



A suspect and non-target approach to unveil the chemical fingerprint of a multi-environment indoor dust

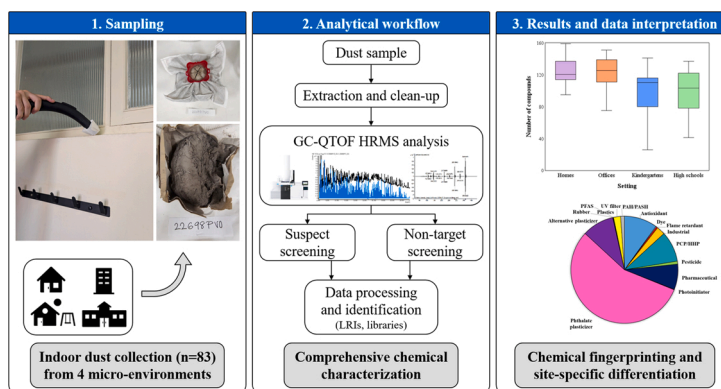
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HIGHLIGHTS

- Combined SS/NTS identified 269 contaminants in indoor dust across four settings.
- Homes showed the highest chemical complexity and pollutant detection frequencies.
- Educational settings were enriched with phthalates and alternative plasticizers.
- Emerging contaminants such as TBPH, AO168=O and 6PPD were detected in all settings.
- Elevated-surface settled and floor dust showed partly different chemical profiles.

GRAPHICAL ABSTRACT



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ABSTRACT

Indoor dust accumulates hundreds of chemicals that may pose a risk to human health. This work extensively characterized Persistent Organic Pollutants (POPs) and emerging contaminants in indoor dust from residential, occupational, and educational settings. A combined suspect and non-target screening (SS/NTS) workflow using gas chromatography quadrupole time-of-flight mass spectrometry was developed to explore the occurrence of 269 suspect contaminants identified or annotated with confidence levels 1–3. A high number of compounds were detected per sample (26–159) with widespread presence of synthetic chemicals and polymer-derived compounds such as classic and alternative plasticizers, antioxidants, flame retardants, or rubber-related additives. Among the latter, this study provides the first evidence of 6PPD and other tire-wear related additives in Spanish indoor dust from conventional settings, highlighting the potential infiltration of outdoor-derived particles. Homes exhibited the highest chemical complexity and chemical burden in terms of number of compounds and individual normalized instrumental responses (NIRs), characterized by antioxidants such as *tris*(2,4-di-*tert*-butylphenyl) phosphate (AO168=O). In educational environments, although the number of contaminants was lower, the results revealed a higher prevalence of phthalates and alternative plasticizers (e.g. 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate, TXIB). Statistical characterization further characterized that polycyclic aromatic hydrocarbons

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(PAHs) and polychlorinated biphenyls (PCBs) were key markers in residential and occupational buildings, while certain personal care products and plastic-related compounds predominated in educational settings. Overall, this study establishes qualitative indoor-dust chemical fingerprints through a multi-tiered screening framework to support potential source identification and contaminant prioritization across diverse exposure-relevant indoor media.

1. Introduction

Indoor dust is a reflection of our lifestyle and the environment around us. Since the mid-20th century, acceleration of production processes and societal modernization have drastically changed dust composition which nowadays is characterized by a high proportion of synthetic fibers, polymeric materials, and a diverse array of chemical additives. This plethora of compounds originates from multiple sources such as consumer goods, furniture, materials, or daily activities like cleaning or personal care, involving both indoor and outdoor inputs [1]. Dust content is therefore dynamic and heterogeneous, depending on the indoor environment and whether it stems from the floor or from elevated surfaces [2]. Many of these changes are reflected at temporal and regional levels driven by shifting in habits, material technologies and regulatory frameworks [3,4]. Depending on the toxicity of these pollutants it may pose a significant health risk [5], which is exacerbated by different exposure pathways [6] and prolonged duration that humans spend in indoor environments [7,8].

Given the constant changes in composition, chemical complexity of these mixtures and potential synergistic toxic effects, exhaustive investigation of indoor contaminants is imperative to accurately assess the potential exposure sources associated with modern indoors. Target analysis remains the preferred option for this type of study and has been used for the determination of ubiquitous dust contaminants such as flame retardants (FRs) [2,6,9], plasticizers [9–12], pharmaceuticals [13], or pesticides [14]. However, the application of these analyses is insufficient when it comes to comprehensive characterizations and the discovery of novel contaminants.

