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Sulfonated-PCBs and OH-sulfonated-PCBs: An insight into their environmental formation and identification

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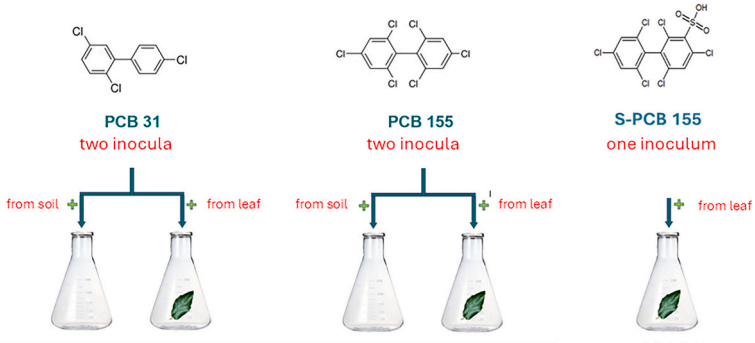
HIGHLIGHTS

- Environmental formation of sulfonated-PCBs from single congeners was obtained.
- Treatments used inocula from PCB contaminated site and phyllosphere.
- Degradation products for PCB 31 and 155 are formed as day 2.
- Number of congeners found is different in the two treatments.
- Formation of OH-sulfonated-PCBs from sulfonated-PCB was confirmed.

GRAPHICAL ABSTRACT



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ABSTRACT

Sulfonated-PCBs (-SO_3H) or S-PCBs, and OH-sulfonated-PCBs (−OH, −SO_3H) or OH-S-PCBs are recently discovered PCB metabolites, deriving from PCB degradation. For these chemicals their precise chemical identity, measured physico-chemical properties, as well as their potential ecotoxicological and toxicological effects, are still unknown. Here, the formation of these new environmental contaminants was first explored by performing single congener (PCB 31 and PCB 155) degradation experiments using two different microbial inocula. In an additional experiment, S-PCB 155 was used as parent compound to verify the production of OH-S-PCBs. The overall aim was to further investigate the array of sulfonated metabolite congeners which can originate from a known single parent compound and furnish some additional evidence on their identity. The results obtained reveal that di- and tri- metabolite congeners were formed from a tri-PCB, and penta-, and hexa- metabolite congeners from a hexaPCB. In general, however, the sulfonated-PCB class is the least produced in terms of the number of congeners, compared to both OH-sulfonated-PCBs and OH-PCBs. An additional experiment revealed the probable production of OH-S-PCBs, obtained starting with S-PCB 155 as parent compound.

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1. Introduction

More than one hundred environmental contaminants belonging to the new classes of sulfonated (-SO_3H) and OH-sulfonated (−OH, −SO_3H) PCBs were recently discovered in a heavily PCB contaminated site located in Northern Italy (SIN Brescia-Caffaro)(Bagnati et al., 2019). Sulfonated- and hydroxy-sulfonated-PCBs originate from PCBs and represent about 1 % of their parent compounds. Being novel chemicals, their chemical identity, their measured physico-chemical properties as well as their potential ecotoxicological and toxicological effects are not known yet. Sulfonated-PCBs were identified for the first time in polar bear serum(Liu et al., 2018) together with other unknown halogenated contaminants. In 2021 Li and coworkers (Li et al., 2021) showed the production of sulfonated-PCB in mice with and without a gut microbiome by feeding them with a PCB mixture. In the environment, sulfonated and OH-sulfonated-PCBs were shown to be able to bioaccumulate in earthworms (Palladini et al., 2022) and plant roots (Palladini et al., 2023). In addition, it appears that their degradation is as slow as that of their parent compounds, and that they can be easily transported by runoff or percolating water in soil(Palladini et al., 2023). In fact, the authors demonstrated they have a lower organic carbon-water partition coefficient and thus a lower affinity for soil than PCBs. These properties show a much higher mobility potential in soil layers than their parent compounds, possibly reaching lower depths and move towards groundwater. In a recent study (Palladini et al., 2025), a series of treatments with microbial inocula from different sources were tested for the first time in the formation of these two new classes of metabolites. All inocula were exposed to a PCB mixture and showed the ability to biotransform PCBs into OH-, OH-sulfonated- and sulfonated-PCBs. In the current work, two microbial inocula out of the eight tested in this preliminary study (Palladini et al., 2025) were used to further explore the degradation process of PCBs. To achieve this goal, fresh leaves of *Quercus ilex* and the culturable microbial community from the SIN Brescia-Caffaro soil were exposed to PCB 31 and PCB 155, used as individual congeners.

