33.6 | n.d - 43.2 | n.d - 76.0 |
| | %DF | 0 | 0 | 0 | 0 | 25 | 25 | 50 | 100 | 50 | 50 | 0 | 25 | 25 | 25 | 50 |
| Blue whiting | mean | n.d | 4.6 | 3.2 | n.d | 48.2 | n.d | 119.5 | 116.1 | 8.7 | 2.1 | 0.01 | 8.1 | 7.0 | n.d | 380.7 |
| *Micromesistius poutassou* | range | n.d | n.d - 18.3 | n.d - 12.6 | n.d | n.d - 192.8 | n.d | n.d - 477.8 | 7.1 - 375.3 | n.d - 34.7 | n.d - 8.4 | n.d | n.d - 32.1 | n.d - 27.9 | n.d | n.d - 1260.2 |
| | %DF | 0 | 25 | 25 | 0 | 25 | 0 | 25 | 100 | 25 | 25 | 0 | 25 | 25 | 0 | 50 |
| Sea bream | mean | n.d | 4.7 | 7.5 | 3.8 | 228.0 | n.d | 346.1 | 288.9 | 3.7 | 38.01 | 0.01 | 0.01 | 4.1 | n.d | 299.3 |
| *Sparus aurata* | range | n.d | n.d - 18.8 | n.d - 27.4 | n.d - 14.9 | n.d - 911.8 | n.d | n.d - 1119.5 | 4.6 - 1072.8 | n.d - 14.6 | n.d - 152.2 | n.d | n.d | n.d - 16.3 | n.d | n.d - 1041.1 |
| | %DF | 0 | 25 | 50 | 25 | 25 | 0 | 50 | 100 | 25 | 25 | 0 | 0 | 25 | 0 | 50 |
| Swordfish | mean | n.d | n.d | n.d | n.d | 15.5 | 0.6 | 36.2 | 7.7 | 11.0 | 0.01 | 38.1 | 20.2 | 5.0 | 14.9 | 656.5 |
| *Xiphias gladius* | range | n.d | n.d | n.d | n.d | n.d - 62.0 | n.d - 2.3 | n.d - 144.8 | n.d - 19.1 | n.d - 30.9 | n.d | n.d - 152.1 | n.d - 72.0 | n.d - 20.0 | n.d - 59.3 | n.d - 2429.7 |
| | %DF | 0 | 0 | 0 | 0 | 25 | 25 | 25 | 50 | 50 | 0 | 25 | 50 | 25 | 25 | 50 |
| Sea bass | mean | n.d | n.d | 0.7 | n.d | 94.1 | n.d | 246.8 | 201.0 | 4.0 | 5.0 | 17.6 | 23.0 | 10.5 | 9.8 | 102.8 |
| *Dicentrarchus labrax* | range | n.d | n.d | n.d - 2.9 | n.d | n.d - 376.1 | n.d | n.d - 821.6 | n.d - 596.9 | n.d - 15.8 | n.d - 19.7 | n.d - 70.2 | n.d - 68.1 | n.d - 42.1 | n.d - 39.0 | n.d - 410.9 |
| | %DF | 0 | 0 | 25 | 0 | 25 | 0 | 50 | 75 | 25 | 25 | 25 | 50 | 25 | 25 | 25 |
| Atlantic bluefin tuna | mean | n.d | n.d | n.d | n.d | 13.8 | n.d | 875.8 | 6.7 | 11.4 | 0.01 | 53.4 | 57.4 | 11.2 | n.d | 31.5 |
| *Thunnus thynnus* | range | n.d | n.d | n.d | n.d | n.d - 55.3 | n.d | n.d - 3227.8 | 0.14 - 21.6 | n.d - 38.2 | n.d | n.d - 213.4 | n.d - 149.8 | n.d - 44.6 | n.d | n.d - 126.0 |
| | %DF | 0 | 0 | 0 | 0 | 25 | 0 | 50 | 100 | 50 | 0 | 25 | 50 | 25 | 0 | 25 |
| Rooved carpet shell | mean | 38.3 | 4.6 | 12.2 | n.d | 49.6 | n.d | 276.0 | 4.8 | 5.7 | 0.01 | 22.0 | 23.3 | 13.1 | 9.4 | 1001.7 |
| *Ruditapes decussatus* | range | n.d –140.8 | n.d - 18.5 | n.d - 20.0 | n.d | n.d - 127.9 | n.d | n.d - 871.6 | n.d - 13.7 | n.d - 22.9 | n.d | n.d - 52.4 | n.d - 93.1 | n.d - 52.2 | n.d - 37.7 | n.d - 2441.0 |
| | %DF | 50 | 25 | 75 | 0 | 50 | 0 | 50 | 50 | 25 | 0 | 50 | 25 | 25 | 25 | 50 |
| European squid | mean | 20.3 | 4.8 | 8.5 | n.d | 30.4 | 5.5 | 0.5 | 53.1 | 2.3 | 0.01 | 0.01 | 17.9 | n.d | n.d | 316.0 |
| *Loligo vulgaris* | range | n.d - 81.1 | n.d - 19.1 | n.d - 27.1 | n.d | n.d - 121.4 | n.d - 21.9 | n.d - 2.1 | n.d - 195.9 | n.d - 9.2 | n.d | n.d | n.d - 71.6 | n.d | n.d | n.d - 1257.9 |
| | %DF | 25 | 25 | 50 | 0 | 25 | 25 | 25 | 50 | 25 | 0 | 0 | 25 | 0 | 0 | 50 |
| Atlantic mackerel | mean | n.d | 5.2 | n.d | n.d | 9.7 | 21.1 | 0.8 | 242.7 | 405.2 | 6.0 | 37.3 | 238.6 | 4.0 | 163.4 | n.d |
| *Scomber scombrus* | range | n.d | n.d - 20.9 | n.d | n.d | n.d - 38.5 | n.d - 84.1 | n.d - 3.1 | n.d - 891.0 | n.d - 1620.8 | n.d - 21.3 | n.d - 127.9 | n.d - 935.5 | n.d - 15.9 | n.d - 653.3 | n.d |
| | %DF | 0 | 25 | 0 | 0 | 25 | 25 | 25 | 50 | 25 | 50 | 50 | 50 | 25 | 25 | 0 |
| Sardine | mean | 57.9 | 5.6 | 117.2 | 19.0 | 98.6 | 19.2 | 137.5 | 731.7 | 374.8 | 80.2 | 547.6 | 78.5 | 1.5 | 179.0 | 149.8 |
| *Sardina pilchardus* | range | n.d - 140.0 | n.d - 22.5 | n.d - 468.7 | n.d - 75.8 | n.d - 394.2 | n.d - 47.9 | n.d - 549.8 | 90.6 - 1837.7 | 31.4 - 910.1 | 3.6 - 267.6 | n.d - 1851.5 | n.d - 121.6 | n.d - 5.8 | n.d - 640.2 | n.d - 599.0 |
| | %DF | 75 | 25 | 25 | 25 | 25 | 50 | 25 | 100 | 100 | 100 | 75 | 75 | 25 | 75 | 25 |
| All | mean | 11.6 | 3.0 | 14.9 | 2.3 | 63.0 | 5.4 | 206.0 | 186.0 | 82.8 | 13.2 | 71.6 | 46.9 | 6.5 | 38.7 | 579.0 |
| | range | n.d - 140.8 | n.d - 22.5 | n.d - 468.7 | n.d - 75.8 | n.d - 911.8 | n.d - 84.1 | n.d - 3227.8 | n.d - 1837.7 | n.d - 1620.8 | n.d - 267.6 | n.d - 1851.5 | n.d - 935.5 | n.d - 52.2 | n.d - 653.4 | n.d – 2441.0 |
| | %DF | 15 | 15 | 23 | 5 | 28 | 15 | 30 | 78 | 40 | 25 | 25 | 38 | 23 | 18 | 37 |
| | Total mean | 19.0 | | | | | 123.3 | | | | | 92.9 | | | | |