Suspect (SS) and non-target (NTS) screening are appropriate options for the characterization of complex samples due to their inherent capability to simultaneously detect a vast range of contaminants. Both liquid chromatography (LC) and gas chromatography (GC), especially when coupled with high-resolution mass spectrometry (HRMS), offer significant power to capture the complex chemical footprint of indoor environments [3,7,8,15,16,17]. LC has extensively been used in recent years for SS/NTS approaches due to several reasons such as (i) the availability of accurate mass libraries, (ii) the preservation of the molecular ion under soft ionization sources, and (iii) the advanced development of specialized data processing algorithms and methods [8,16]. However, LC applicability may fall short for the identification of many of the expected non-polar and semi-volatile organic compounds (SVOCs) potentially present in dust. In that sense, GC is considered a particularly suited alternative for their analysis offering analytical strengths for contaminant screening such as superior reproducibility, robust mass fragmentation in electron ionization sources (EI) and high retention stability [18–20]. A reliable framework for suspect identification is provided by performing analyses under chromatographic conditions identical to those of reference spectral libraries [18]. Nonetheless, beyond fixed conditions, adopting linear retention indices (LRIs) is generally preferred, as it ensures a more universal and instrument-independent approach to obtain accurate retention parameters, thereby providing an additional layer of identification confidence [17]. As a result, its use is gaining traction for comprehensive environmental screening using GC-HRMS-based analyses [3,8]. In such approaches, a significant bottleneck is the generation of immense datasets. For that reason, the integration of multivariate statistical tools is indispensable to extract meaningful information, resolve site-specific chemical fingerprints, and elucidate differences or similarities among

complex samples [1,3,7,21].

Building upon these considerations, while numerous studies have focused on isolated indoor microenvironments or pre-selected target compounds, there remains a critical need to evaluate chemical diversity holistically across the full spectrum of daily human occupancy. The novelty of this study resides in the extensive, exploratory, and qualitative application of a multi-tiered screening framework combining suspect and non-target screening (SS/NTS) workflow across a robust suite of dust samples spanning residential, occupational, and educational environments. By contrasting these diverse settings, each characterized by distinct material uses, activities, and occupant vulnerabilities, this work provides an integrated framework for mapping indoor chemical fingerprints, identifying potential sources, and prioritizing emerging contaminants. Qualitative indicators were employed to evaluate the contaminant prevalence and assess the relative chemical load across the different settings in terms of the number of detected compounds, chemical diversity, and cumulative instrumental responses. The aging of dust, related to the transformation of key additives and the differential distribution of contaminants between floor and elevated-surface settled dust was investigated. Finally, multivariate analysis tools were integrated to highlight crucial pollutants and characteristic chemical signatures for each environment.

2. Material and methods

2.1. Sample information and preparation

Indoor dust samples ($n = 83$) were collected in 2022 from different residential and occupational settings across Spain, comprising homes (H, $n = 14$), offices (O, $n = 22$), kindergartens (K, $n = 21$), and high schools (HS, $n = 26$). Specifically, offices were located in government and private buildings, research centers, and university departments. Within each category, sampling sites were chosen to characterize chemical diversity related to typical indoor activities, varying material compositions, and different age-specific occupant groups (infants, adolescents, and adults). Floor and settled dust from elevated surfaces (>0.5 m above the ground) in non-residential settings was collected separately by the research team using a standardized protocol involving a vacuum cleaner with a paper filter coupled to the vacuum tube [13]. In domestic environments, each participant took composite samples from the entire home without differentiation for separately collecting floor or elevated-surface settled dust. Information regarding building characteristics, surrounding environments, and occupant habits was gathered in a previous work [13].

After collection, bulk dust samples were sieved ($500\ \mu\text{m}$) to remove the coarsest particles homogeneously in all samples while maintaining their nature and representativeness [7,13], then homogenized and stored in polyethylene containers at -20°C until treatment. Extracts previously prepared [14] subsequently re-analyzed using SS and NTS workflows to enhance the characterization of potential contaminants. Extraction was carried out using a QuEChERS based method as detailed in the [Supplementary Material](#) (SM, Text S1) [14]. Samples were spiked with 50 ng of metolachlor-d6 as internal standard (ISTD) and 1 ng of ^{13}C -PCB 15 and ^{13}C -PCB 70 as injection standards (ISS). Where necessary, appropriate dilutions were applied to balance high-abundance signals.