The aim of this study is to test for the first time, the pattern and timing of S-PCBs, and OH-S-PCBs production by microbial communities using single congeners as inocula. No attempts were made to identify microbial species or consortia, specific metabolite concentrations nor pathways. In addition, these experiments were planned to confirm the production of OH-S-PCBs versus sulfated-PCBs, another PCB metabolite class.

2. Materials and methods

2.1. Experimental design and setup

Two experiments were performed, in aerobic conditions: in the first one, two inocula, selected in a previous experiment (Palladini et al., 2025), were tested with two native PCB congeners (PCB 31 and PCB 155), used as individual contaminants. The reason for using single native congeners, instead of a PCB mix, was to reduce the complexity of the system and to facilitate congener identity recognition. Later, in the second experiment, the newly synthetized S-PCB 155 (Maspero et al., 2023) was used as parent compound to evaluate the production of metabolites and tentatively identify degradation products, especially OH-S-PCBs.

In the first experiment, L1 (fresh leaves of *Quercus ilex*) and M1 (culturable bacterial and fungal community from the SIN Brescia-Caffaro) were selected as microbial inocula for their different ability to form sulfonated- and hydroxy-sulfonated-PCBs (Palladini et al., 2025). PCB 31 and PCB 155 (dissolved in acetone) were singularly used (at concentrations of 2 μg/mL and 12 μg/mL respectively) to contaminate two 250 mL flasks each filled with 100 mL of M9 mineral medium. The inocula consisted in 3 fresh leaves of *Q. ilex* or in the culturable fraction of microorganisms from the SIN (Palladini et al., 2025). Three additional flasks were also prepared as control samples with sterilized mineral medium and a native PCB mix (4 μg/mL), to assess photodegradation. Flasks were kept at 20 ± 1 °C and continuously stirred with a magnetic stirrer at 250 rpm in aerobic conditions. All treatments were sampled 2, 40, 86, and 249 days from the start of the experiment. One control flask was sacrificed immediately after being spiked, while the other two were extracted 21 days from the start of the experiment. The experiment ended on day 249 when all treatments were sacrificed and thoroughly extracted to remove potentially formed metabolites. This included the extraction of mineral medium, leaves and pellet obtained after centrifugation (RCF = 1100 for 15 min), but also rinsing flask walls and stirrer.

Experiment 2 was assembled to further verify and identify the production of OH-S-PCBs, starting from S-PCB 155 (Table 1), given the symmetric nature of S-PCB 155, where only 3 meta- positions are available for substitutions. Here two flasks (250 mL) were filled with 100 mL of M9 sterilized mineral medium, 3 fresh leaves of *Quercus ilex* as inoculum and spiked with sulfonated-hexaPCB dissolved in acetone, to reach a final concentration of 10 μg/mL. Temperature and stirring conditions were as in Experiment 1. Leaves, mineral medium and flasks were extracted and analyzed to detect sulfonated metabolites 20 days after the start of the experiment. Blanks and standards were also analyzed to detect sulfonated metabolites.

Carbon sources were PCB 31 or PCB 155 in Experiment 1 for both L1 and M1, or S-PCB155 In Experiment 2. An additional carbon source in L1 and in Experiment 2 were the leaves themselves since they could have contributed with their own tissues to raise the available carbon level in time.

Details on the chemicals employed and sample extraction are given in Text SI-1.

2.2. Analysis of PCB metabolites

After being extracted, all samples were concentrated with a rotary evaporator, then with a gentle stream of nitrogen, and reconstituted with 1 mL of acetonitrile before being analyzed with HPLC-HRMS using a Thermo Fisher Scientific (USA) Vanquish VC-P20-A-01 LC system coupled to an Orbitrap Exploris 120 high resolution mass spectrometer, run at 60,000 resolution. More details on the analytical procedure are given in Text SI-1, as well as the extracted ion chromatograms for the different compounds in the two treatments (Figs. SI-1 to SI-34). L1 concentrations are referred to the sum of extracted leaf and mineral medium.