n.d.: not detected. BT: benzothiazole 5-chloro-1-benzothiazole; ClBT: 2-(methylthio)-benzothiazole; MeSBT: 2-hydroxybenzothiazole; OHBT: 2-aminobenzothiazole; NH2BT: benzosulfonamide; BSA: ortho-toluesulfonamide; o-TSA Me-p-TSA: N-methyl-para-toluesulfonamide; p-TSA: N-ethyl-para-toluesulfonamide; Et-p-TSA: para-toluesulfonamide; ATII: Traseolide; DPMI: Cashmeran; HHCB: Galaxolide; AHTN: TonalideHHCB-lactone: Galaxolidone.

**Table 2 –** Mean and range of concentrations in ng/g (dw) and percentage of detection frequency (%DF) of organophosphate esters and phthalates.

| Species | | *Organophosphate esters* | | | | | | | | | *Phthalates* | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | TEP | TBP | TiBP | TCPP | TCEP | TEHP | EHDPP | TPP | TTP | DEP | DiBP | DMP | DEHA | DEHP | DnOP |
| European hake | Mean | 14.7 | 18.6 | 0.1 | 1.45 | n.d | 0.2 | n.d | 229.8 | 100.5 | 81.1 | 110.7 | 63.8 | 1.1 | 0.1 | n.d |
| *Merluccius merluccius* | Range | n.d - 58.9 | n.d - 74.4 | n.d - 0.4 | n.d - 5.8 | n.d | n.d - 0.6 | n.d | n.d - 897.9 | n.d - 363.3 | n.d- 322.0 | n.d - 442.6 | 0.1 - 116.2 | n.d - 4.2 | n.d - 0.3 | n.d |
| | %DF | 25 | 25 | 25 | 25 | 0 | 25 | 0 | 50 | 75 | 50 | 25 | 100 | 25 | 25 | 0 |
| Blue whiting | Mean | 13.5 | 7.7 | n.d | 197.8 | n.d | 6.2 | 29.5 | 6.8 | 144.0 | 5.0 | 137.2 | 65.4 | 655.5 | 1468.2 | 9.9 |
| *Micromesistius* | Range | n.d - 53.9 | n.d - 30.6 | n.d | n.d - 791.3 | n.d | n.d - 19.3 | n.d - 115.8 | n.d - 21.9 | 13.6 - 378.9 | n.d - 19.8 | n.d - 464.5 | 0.1 - 161.2 | n.d - 1971.8 | n.d - 5530.1 | n.d - 39.5 |
| *poutassou* | %DF | 25 | 25 | 0 | 25 | 0 | 50 | 50 | 50 | 100 | 25 | 50 | 100 | 50 | 50 | 25 |
| Sea bream | Mean | 19.6 | 3.8 | 1.4 | 317.2 | n.d | 28.0 | 51.3 | 365.5 | 184.3 | 69.4 | 2.3 | 16.5 | 113.6 | 379.9 | 8.7 |
| *Sparus aurata* | Range | n.d - 57.3 | n.d - 15.3 | n.d - 5.6 | n.d - 1259.2 | n.d | n.d - 104.6 | n.d - 205.1 | n.d - 1441.0 | n.d - 692.0 | n.d - 275.3 | n.d - 9.2 | n.d - 58.7 | n.d - 451.4 | n.d - 1519.7 | n.d - 34.6 |
| | %DF | 50 | 25 | 25 | 50 | 0 | 50 | 25 | 50 | 75 | 50 | 25 | 50 | 50 | 25 | 25 |
| Swordfish | Mean | 13.8 | n.d | n.d | 7.7 | n.d | n.d | 0.2 | 0.9 | 74.2 | 0.05 | 126.7 | 59.0 | 1271.4 | 1307.5 | 21.6 |
| *Xiphias gladius* | Range | n.d - 53.0 | n.d | n.d | n.d - 30.8 | n.d | n.d | n.d - 0.8 | n.d - 3.7 | n.d - 294.3 | n.d - 0.2 | n.d - 400.8 | n.d - 158.9 | n.d - 4693.2 | n.d - 5158.9 | n.d - 86.2 |
| | %DF | 50 | 0 | 0 | 25 | 0 | 0 | 25 | 25 | 75 | 25 | 50 | 75 | 50 | 50 | 25 |
| Sea bass | Mean | 20.9 | 3.1 | 1.0 | n.d | n.d | 2.2 | 0.8 | 1878.3 | 308.3 | 159.6 | 173.0 | 39.0 | 0.03 | 1.3 | n.d |
| *Dicentrarchus labrax* | Range | n.d - 60.3 | n.d - 12.5 | n.d - 3.8 | n.d | n.d | n.d - 8.7 | n.d - 2.4 | n.d - 7480.3 | n.d - 909.1 | n.d - 399.4 | n.d - 692.0 | n.d - 66.8 | n.d - 0.1 | n.d - 5.1 | n.d |