2.2. Instrumental analysis

Dust extracts were analyzed by gas chromatography coupled to time-of-flight high resolution mass spectrometry (GC-QTOF-HRMS) comprising on an 8890 gas chromatograph and a 7250 QTOF MS spectrometer from Agilent Technologies (Wilmington, DE, USA). Chromatographic conditions and instrument configuration were based on those used in the commercial library *GC/Q-TOF Pesticide Personal Compound Database Library (PCDL)* (Agilent Technologies) [22], using two HP-5MS-UI columns (15 m x 0.25 mm x 0.25 μ m; Figure S1). Specific details on instrumental parameters are included in the SM (Text S2 and Tables S1 and S2). Maintaining such conditions preserves experimental retention times (RTs) in comparison with the library and, hence, increases identification confidence to minimize the number of false positives. Carrier gas flow (He, 1 mL/min) was adjusted using RT locking through replicate chlorpyrifos-d10 injections to minimize differences between runs and ensure a better RT match with the library.

2.3. Data processing

The data processing workflow combined both SS and NTS procedures to accomplish a detailed characterization of the indoor dust (Figure S2). Both procedures were based on the comparison of detected features against diverse reference libraries combining vendor databases, open-source repositories [19] and NIST mass spectral library to achieve identification confidence (IC) 2 or 3 as proposed for GC-HRMS [8]. IC 2 describe compounds for which there is sufficient information to consider probable structure identification based on mass spectra and retention data (RT or LRI), while IC 3 analytes also showed good spectral and/or experimental agreement on retention data, but lacked sufficient orthogonal information to assign a single structure. A small set of compounds was confirmed as IC 1 using commercially available analytical standards.

Suspect screening. Initial SS was performed using Mass Hunter TOF Quantitative Analysis and the GC screener tool to explore and identify the samples with the highest number of detected compounds. An initial suspect list was derived from the Agilent GC/Q-TOF PCDL (>1000 pesticides and environmental contaminants such as polycyclic aromatic hydrocarbons, PAHs, and plasticizers) and was subsequently refined to remove early-eluting compounds, analytes with insufficient data (i.e. RT or LRI), or previously characterized in our laboratory in this type of matrix. Retention data, quantifier ion, and three qualifier ions were selected and included for each suspect in the data processing method. Features were annotated based on (i) RT deviation within ± 0.25 min, (ii) library match > 75%, (iii) signal-to-noise > 3, (iv) mass accuracy < 5 ppm, and (v) coelution of at least 2 ions.

Non-target screening. A discovery subset of 24 dust samples was selected, including 6 dust samples of each environment (Figure S3). The primary criteria for sample selection were the preliminary number of detected compounds and dust type in the initial SS. This approach represented a deliberate, necessary practical compromise between achieving sufficient chemical diversity and managing the substantial manual time investment required for NTS data processing, acknowledging that minor, rare, and site-specific compounds with low ubiquity may have been missed. These samples were reprocessed using Agilent Unknown Analysis software (Figure S3). The SureMass algorithm was selected for peak detection and mass spectral deconvolution. An alkane mix (C₈-C₄₀, iso-octane; Dr. Ehrenstorfer) was injected before each sequence to check system performance, reproducibility, and to calculate LRIs [16]. LRIs and mass spectra were compared against mass spectral libraries of unit and accurate mass resolution. Data sets were manually aligned and carefully inspected to confirm identifications and minimize false positives, since the software does not provide automatic alignment. Besides, different match names or reference *m/z* (quantifier) can be retrieved for a given feature [16,18]. More information about software functionality and limitations was carefully addressed by Moschet et al.

[16]. Identification was prioritized for features meeting the following thresholds: (i) shape quality > 70, (ii) library match > 70%, and (iii) LRI deviation within $\pm 2\%$. Features detected in at least three samples were preserved and their curated mass spectra were added to an in-house mass spectral library.