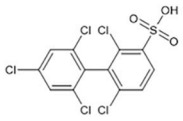
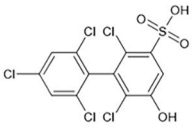
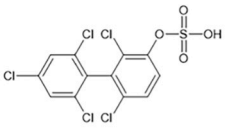
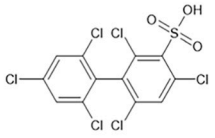
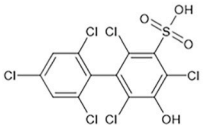
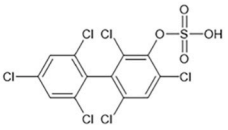
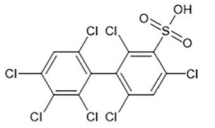
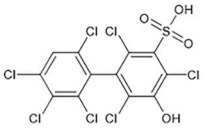
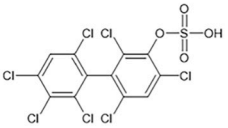
2.3. Rationale on degradation product identification

The confidence levels of these identifications were based on the paper of Schymanski et al. (Schymanski et al., 2014) and were: “level 1b” (confirmed by the synthesis of a mixture of isomers) for sulfonated-PCBs and “level 3” (tentative candidates) for OH-sulfonated-PCBs.

2.4. Quality Assurance/Quality Control (QA/QC)

OH-PCB-187 and sulfonated-PCB 155 were used to quantify the detected metabolites (more information on the quantitative analysis is given in Text SI-1). To evaluate possible cross-contamination, laboratory blanks (solvents) were included at a rate of one per sample batch and extracted following the same procedures as for samples. The extraction recovery of internal standard from the aqueous phase was complete (139 ± 15 %) (Palladini et al., 2023), whereas it was 75 ± 10 % for leaves, and pellet samples(Bagnati et al., 2019).

Table 1
Parent sulfonated PCBs and likely/unlikely metabolites formed in experiment 2.

Chlorination class	Parent Compound (S-PCB)	Likely metabolite (OH-S-PCB)	Unlikely metabolite (sulfated-PCB)
Penta			
Hexa			
Hepta			

Note: for all structures but the hexaCl-S-PCB, the exact positions of -OH, -SO_3H, and -SO_4H groups were not chemically established and the structures presented are for illustrative purposes. Also, for penta- and hepta- parent compounds and metabolites the chlorine atoms positions are given for illustrative purposes, since their exact location is not currently known.

3. Results and discussion

3.1. Reasons for chemical selection for the experiments

PCB 31 and PCB 155 were selected being a tri- and a hexachlorinated congener, respectively, characterized by a different degradability (Grimm et al., 2015; Ritter et al., 1995; Viney and Bewley, 1990). The reason for selecting higher concentrations of the hexa-PCB stands in the fact that, being more hydrophobic than the tri-PCB, the added amount had the role of keeping the bioavailable concentrations in water as high as possible to compensate for the adsorption to glass walls and leaves. In addition, PCB 31 is among the PCB present in the SIN Brescia-Caffaro soil at higher concentrations than other tri-chlorinated congeners (i.e. PCB 16, PCB 18, PCB 19, PCB 22, PCB 33 and PCB 37) (Di Guardo et al., 2020, 2017). PCB 155, on the other hand, is not present in that soil, but represents the hexa-chlorinated PCB family, one of the most abundant (Di Guardo et al., 2020, 2017). In addition, it was already used as a model compound in previous experiments (Palladini et al., 2025, 2022). PCB 155 is also peculiar since Cl-substituents occupy all ortho- and para-positions on the biphenyl, leaving 4 meta- positions H-substituted. Any single substitution of these H-atoms with, e.g. -SO_3H group, will produce just one type of sulfonated-hexachloro biphenyl, reducing the potential formation of isomers and facilitating the recognition basing only on the number of chlorine atoms detected from the MS peak of the molecular ion. For this reason, S-PCB 155 was used as parent compound for experiment 2.

3.2. Metabolite concentrations and congeners detected in Experiment 1

No metabolites were produced in control samples. Concentrations of PCB 31 and PCB 155 metabolites formed in all treatments were generally comparable, with the exception of PCB 31 in L1, for which no sulfonated metabolites were found. (Fig. 1). Among the metabolites formed we indicate some as OH-sulfonated-PCBs to direct the discussion and refer to previous papers (Bagnati et al., 2019; Palladini et al., 2025). However, based on their exact mass they could also be sulfated-PCBs. This issue is further discussed in some of the following sections.

This is not surprising as it is well known that the biodegradability of PCBs is inversely proportional to the number of chlorine atoms, as well as their position on the biphenyl, and that ortho-substituted PCBs (on the same ring or in both rings) are more resistant to biodegradation (Furukawa et al., 1979; Furukawa and Fujihara, 2008). However, L1-PCB 31 and M1-PCB 31 produced more OH- and OH-sulfonated-PCBs than PCB 155 treatments, especially M1-PCB 31. Sulfonated-PCBs are an exception, as more congeners are derived from PCB 155 ($n = 3$, 2 penta-Cl and 1 hexaCl) than from PCB 31 ($n = 2$, 2 tri-Cl-) (Fig. 1 and Table SI-1).