| | %DF | 50 | 25 | 25 | 0 | 0 | 25 | 50 | 50 | 100 | 50 | 25 | 75 | 25 | 25 | 0 |
| Atlantic bluefin tuna | Mean | 15.8 | n.d | n.d | n.d | n.d | 0.9 | 2.3 | 6.5 | 558.6 | 105.2 | 150.4 | 28.8 | 1091.8 | 621.8 | 99.2 |
| *Thunnus thynnus* | Range | n.d - 63.2 | n.d | n.d | n.d | n.d | n.d - 3.4 | n.d - 9.0 | n.d - 25.9 | n.d - 2016.9 | n.d - 345.0 | n.d - 439.0 | n.d - 58.4 | n.d - 2324.8 | n.d - 1349.6 | n.d - 396.9 |
| | %DF | 25 | 0 | 0 | 0 | 0 | 25 | 25 | 25 | 75 | 50 | 50 | 75 | 50 | 50 | 25 |
| Rooved carpet shell | Mean | n.d | 1.4 | n.d | 1.1 | n.d | 1.5 | n.d | n.d | 11.4 | 201.5 | 105.0 | 0.6 | 380.8 | 760.8 | 66.4 |
| *Ruditapes decussatus* | Range | n.d | n.d - 5.6 | n.d | n.d - 4.3 | n.d | n.d - 6.1 | n.d | n.d | n.d - 45.5 | n.d - 806.0 | n.d - 420.0 | n.d - 2.1 | n.d - 1485.9 | n.d - 3042.8 | n.d - 265.5 |
| | %DF | 0 | 25 | 0 | 25 | 0 | 25 | 0 | 0 | 25 | 50 | 25 | 50 | 50 | 50 | 25 |
| European squid | Mean | 6.2 | 2.5 | n.d | 465.6 | n.d | 1.2 | 4.8 | 16.8 | 713.6 | 0.02 | 10.0 | 207.9 | 1407.8 | 1696.6 | 166.8 |
| *Loligo vulgaris* | Range | n.d - 24.8 | n.d - 10.0 | n.d | n.d - 1862.2 | n.d | n.d - 4.7 | n.d - 19.0 | n.d - 39.5 | n.d - 2834.8 | n.d - 0.1 | n.d - 40.1 | n.d - 804.3 | n.d - 2946.9 | n.d - 3021.6 | n.d - 344.2 |
| | %DF | 25 | 25 | 0 | 25 | 0 | 25 | 25 | 50 | 50 | 25 | 25 | 50 | 75 | 75 | 50 |
| Atlantic mackerel | Mean | n.d | n.d | n.d | 8.9 | n.d | n.d | 2.9 | 12.6 | n.d | n.d | 66.6 | 25.8 | 1383.7 | 987.6 | 336.5 |
| *Scomber scombrus* | Range | n.d | n.d | n.d | n.d - 27.2 | n.d | n.d | n.d - 11.4 | n.d - 50.5 | n.d | n.d | n.d - 266.5 | n.d - 64.1 | n.d - 3402.8 | n.d - 2775.6 | n.d - 1057.3 |
| | %DF | 0 | 0 | 0 | 50 | 0 | 0 | 25 | 25 | 0 | 0 | 25 | 75 | 75 | 75 | 50 |
| Sardine | Mean | 4.7 | 9.9 | n.d | 375.2 | n.d | 1.8 | n.d | 169.3 | 48.5 | 59.8 | 0.05 | 51.7 | 452.6 | 184.2 | n.d |
| *Sardina pilchardus* | Range | n.d - 18.9 | n.d - 39.5 | n.d | n.d - 1436.9 | n.d | n.d - 7.1 | n.d | n.d - 677.3 | n.d - 193.8 | n.d - 239.2 | n.d - 0.2 | 0.2 - 116.3 | n.d - 1527.1 | n.d - 736.6 | n.d |
| | %DF | 25 | 25 | 0 | 50 | 0 | 25 | 0 | 25 | 25 | 50 | 25 | 100 | 50 | 50 | 0 |
| All | Mean | 10.9 | 4.7 | 0.25 | 137.5 | n.d | 4.2 | 9.2 | 268.7 | 214.3 | 68.2 | 88.2 | 55.9 | 675.8 | 740.8 | 70.9 |
| | Range | n.d - 63.2 | n.d - 74.4 | n.d - 5.6 | n.d - 1862.2 | n.d | n.d - 104.6 | n.d - 205.1 | n.d - 7480.3 | n.d - 2834.8 | n.d - 806.0 | n.d - 692.0 | n.d - 804.3 | n.d - 4695.2 | n.d - 5530.1 | n.d - 1057.3 |
| | %DF | 25 | 18 | 8 | 28 | 0 | 25 | 23 | 35 | 60 | 37 | 32 | 77 | 50 | 47 | 23 |
| | Total mean | 72.2 | | | | | | | | | 283.3 | | | | | |