Selection of relevant features from NTS and integration into SS workflow. Annotated NTS candidates were merged with the initial suspect list to create a final processing method containing 1120 compounds (Table S3). This expanded list allowed for a streamlined, selective re-evaluation of all 83 samples using consistent reference ions and RTs. The area of each feature was normalized by the ISTD to minimize fluctuations in sample volume and instrumental analysis and is expressed as 'Normalized Instrumental Response' (NIR) [4,23]. Features with NIRs less than 10 times the area observed in the blanks were discarded. Some peaks were frequently detected in blanks (Table S4) though blank contributions were below 7% and were retained as tentative identifications subtracting the corresponding blank NIR for each compound [16]. Detection frequency (DF) was calculated for each suspect feature, defined as the number of detections in all samples divided by the total number of samples.

Additional information about strengths and limitations of the analytical workflow are provided in Text S3.

2.4. Quality assurance and calculations

A NIST SRM 2585 dust reference material was prepared by triplicate (*n* = 3) for quality assurance and optimization of the data processing workflow. Its application resulted in the identification and annotation in the reference material of the 156 compounds listed in Table S5. Principal Component Analysis (PCA) showed that subsamples from SRM 2585 clustered closely with most dust samples (Figure S4A). Although the first two components explained only approximately the 30% of the variance (likely due to the high number of features included in the analysis) [16, 18], replicate injection grouped together with similar weights. This demonstrates the accuracy of the sample preparation and data processing for compound detection and area normalization across subsamples [16]. Furthermore, the relative standard deviation (%RSD) for the NIRs was below 20% for 155 out of 156 identified/annotated compounds (Table S5; Figure S4B). Procedural field blanks were prepared at the field using diatomaceous earth collected with the same vacuum cleaner, stored, and treated in the same way as the samples [13]. Instrumental blanks with iso-octane injections were included after each sample injection to check carry-over and cross-contamination of the chromatographic system.

NIRs, number of detected compounds, and individual signal-based apparent Transformation Fractions (TFs) were further investigated through statistical analyses (Text S4). The scope of proposed suspect approach is strictly qualitative and does not intend to approach quantitation or semi-quantification of the identified compounds since NIRs cannot substitute for absolute concentrations. Hence, the number of detected compounds, DFs, TFs, or NIRs have been used to establish general comparisons and to assess differences and trends among samples from different locations.

TFs were calculated for the parent compound of certain contaminants and its transformation products (TPs) as a qualitative and exploratory indicator of environmental degradation without considering absolute molar conversion. The TF for each specific TP was defined as the ratio of its NIR to the sum of the NIRs of the parent compound and the respective TP according to Eq. 1:

$$TF = \frac{NIR_{TP}}{NIR_{parent} + NIR_{TP}} \quad (1)$$

In cases where the parent compound was not detected, a value of zero was assigned to the parent compound to represent a complete apparent transformation (TF=1). This approach allows for a joint interpretation of the chemical transformation of dust; a TF close to

0 indicates parental compound preservation, while a TF approaching 1 reflects a plausible degradation in the indoor environment. Comparison of TF has been carried out individually for each compound to discern statistical differences among samples. TFs of different compounds are not directly compared to avoid potential differences in the instrumental response factors when comparing compounds with distinct characteristics, MS responses, and/or recoveries.

Multivariate analyses such as PCA and Hierarchical Cluster Analysis (HCA) were also carried out to explore site-specific chemical patterns and sample similarities (Text S4).

3. Results and discussion

3.1. Compound occurrence in indoor dust

Application of the described integrated workflow resulted in the identification or annotation of 269 compounds at confidence levels 1–3 from the initial list of 1120 suspects ranging from 26 to 159 compounds per sample. Overall, the majority of them represent compounds identified by library match (IC=2, 175 compounds), while 88 remain tentatively annotated as IC= 3, mainly comprising several isomers with close elution, since standards were not available for unambiguous identification [21]. For the discussion, IC 3 compounds were grouped and treated according to their chemical family and were not used for individual compound comparisons. Some of the annotated substances (6) were retrospectively identified by purchasing new standards, taking into account availability and time [4,8,21]. These substances were categorized according to their main use into 15 chemical families (Fig. 1), including industrial compounds (n = 78), pesticides (n = 35), personal care or household products (PCP/HHPs, n = 35), PAHs and sulfur-containing PAHs (PAHs/PASHs, n = 31), antioxidants (n = 19), FRs (n = 18), phthalates (n = 6) and alternative plasticizers (APs, n = 13), other plastic (n = 2) and rubber-related compounds (n = 7), pharmaceuticals (n = 9), UV filters (n = 6), dyes (n = 4),

photoinitiators (PIs, n = 3), and PFAS (n = 3). Table S6 depicts all compounds including information about chemical subclasses highlighting polychlorinated biphenyls (PCBs, n = 51), PAHs (n = 26), and organophosphate esters (n = 19).