In general, the concentration of all the chlorination families detected in samples increased with time (Fig. 2), except for di- and tri-OH-sulfonated-PCBs in M1-PCB 31 and mono-, penta- and hexasulfonated-PCBs in M1-PCB 155. All congeners detected in samples are reported in Table SI-1.

Metabolites mainly appeared after 40 days (Fig. 2), apart from hexaOH-PCBs and hexasulfonated -PCBs which were detected much earlier (at $t = 2$ d).

3.3. Metabolite concentrations and congeners detected in Experiment 2

This is the first degradation experiment we are aware of in which S-PCBs are used as parent compounds: the S-PCB 155 standard employed contained minor amounts of other S-PCBs (Text SI-1): heptachlorinated-S-PCB (heptaCl-S-PCBs), and pentachlorinated-S-PCB (pentaCl-S-PCBs), resulting in three sulfonated-PCB classes as parent compounds. At the end of the experiment (day = 20) several products were found (Table SI-2). The HexaCl-OH-PCB formed could result from the desulfuration and hydroxylation of the parent HexaCl-S-PCB or the dechlorination, desulfuration, and hydroxylation of the parent HeptaCl-S-PCB, although less likely. Four additional compounds were formed and attributed to OH-S-PCBs, as discussed in the following section.

3.4. Tentative identification of metabolites of PCB 155 in Experiment 1

Some considerations can arise starting from PCB 155 degradation. In both inocula the sulfonated-PCB formed is just one isomer, as expected,