n.d.: not detected. TEP: triethyl phosphate; TBP: tributyl phosphate; TiBP: tri-isobutyl phosphate; TCPP: tris (2-chloroisopropyl) phosphate; TCEP: tris (2-chloroethyl)-phosphate; TEHP: tris (2-ethylhexyl)-phosphate; EHDPP: 2-ethylhexyl-diphenyl-phosphate; TPP: triphenyl phosphate; TTP: tritolyl phosphate; DEP: dimethyl phthalate; DiBP: diethyl phthalate; DMP: isobutyl phthalate; DEHA:di-(2-ethylhexyl)-adipate; DEHP: di-(2-ethylhexyl)-phthalate; DnOP: di-n-octyl phthalate.

The organophosphate esters have the following frequency of detection: TTP > TPP > TCPP > TEP > TEHP > EHDPP > TBP > TiBP > TCEP, with a mean concentration ranging from 0.3 ng/g dw for TiBP to 268.7 ng/g dw for TTP. The difference between contaminants can also be attributed to their different physical and chemical characteristics (van der Veen and de Boer, 2012). For example, TCEP demonstrates high solubility in water, but it is not considered a bioaccumulative compound (RSC, 2024). This is why many studies show a high concentration of TCEP in water, but a low concentration in marine species. This could explain why it is not found in the seafood samples in our study, but in other studies it has been found in marine waters. Another relevant aspect for understanding why TCEP is detected in marine waters is that wastewater treatment plants (WWTPs) are not able to remove this compound. For example, Reemtsma et al. (2008) looks at the concentrations at both the inlet and outlet of a WWTP, as well as the elimination percentage. TiBP, found in this study at low concentrations, shows an elimination percentage of 86 % in WWTPs. The authors also examine TCEP, which is not eliminated; however, this observation aligns with the high concentrations found in other previous water studies (Hao et al., 2018; Regnery and Püttmann, 2010).

Organophosphate esters have been found in fish samples in another study (Santín et al., 2016) in which 13 OPEs were detected in fish samples from the Llobregat River, Spain. The total concentrations were 2423 ng/g ww and the mean value was 677 ng/g ww. Compounds such as TEHP stood out with concentrations between 37 and 326 ng/g ww. Other studies showed lower concentrations of contaminants, such as Castro et al. (2023a), which found a similar chain of detection frequencies: TTP > TiBP > TBP > EHDPP > TTP > TCPP > TCEP, between the mean concentrations of 1.7 and 18.0 ng/g ww.

The PAEs have the following distribution of detection frequencies: DEHP > DEHA > DiBP > DnOP > DEP > DMP, with a mean concentration between 55.8 ng/g dw (DMP) and 740.7 ng/g dw (DEHP). In previous research (Hidalgo-Serrano et al., 2021), similar concentration levels were observed for PAEs, with the highest concentrations detected in sole and shrimp samples, particularly for DEHP (978 ng/g dw) and DEP (982 ng/g dw). These results are in line with others (Xu et al., 2018) that reported concentrations of up to 384 ng/g dw for DBP and up to 763 ng/g dw for DEHP in 60 randomly selected fish samples.

If we compare the results of different species, squid appears as the predominant species with a total mean concentration of all compounds of 266.1 ng/g dw. The mean concentration value is higher due to a single squid sample in which higher values of contaminants than the rest of the samples were found. The next two species with the highest mean concentrations were mackerel and sardine with the same total mean concentration of 131.8 ng/g dw. The lowest total mean concentration was found in hake, with a value of 31.4 ng/g dw.