Residential and office dust showed significantly higher complexity in terms of number of compounds ($p < 0.05$), probably related to more diverse activities and internal sources [24]. The total number of compounds in both microenvironments was 240 and 244, respectively, where half of them (120 and 121) were detected in 50% of the samples. In educational settings, the number of identified and annotated substances was lower with 213 for kindergartens and 205 for high schools with individual samples showing greater variability (Figure S5). Despite high schools contained fewer compounds, summed NIRs were comparable to other settings and significantly higher than those in offices (Fig. 1), largely due to the contribution of phthalate plasticizers as shown in Figure S5B. Consistent with our findings (Figure S6), Christia et al. [25] found higher plasticizer concentrations in non-domestic environments [26], while Velazquez-Gomez et al. [27] reported that Spanish high schools were the environment with the highest levels of phthalates. Although environmental levels can vary widely across international studies due to differences in sampling designs, building ages, and regional regulations, these elevated signals could be potentially linked to specific structural and usage factors, such as PVC flooring, high occupancy rates, and extensive electronic equipment usage [28]. In kindergartens, phthalate levels are lower and there is a shift toward the use of alternative plasticizers. Homes, on the other hand, showed a higher average contribution of antioxidants and PCP/HHPs, while offices exhibited a higher contribution of tobacco-derived alkaloids than other settings.

Overall, although NIRs direct comparison should be interpreted cautiously, collectively considering the number of compounds, their DFs, and the cumulative NIRs (Figure S7), homes can be considered the most complex environment among all the studied settings.