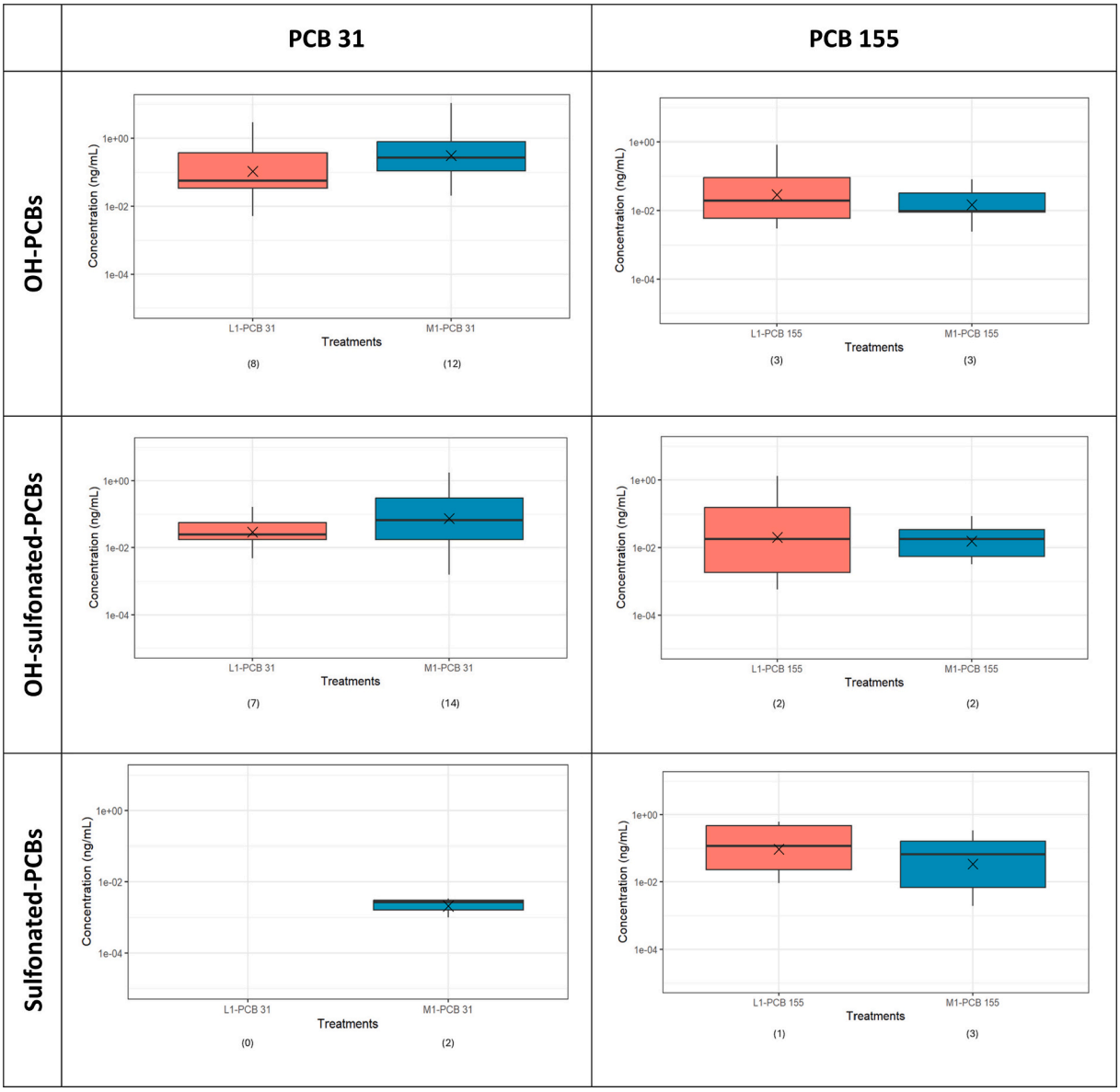


Fig. 1. Box plots of concentrations (ng/mL) of OH-PCBs, sulfonated-PCBs, and OH-sulfonated-PCBs in experiment 1, on a log scale (data from all times). The numbers in brackets below each box plot indicate the total number of congeners detected for each class.

since PCB 155 is a highly symmetric molecule with only meta positions available for substitution. This could explain the higher initial concentration (Fig. 3 top and Fig. 2) for this sulfonated chemical. The identity of the sulfonated-PCB 155 was also confirmed by the retention time, since for this metabolite a pure standard was synthetized by our group (Maspero et al., 2023). In a previous degradation experiment in flask (Palladini et al., 2025) many sulfonated-hexaPCB were formed, however, their formation could have derived from other PCBs present in the initial parent compound mixture (such as hepta-, octa-, and deca-PCB). Therefore, the results presented here allow to precisely relate the formation of the hexasulfonated PCB as directly derived from its parent compound, PCB 155.

Similarly, the number of isomers of OH-PCB 155 formed in the two experiments (L1 and M1) is one, so it is reasonable to assume that the OH-substitution took place in the meta-position as well. Both these degradation products appeared very soon, at $t = 2$ d, together with the dechlorination products SO_3-penta-PCB (only in M1). Here two isomers appear, probably depending on the removal of the Cl atoms either in para- or in ortho- positions. Similar consideration can be drawn for the two OH-Penta-PCB. However, these sulfonated and hydroxylated penta-Cl-PCBs could in theory also be derived from penta-Cl-PCB impurities possibly present in PCB 155 standard.

The two pentaCl-OH-S-PCBs (indicated as SO3 + OH-Penta-Cl in Fig. 3) can be identified being two out of many possible isomers of a OH-sulfonated-pentachlorobiphenyl or hypothetically, as two sulfated metabolites. However, these are the same two chemicals (same retention times and same exact masses) as the chemicals tentatively identified as pentaCl-OH-S-PCBs of experiment 2.

3.5. *Tentative identification of metabolites of PCB 31 in Experiment 1*

The situation is more complex to decode for PCB 31, having less chlorine substituents and at different positions on the biphenyl. Two trichlorinated-sulfonated products are formed (only in M1) (Fig. 3, bottom). While their identity of S-PCBs can be confirmed by their exact mass, a precise substitution position for the -SO_3H group on the biphenyl could not be given. The number of OH-tri-PCB formed in L1 (5 isomers) is compatible with the substitution of the ortho- meta- and para-