Fig. 2 shows a convex curvature for species with low lipid levels in grey and for species with high lipid levels in blue. This graph shows an overlap, meaning there is no difference in HPVC concentrations in species with low and high lipid levels, as some samples from species with high lipid content have concentrations similar to those from species with low lipid content and vice versa. This may be due to additional factors, such as diet and environmental conditions that may influence lipid composition. It can also be deduced from Fig. 2 that the high lipid species samples show a higher dispersion compared to the other samples. This is evidenced by the presence of two sample points in the graph that are distant from the others. This principal component plot shows the two principal dimensions (PCA) that described the variation in the data optimally in the two-dimensional plane of the PCA plot. PC1 (21.3 %) and PC2 (13.9 %) of the plot are slightly low, but the plot helps us to see an overview of all samples.

In general, considering all the samples, no clear difference between species or contaminants were observed; however, when we look at specific compounds, a small difference can be observed according to the physical and chemical characteristics of some HPVC (van der Veen and de Boer, 2012). This difference can be observed in a few compounds. For example, compounds such as PAEs are more influenced by fat (lipophilic), whereas OPEs are thought to have lipophobic properties. Fig. 3 shows a subplot that shows multiple data visualizations within the same figure, which facilitates comparison. PAE values make minimal contributions, which indicates that PAEs do not aid in the differentiation between samples, as they are present in all of them (shown in the center of the graph). Most of the contributions come from OPE compounds, predominantly aligned with PC2, which exhibit significant variability in that direction. EHDPP and TiBP, recognized as non-lipophilic, are notable. Apart from OPEs, compounds such as benzosulfonamides (Me-p-TSA and p-TSA) make relevant contributions on the PC1 axis, leading to a pronounced variability in that dimension. These compounds show more prominence and have a high tendency to be found in the same sample. The specificity of these compounds might help us in separating samples as they tend to be more specific between species. Unfortunately, it is necessary to obtain more data to get a better understanding and to ensure that these compounds exhibit this specificity as well as to facilitate separating high and low lipid content species.

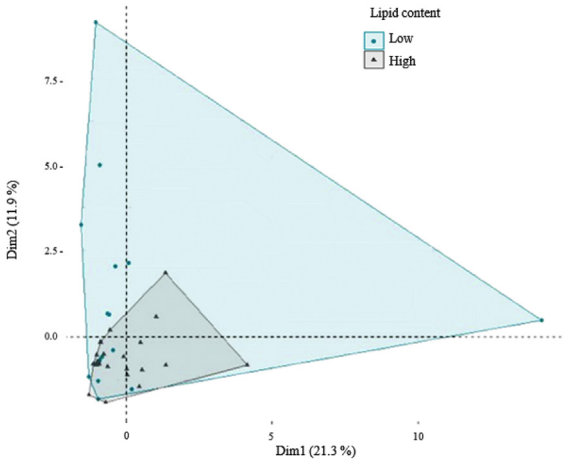


**Fig. 2 –** Convex hulls for low (grey) and high (blue) lipid content species.

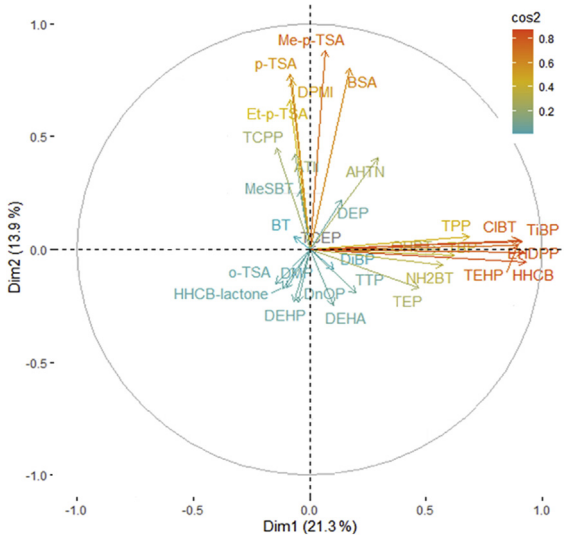


**Fig. 3 –** Subplots show the loadings and contributions of the congeners.

### 3.3. Exposure and risk characterization

Two scenarios were considered for the dietary exposure index based on the data collected in the monitoring stage: a low-bond (LB) and a high-bond (HB) scenario. The two scenarios allow us to represent dif-

ferent levels of exposure to the contaminants. The LB scenario assumes that individuals have a lower exposure to the contaminant and the HB scenario would be the worst-case situation in which a person is highly exposed to the contaminant. Consumption data was obtained from the survey of Spanish Government SG (2023). Certain species stand out from among the selected species with the highest consumption. With a consumption of 2.24 kg per person per year, Atlantic tuna is the most consumed species by the Spanish population. After Atlantic tuna there are the other analyzed species such as hake, sea bream, sea bass, mackerel, sardine, shellfish, squid, swordfish and blue whiting. The survey allowed us to determine the consumption data of the population and subsequently estimate the exposure to the contaminants under investigation. The exposure results for the low-bond scenario can be seen in **Appendix A Fig. S1a** and for the high-bond scenario in **Appendix A Fig. S1b.**