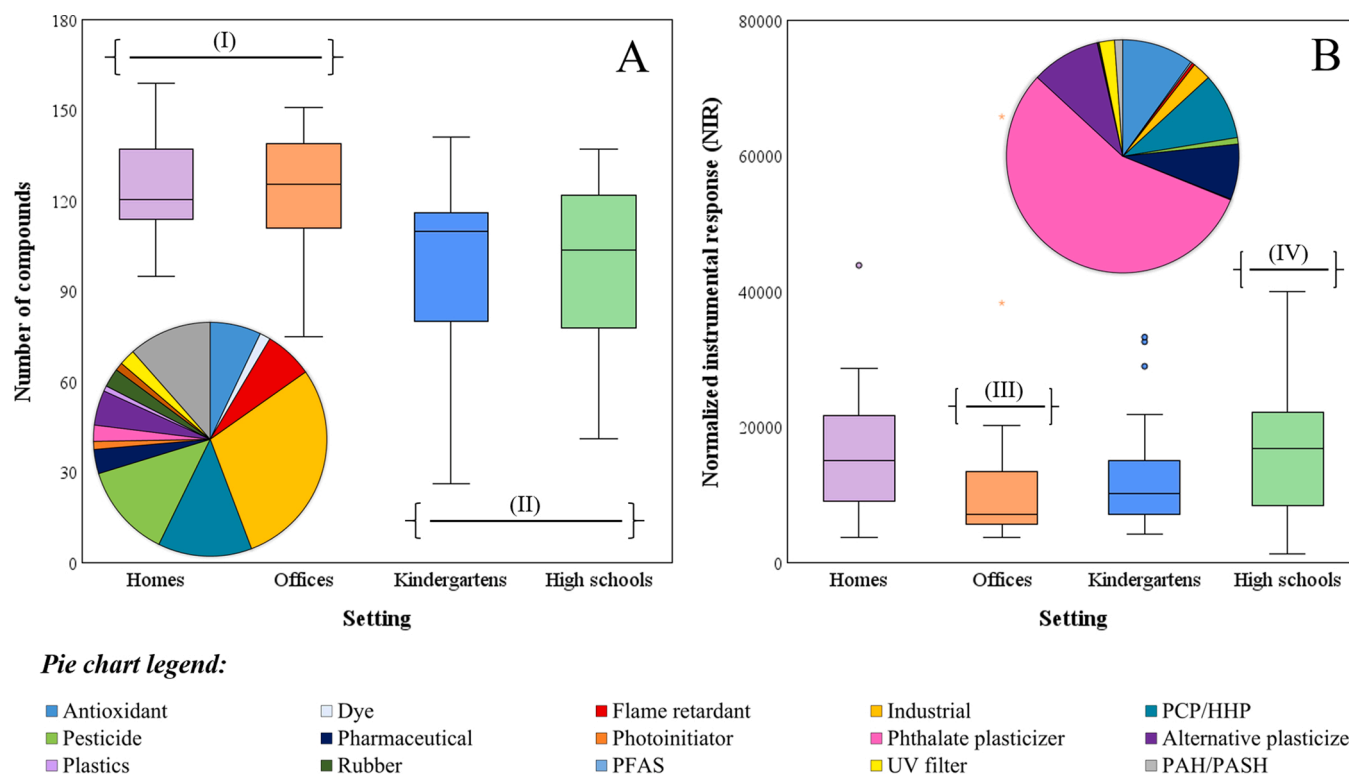


Fig. 1. Number of identified and annotated compounds and cumulative NIRs in the indoor dust samples. Significant intergroup differences were observed between groups (I) and (II) (One-way ANOVA) and (III) and (IV) (Kruskal-Wallis).

3.2. Major chemical classes and trends

3.2.1. Phthalate plasticizers

Phthalate plasticizers were detected in all dust samples from homes, offices, kindergartens, and high schools. Despite comprising only six compounds, this class dominated the total NIRs with median values exceeding 50%, highlighting dibutyl phthalate (DBP, DF=99%), benzyl butyl phthalate (BBP, 98%), bis(2-ethylhexyl) phthalate (DEHP, 95%), diisobutyl phthalate (DiBP, 92%), and diethyl phthalate (DEP, 92%). Phthalates are extensively incorporated to plastics to impart elasticity, transparency, or flexibility. Some of them, such as *ortho*-substituted phthalates (BBP, DEHP, DBP, and DiBP) are particularly harmful and have shown negative effects in endocrine disruption, reproduction, or neurodevelopment [5]. Their use has been gradually regulated in the European Union (EU) since they were identified as Substances of Very High Concern (SVHC), with regulations for children's toys in the early 2000s and more recently on electronics (2019) and consumer goods (2020) [29]. However, their long-standing historical use, coupled with the long lifespan of consumer products and the influence of circular economy (recycled plastics), render these compounds pervasive in indoor dust across EU countries [12,27,30]. While GC-QTOF-HRMS provides high-resolution data for these compounds, their extreme abundance relative to other families, combined with inherent challenges such as blank contributions and potential detector saturation, can bias the overall statistical interpretation of the chemical footprint [8,23,24,31]. Consequently, while a potential overestimation in peak intensities cannot be entirely ruled out, these analytical nuances have been

carefully controlled through strict blank-subtraction thresholds ($10 \times$). Due to the possible analytical limitations and their disproportionately high contributions, to ensure a balanced assessment of the broader indoor chemical behavior and to avoid masking the trends of less abundant contaminants, phthalates were excluded from the subsequent multivariate statistical analyses. The median contributions of the remaining families are shown in Figure S8.

3.2.2. Alternative plasticizers

Thirteen APs showed high detection frequencies in all environments, denoting citrates, butyrates, organophosphates, adipates, or trimellitates (Fig. 2). Although their indoor ubiquity has been previously described [32,33], their comparative presence in dust across different microenvironments has been scarcely reported in European settings and, specifically, in Spain [34]. Notably, APs followed a distinct trend compared to classic plasticizers, with generally individual NIRs in kindergartens $\approx$ high schools > homes > offices (Figure S8 and S9). This distribution is likely linked to the strict restrictions and replacement of phthalates in children's toys and school materials, as well as the widespread use of modern synthetic flooring and materials in these educational facilities, giving that building typology and contemporary components heavily shape alternative plasticizer profiles [11]. Among them, dioctyl terephthalate (DOTP) and tri(2-ethylhexyl) trimellitate (TOTM) are considered direct replacements for DEHP. TOTM, suggested to be an endocrine disruptor with persistent bioaccumulative properties [32,33], was widely dispersed (DF=99%) in all settings. DOTP is considered to have lower toxicity and higher stability, but there are also