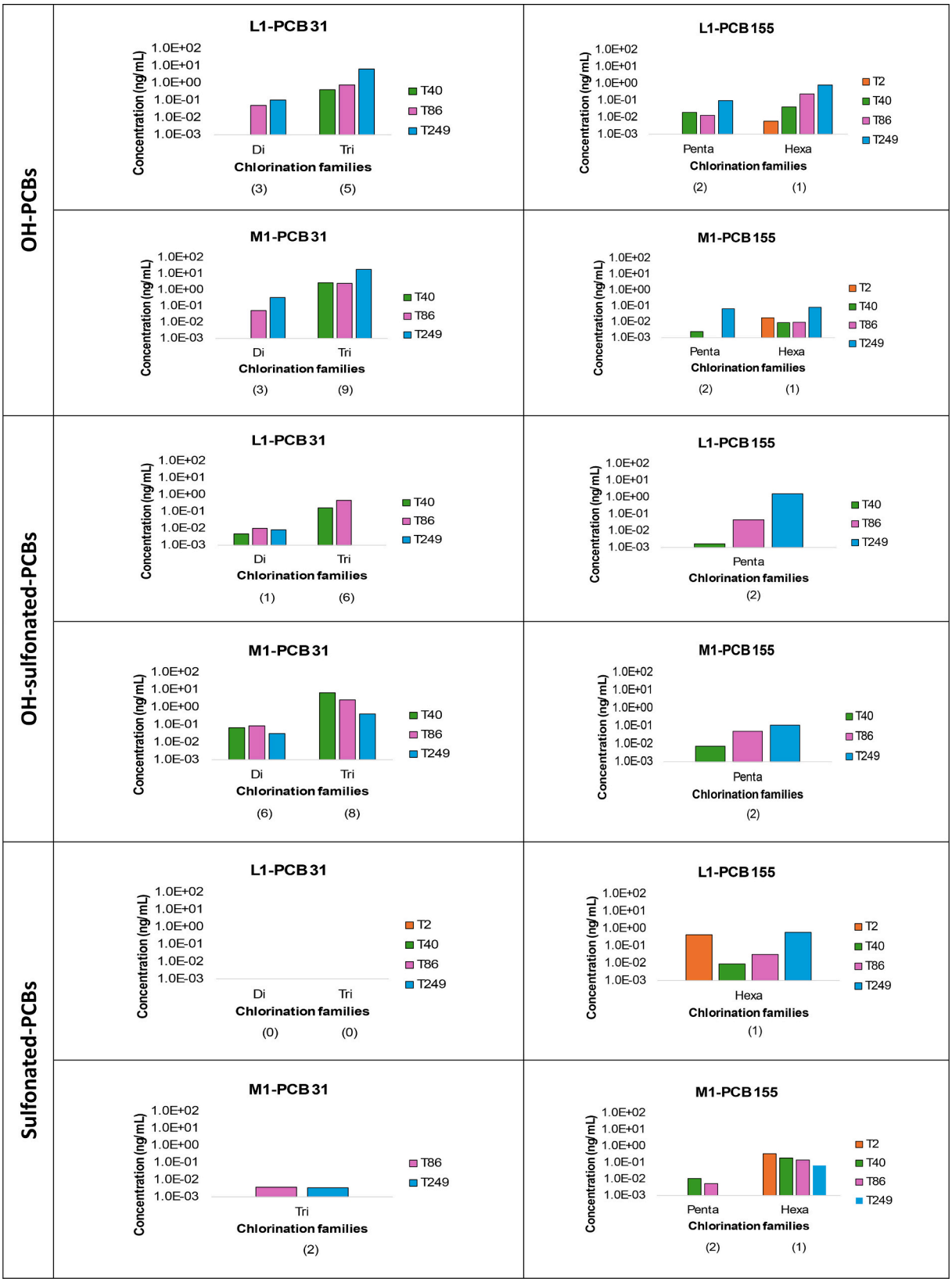


Fig. 2. Appearance of congeners of OH-, OH-sulfonated- and sulfonated-PCBs at the different collection times. Numbers in brackets below each family represent the number of different congeners found.