The LB scenario shows mean dietary intake values ranging from $1.0 \times 10^{-3}$ to $1.4 \times 10^{-1}$ ng/(kg bw·day) and the HB shows a range from $6.8 \times 10^{-1}$ to 14.0 ng/(kg bw·day). If we look at the exposure of each group of compounds, we can conclude that the exposure to BTs has the highest values with a mean exposure of $1.2 \times 10^{-3}$ ng/(kg bw·day) for LB and $7.7 \times 10^{-1}$ ng/(kg bw·day) for HB. Many studies show BT as one of the compounds with the highest exposure in the diet, with values of 25.7 ng/(kg bw·day) in Castro et al. (2023a) and a value of 11.0 ng/(kg bw·day) in Trabalón et al. (2017). BT are one of the most widely studied compounds as the WHO has established a maximum level of 5.1 mg/(kg bw·day). Fortunately, these values are not exceeded by any contaminant in any sample.

BSAs have the highest mean exposure value in the LB of $1.0 \times 10^{-1}$ ng/(kg bw·day). In the HB the mean exposure value is 4.7 ng/(kg bw·day). In Castro et al. (2023a) BSAs have a maximum exposure value of 38.4 ng/(kg bw·day), which is higher than that found in our study. The limited number of studies in which these contaminants are determined in fish samples makes comparison difficult.

For the OPEs, the mean exposure values are $2.7 \times 10^{-2}$ to 7.4 ng/(kg bw·day) for the LB and HB, respectively. The study by Sala et al. (2022) shows exposure results for OPEs, with a sum of values of 16.9 ng/(kg bw·day) for the LB scenario and 37.1 ng/(kg bw·day) for the HB scenario.

Musk fragrances have a value of $2.6 \times 10^{-2}$ ng/(kg bw·day) for the LB scenario and a value of 3.9 ng/(kg bw·day) for the HB scenario. In Trabalón et al. (2015) similarities with the average exposure are found for the compounds AHTN, DPMI and ATII (1.1 ng/(kg bw·day) and 3.7 ng/(kg bw·day), respectively). HHCB and HHCB-lactone showed the highest exposure results among the individual compounds, with mean values of 19.7 ng/(kg bw·day) and 6.8 ng/(kg bw·day), respectively.

PAEs have a value of $4.1 \times 10^{-2}$ ng/(kg bw·day) for the LB scenario and a value of 8.3 ng/(kg bw·day) for the HB scenario, which is the highest. DEHP is one of the most frequently detected compounds as it has been found to have values between 50 and 1390 ng/(kg bw·day) (Castro et al., 2023a), which agrees with other studies that calculated the dietary exposure to those compounds that come into contact with fish, such as phthalates (Aquilina et al., 2017). The highest exposure for the phthalate group is between 0.9-7.2 and 1.6-11.7 μg/(kg bw·day) for medium and heavy users, respectively, and contributes to 23 % of the worst-case group TDI.

Regarding species in the LB scenario, sardines are the species with the highest exposure index, with a ΣHPVC value of $6.5 \times 10^{-1}$ ng/(kg bw·day), followed by sea bream ($3.6 \times 10^{-1}$ ng/(kg bw·day)) and Atlantic tuna ($3.5 \times 10^{-1}$ ng/(kg bw·day)). In the HB scenario, Atlantic tuna (85.8 ng/(kg bw·day)) is in first position followed by sea bream (43.3 ng/(kg bw·day)) and sea bass (35.7 ng/(kg bw·day)).

To calculate the risk factor, we differentiated between carcinogenic and non-carcinogenic compounds. For carcinogenic compounds the study was performed for the compounds TBP, TCEP, DEHA, TEHP and DEHP, which have carcinogenic properties. For the non-carcinogenic compounds, we calculated the risk factor for TEP, BT, DMP, TiBP, DEP,

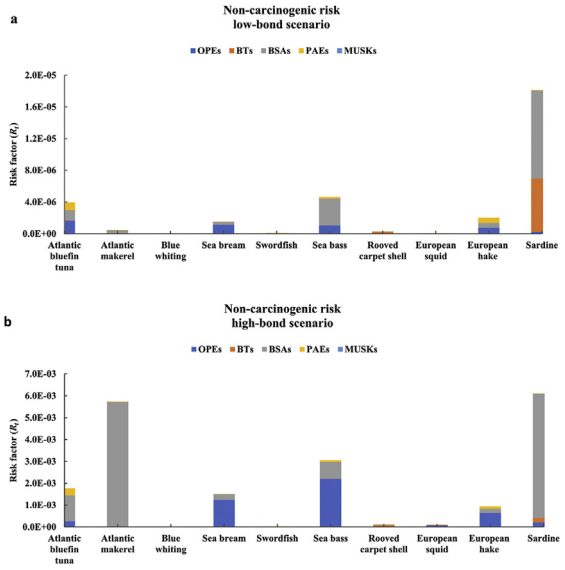


**Fig. 4 –** Risk factor ($R_t$) for non-carcinogenic compounds for the low-bond scenario (a) and the high-bond scenario (b).

HHCB, $NH_2$BT, Et-p-TSA, p-TSA, EHDPP, TPP, DnOP and TTP. It was not possible to calculate the risk for the musk fragrances because none of the contaminants had NOEAL or BMD values available.