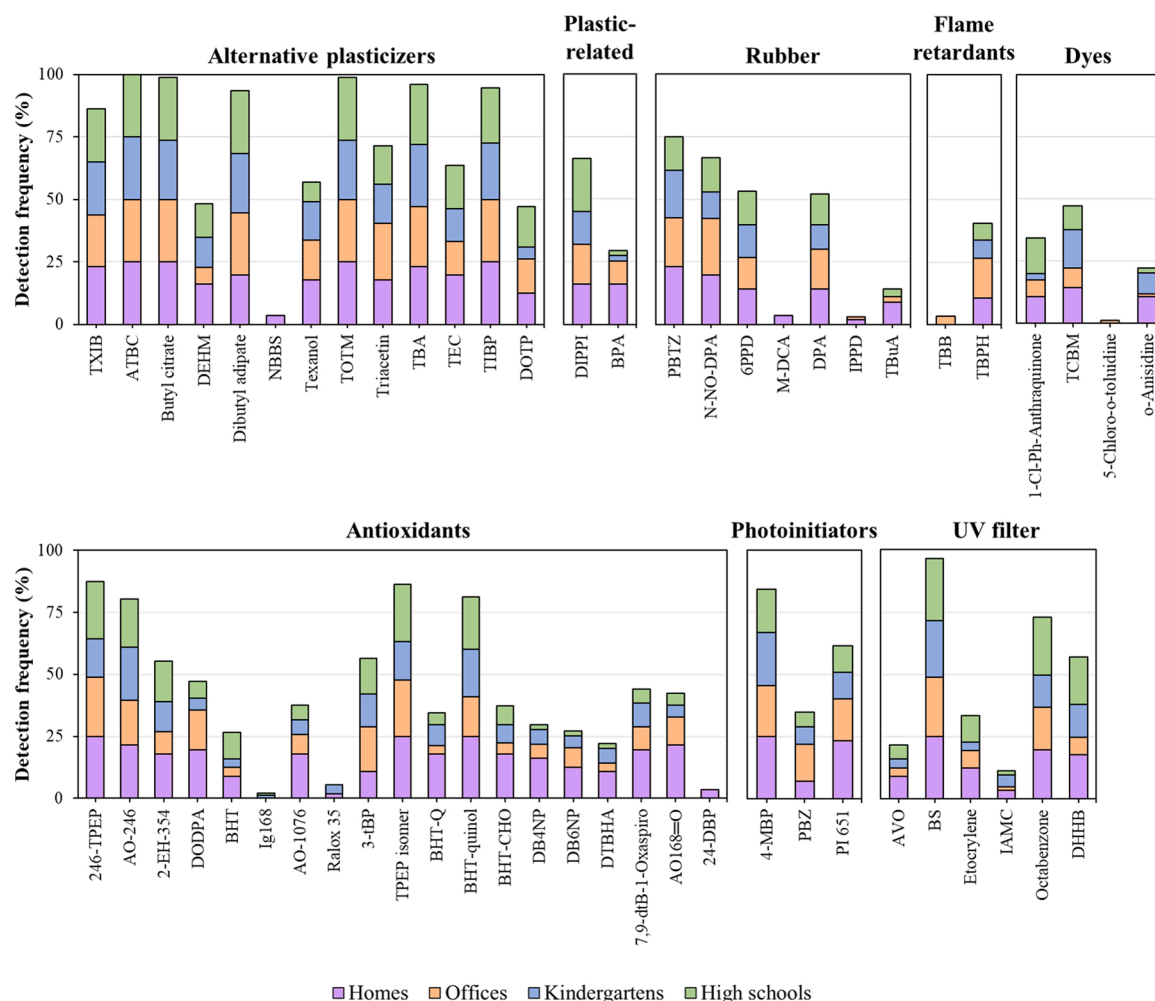


Fig. 2. Detection frequencies (DFs, %) per setting of the main chemical families identified in indoor dust.

concerns about potential negative health effects and high migration from parent materials [35]. Conversely, DOTP was less frequent (DF=48%) but highly variable in kindergartens, potentially reflecting disparities in material age or usage habits [32]. Other APs such as citrates (acetyl tributyl citrate, ATBC; butyl citrate; triethyl citrate, TEC; and tributyl aconitate; TBA) were frequently detected with major contributions to AP's summed NIRs. Butyl citrate and ATBC are probably the most studied citrate plasticizers and presented significantly lower ($p < 0.05$) levels in offices. On the other hand, TBA which was recently identified in indoor dust from China [36], was also widespread with no differences between environments ($p > 0.05$).