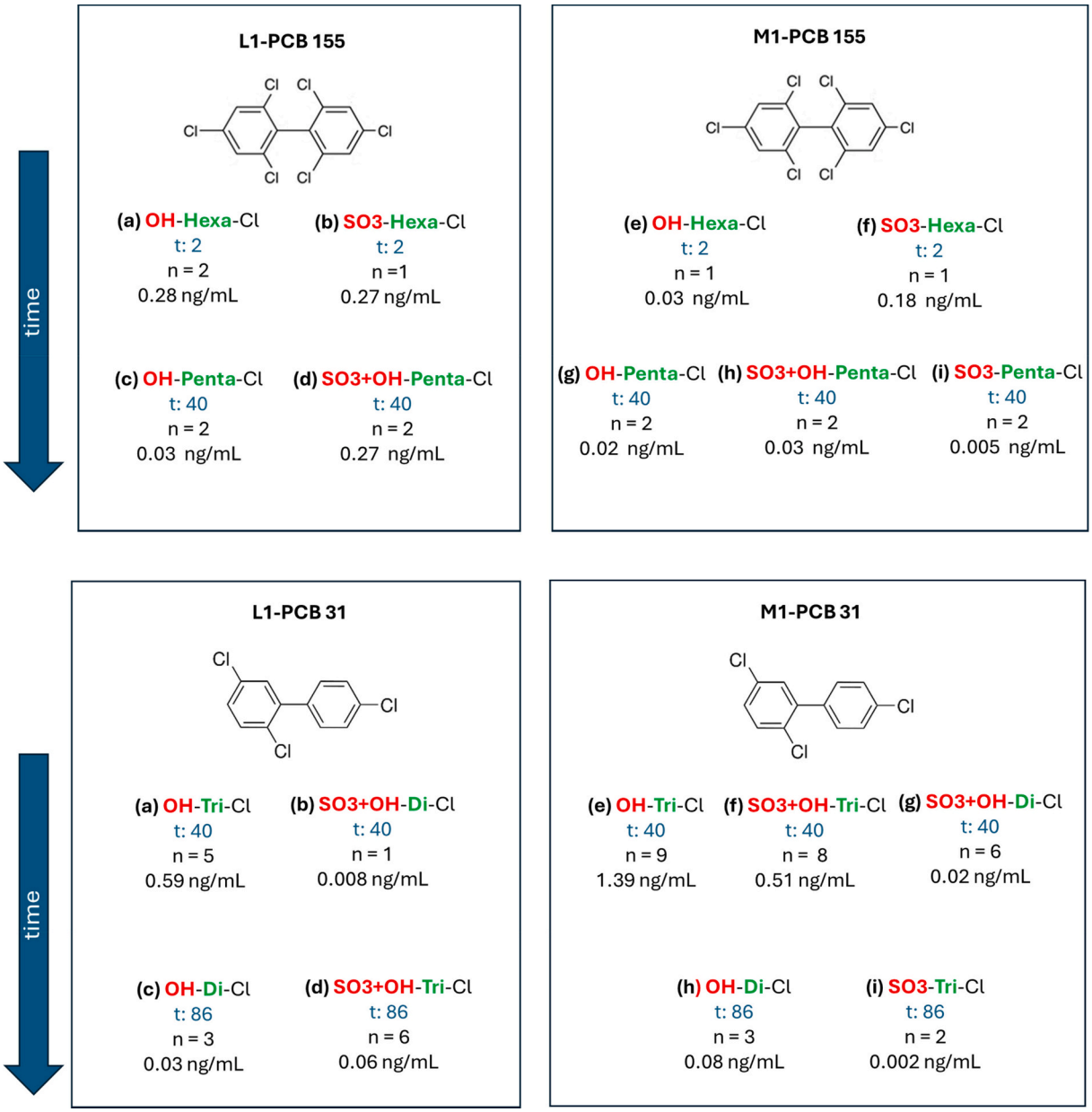


Fig. 3. Timing of formation and concentrations of degradation products in the two treatments for PCB 155 (top) and PCB 31 (bottom). The blue arrows show the increasing time of formation; t is time in days, n is the number of isomers formed. Concentrations are averages for chlorination family.

positions on the biphenyl. However, looking at M1, 9 isomers were found, and this is only compatible with the same substitution for the L1 case but also situations in which Cl- groups are rearranged, leading to more potential isomers. These metabolites could be formed via a concerted oxidation mechanism involving an arene oxide, which would rearrange spontaneously to form the hydroxylated intermediate through a (1,2)-chlorine shift (NIH) mechanism (Daly et al., 1972). The number of OH-di-PCB isomers found is 3 in both experiments and this is compatible with the removal of one of the three chlorine atoms in the biphenyl. However, these sulfonated and hydroxylated di-Cl-PCBs could in theory also be derived from di-Cl-PCB impurities possibly present in PCB 31 standard. The situation is again more complex for the remaining degradation products: The so called SO3 + OH-tri-Cl formed are 6 in L1 and 8 in M1. Assuming that only the available positions could be substituted by sulfate groups (-SO_4H), only five isomers would be theoretically possible. Having instead six isomers in L1 and eight in M1 the probability that they could be OH-sulfonated-PCBs is higher. However, they could also be a mixture of sulfate-PCBs and OH-sulfonated-PCBs. Similar considerations can be drawn for the dechlorinated SO3 + OH PCBs, which are 1 and 6 isomers in L1 and M1, respectively.

3.6. *Tentative identification of S-PCB 155 metabolites in Experiment 2*

Several metabolites were formed (Table SI-2), and some were attributed to OH-S-PCBs, based on their exact mass. This is because it would be very unlikely that the -SO_3H group in the parent compound would be substituted with a -O-SO_3H group (in order to obtain a sulfated-PCB) (Table 1). The most probable event is the addition of an -OH group to the biphenyl, with the production of OH-S-PCBs, as shown in Table 1 and Fig. 4.