Risk factor for non-carcinogenic compounds under the low-bond scenario is shown in Fig. 4**a,** while the corresponding values for the high-bond scenario are presented in Fig. 4**b**. The margin of exposure for carcinogenic compounds under the low-bond scenario is shown in Fig. 5**a**, while the high-bond scenario is presented in Fig. 5**b**. In the case of MUSK fragrances, no NOAEL or BMD values were available, and therefore risk could not be calculated. For there, it has to be considered, that the $R_t$ values have to be close to 1 in this study to be a potential risk to humans.

The risk factor for non-carcinogenic compounds in both the low and high scenarios showed a maximum for BSAs with values between $6.2 \times 10^{-11}$ and $1.1 \times 10^{-5}$ for LB and between $5.0 \times 10^{-9}$ and $5.7 \times 10^{-3}$ for HB. In the LB scenario, the high value of BSAs is followed by BTs and OPEs with maximum values of $6.7 \times 10^{-6}$ and $1.6 \times 10^{-6}$, respectively. Finally, PAEs have the lowest $R_t$ among the other compound families, with a maximum between samples of $9.7 \times 10^{-7}$. In the HB scenario, the risk factor after the BSAs is the OPEs with a very similar $2.2 \times 10^{-3}$ value. And finally, we find PAEs and BTs with values of $3.2 \times 10^{-4}$ and $1.9 \times 10^{-4}$, respectively. Fortunately, no non-carcinogenic risk was observed in the species analyzed because they were considerably lower than the threshold of 1.

Sala et al. (2022) provided risk factor values for some OPEs in samples of sardine, anchovy and hake from the Mediterranean and the $R_t$ values obtained ranged from $5.0 \times 10^{-6}$ to $7.3 \times 10^{-4}$. Bekele et al. (2021) also researched the risk factors of 17 OPEs in ten fish species from northern China, obtaining similar results, with values ranging from $7.1 \times 10^{-5}$ to $1.2 \times 10^{-3}$.

Observing the species that have the highest risk values depending on the compound, we see a difference in the LB scenario ranging between the sardine and the Atlantic tuna. The OPEs and PAEs stand out in the Atlantic tuna and the BTs and BSAs stand out in the sardine species. In the HB scenario, the maximum risk value varied a little more between species. OPEs had their highest value in the sea bass, BTs and BSAs in the sardine and PAEs in the Atlantic tuna. It is observed that the species with the highest exposure are two species with high lipid content, sardine and Atlantic tuna; however, the rest of the species with high lipid content have a similar risk value to those with low lipid content. Therefore, the relation would not be directly proportional to the lipid content but would be more related to the specificity of the fish.