The concentrations per chlorination class of S-PCBs (parent compound) vs. OH-S-PCBs (metabolite produced) in Fig. 4 could also show their close relationship: heptaCl-OH-S-PCBs and hexaCl-OH-S-PCBs are respectively about 10^{-3} and 10^{-2} times lower than their parent compounds. The pentaCl-OH-S-PCBs (2 congeners) concentrations are instead about 0.25 times lower than pentaCl-S-PCBs, possibly indicating

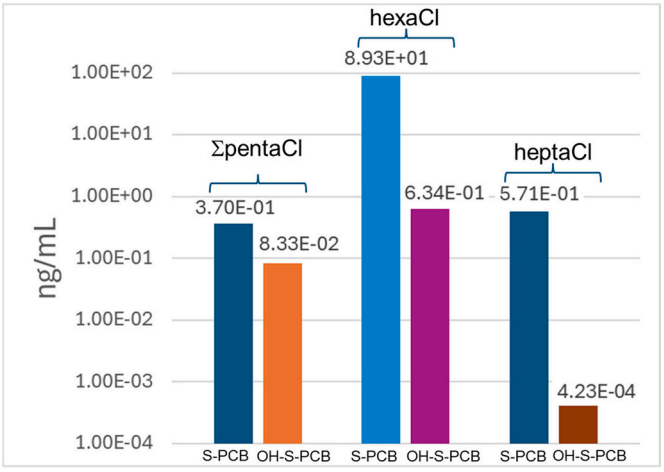


Fig. 4. Concentrations of parent S-PCBs and OH-S-PCBs formed per chlorination class in experiment 2 at $t = 20$ d (average of two replicates).

an easier transformation from the corresponding penta-s-PCB or additional formation from other compounds, such as hexaCl-S-PCBs or hexaCl-OH-S-PCBs.

3.7. Environmental relevance of the metabolite production

The degradation patterns of PCB 31, PCB 155 and S-PCB 155 allowed to better focus the probable metabolite formation and order of appearance than previously shown (Palladini et al., 2025). Additionally, in the degradation of PCB 155, also two pentachloro S-PCBs appear, possibly corresponding to the dechlorination of the ortho or para chlorines present in PCB 155, showing a potential for further chlorine removal in the formation of lower chlorinated sulfonated PCBs. The presence of many isomers of di and tri OH-S-PCBs in the degradation of PCB 31 in M1 may support the potential identity of these degradation products as OH-S-PCBs. Such confirmation could possibly result also from the degradation of S-PCB 155, although more work is needed to validate the formation of OH-S-PCBs vs. sulfated-PCBs.

4. Conclusions

The degradation patterns of PCB 31, PCB 155 and S-PCB 155 showed interesting results on probable formation and order of formation of the metabolites. However, some uncertainty remains on the dependency and the order of formation (which product derives from which). More studies are required as well as the preparation of more model compounds to elucidate and confirm the formation of OH -sulfonated vs. sulfated PCB metabolites. However, these results present for the first time the direct formation of sulfonated-PCB degradation products in environmental samples from single parent PCBs, especially for PCB 155, for which a sulfonated-PCB standard is available (Maspero et al., 2023). As stated in previous studies, much information is still needed to understand the environmental fate as well as the ecotoxicity and human toxicity of these sulfonated metabolites of PCBs (Bagnati et al., 2019; Palladini et al., 2023).

CRediT authorship contribution statement

Jessica Palladini: Writing – review & editing, Writing – original draft, Investigation, Data curation. **Elisa Terzaghi:** Writing – review & editing, Data curation, Conceptualization. **Elisabetta Zanardini:** Resources, Investigation. **Giovanni Palmisano:** Validation, Methodology, Investigation, Formal analysis. **Renzo Bagnati:** Writing – review & editing, Methodology, Investigation, Formal analysis. **Alice Passoni:** Methodology, Investigation. **Antonio Di Guardo:** Writing – review & editing, Supervision, Project administration, Investigation, Funding acquisition, Conceptualization.

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.

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Appendix A. Supplementary data

Additional information about the experimental procedures and methods, LC-HRMS-ORBITRAP extracted ion chromatograms of PCB degradation products in the two treatments, concentrations detected in all treatments in tabular form (PDF). Supplementary data to this article can be found online at doi: https://doi.org/10.1016/j.scitotenv.2025.180176.

Data availability

Data are in SI

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