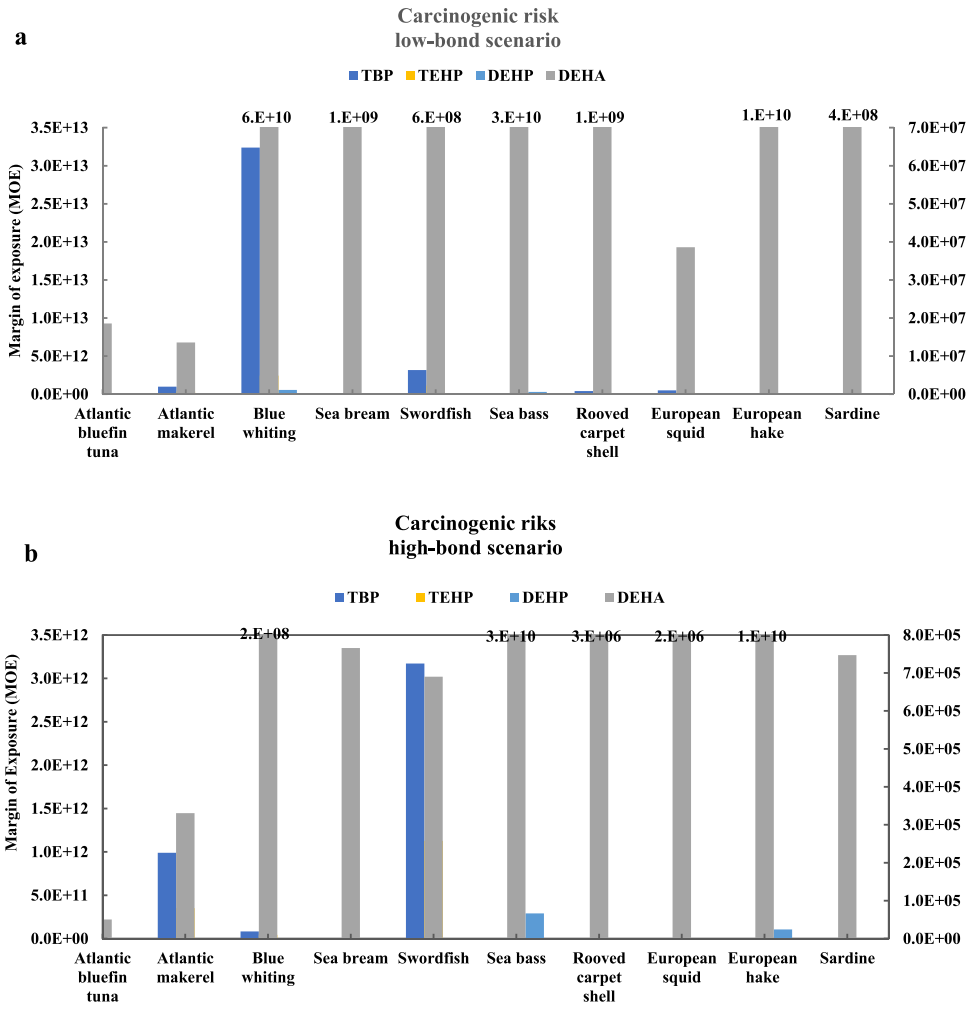


**Fig. 5 –** Margin of exposure (MOE) for carcinogenic compounds for the low-bond scenario (a) and high-bound scenario (b).

Regarding the carcinogenic risk, the exposure margin values for TBP, DEHP, TEHP and DEHA are higher than the 10,000 limit established by the EFSA for carcinogenic compounds (EFSA, 2012b), which establishes that values of MOE below 10,000 are considered to be carcinogenic. All the results can be observed in Fig. 5, which depicts a dual-axis bar graph. The primary axis (left) is for the compounds DEP, TBP, and TEHP, and the secondary axis (right) is for the DEHA. TCEP was not detected in any sample, so the half detection limit value was used; however, these values are much lower and therefore do not present a risk.

In the LB scenario, the compound with the highest risk was DEHA, which ranged from $1.4 \times 10^{7}$ to $5.9 \times 10^{10}$, followed by compounds DEHP and TEHP with values from $2.8 \times 10^{8}$ to $5.5 \times 10^{11}$ and $1.9 \times 10^{9}$ to $2.4 \times 10^{12}$, respectively. The compound TBP was found to have the lowest risk and therefore the highest value ($1.5 \times 10^{10}$). The HB scenario follows the same pattern as the LB scenario. The compound with the highest risk was also DEHA with values between $5.0 \times 10^{4}$ and $2.7 \times 10^{10}$. It was followed by compounds DEHP and TEHP with values from $9.2 \times 10^{5}$ to $2.9 \times 10^{11}$ and $8.7 \times 10^{6}$ to $1.1 \times 10^{12}$, respectively. The compound TBP was found to have the lowest risk and therefore the highest value ($1.5 \times 10^{7}$). In the study by Castro et al. (2020) some OPEs, such as TBP, were determined in fish samples from the Mediterranean, including Atlantic tuna and sea bass, and similar carcinogenic risk values were observed between $4.8 \times 10^{7}$ and $1.1 \times 10^{8}$.

The species with the highest risk are Atlantic mackerel and Atlantic tuna, both for the HB and LB scenarios. This may be due to the high consumption of Atlantic tuna. It can also be observed that most of the risk comes from the phthalate compounds DEHA and DEHP, followed by other carcinogenic compounds (OPEs). As observed earlier, phthalates are more closely associated with lipids than OPEs, which do not have as many lipophilic properties. Fortunately, the analyzed species showed no evidence of carcinogenic risk.

## 4. Conclusions

In this study, a total of thirty high production volume chemicals were examined, of which twenty nine were detected in ten of the most consumed fish species in Spain during a one year sampling period. The mean concentrations across seafood species revealed varying degrees of contamination, with phthalates exhibiting the highest mean concentration (283.3 ng/g dw) and musk fragrances, particularly HHCB-lactone, as the most concentrated individual compound (2441.0 ng/g dw). Intra-family analyses highlighted the prominence of specific compounds, such as DEHP in PAEs, HHCB-lactone in MUSKs, $NH_2BT$ in BTs, o-TSA in BSAs, and TPP in OPEs. Detection frequencies showed that Me-p-TSA and DMP were prevalent in 78 % of samples, whereas TCEP, BT, ClBT, OHBT, BSA and TBP were not detected or detected in very few samples.

PAEs exhibit the highest exposure in the HB scenario (8.3 ng/(kg bw·day)). Species-specific exposure indices identified Atlantic tuna as the species with the highest exposure in the HB scenario with 51.0 ng/(kg bw·day). The risk factors for non-carcinogenic compounds in the LB and HB scenarios were highest for BSAs ($1.1 \times 10^{-5}$ and $5.7 \times 10^{-3}$, respectively). Sardine and Atlantic tuna are the species with the highest risk values in LB, while in HB, the maximum risk value varies more among species. The relation between species and risk values is not proportional to lipid content, but rather it has been found to be more related to fish specificity. The margin of exposure for carcinogenic values was highest

for Atlantic mackerel and Atlantic tuna in both scenarios and most of the risk comes from the phthalates DEHA and DEHP, followed by other carcinogenic compounds (OPEs). However, none value in this study are of concern, according to EFSA criteria.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## CRediT authorship contribution statement

**Sílvia Borrull:** Writing – original draft, Validation, Resources, Investigation, Formal analysis. **Francesc Borrull:** Supervision, Funding acquisition. **Rosa M. Marcé:** Writing – review & editing, Supervision, Methodology, Conceptualization. **Eva Pocurull:** Writing – review & editing, Supervision, Methodology, Conceptualization.

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## Appendix A Supplementary data

Supplementary material associated with this article can be found in the online version at doi:10.1016/j.jes.2025.06.005.

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