3.2.3. Flame retardants

FRs were more frequently found in offices than in other environments, a pattern previously linked to the high density of electronic devices or foam-containing furniture in these settings [10]. Among them OPFRs were prominent, aligning with their reported dispersion and high concentrations in indoor dust [6,16]. Interestingly, bis(2-ethylhexyl) tetrabromophthalate (TBPH) has emerged as a major replacement for polybrominated diphenyl ethers (PBDEs) in technical formulations such as FM-550, FM 600, FM BZ-54, or Uniplex FRP 45 [9]. Given its ubiquity in dust from different indoor spaces [2,9,37], apprehension regarding its toxicity and exposure through ingestion has escalated [38]. Consequently, a proposal was submitted in March 2026 to list TBPH under Annex A of the Stockholm Convention [39]. In this study, TBPH predominated in offices (64%), where 2-ethylhexyl tetrabromobenzoate (TBB, 14%) exhibited a concurrent detection pattern, probably due to their joint presence in commercial mixtures. While studies in Southern Europe have identified TBPH at ng/g concentrations [40], our screening approach highlights its extensive dispersion across various public and domestic spaces. The relatively lower overall detection frequencies of TBB compared to TBPH (4% vs. 40%) may be attributed to regional variations in technical formulations or different degradation rates [41, 42]. Furthermore, the presence of indoor pollutants is highly dependent on the timeframe, consumer goods, and materials. For instance, previous research found that TBPH concentrations were higher in theaters, followed by schools and residences [40], while it was the most abundant halogenated FR, followed by TBB, in Swedish offices [9]. These variations across environments and regions are likely driven by differing emission sources and specific formulation usage patterns [9].

3.2.4. Plastic, resins or foam-related compounds

Bisphenol-A (BPA) and 2,6-diisopropylphenyl isocyanate (DIPPI), related to plastics, epoxy resins or foams, were identified in all settings (DF=25% and 67%, respectively; Fig. 2). Despite stringent global regulations and the shift toward alternatives [5], BPA remains a concern due to its endocrine toxicity and frequent occurrence at indoors [27,30, 31]. In this study, BPA was more frequent in non-educational environments (47% vs. 9%), though median NIRs were higher in high schools (Figure S9), consistent with other studies [27]. Interestingly, no BPA alternatives (e.g. BPS or BPF) were detected suggesting that BPA remains the predominant monomer in these microenvironments despite current regulatory pressures. The detection of DIPPI is noteworthy, as its presence in indoor dust has been scarcely documented. As a transformation product in polyurethane resins [43], its widespread occurrence demonstrates the capability of our SS/NTS workflow to detect and annotate less-common contaminants that may contribute to the overall chemical diversity of indoor spaces.

3.2.5. Rubber-related compounds

Up to six compounds used in rubber-related products including antioxidants, vulcanizers, or stabilizers showed high frequency across the study (Fig. 2). Overall, total contribution was greater at homes, although for individual compounds statistical differences were only observed for 2-phenylbenzothiazole (DF=72%; $H \approx K > O \approx HS$). This compound has been linked to tires [44], but its detection in indoor dust from

conventional residential and educational environments is rare. Also notable was the detection of *p*-phenylenediamine antioxidants (PPDs) in all environments such as N-(1,3-dimethylbutyl)-N'-phenyl-*p*-phenylenediamine (6PPD; 53%, IC=1) and N-isopropyl-N'-phenyl-1, 4-phenylenediamine (IPPD; 2%, IC=1), but their quinone derivatives were not found. PPDs have been reported in residential indoor dust where 6PPD is frequently the predominant compound [45], but to the authors' knowledge, its presence in Spanish indoor environments has not been reported previously. The non-detection of the PPD-quinones is likely more related to a limitation of the GC-based analytical technique rather than an absolute absence in the analyzed samples, since these compounds have been detected in residential dust, but often using LC due to their higher polarity [45]. The occurrence of PPDs suggests possible infiltration of tire-wear particles into indoor spaces via different combined mechanisms, such as direct particle infiltration, deposition and dragging from outdoor surfaces, and/or adhesion to personal items like shoes or clothing [46]. Nevertheless, distinct domestic sources related to rubber-derived products, such as, belts, indoor mats, stored footwear, or specialized flooring remain plausible auxiliary contributions [47]. Given the known environmental toxicity of some rubber-related compounds and its highly toxic TPs (e.g. 6PPD-Q), these results underscore the relevance of monitoring rubber additives as key contributors to indoor dust complexity.

3.2.6. Synthetic antioxidants

Nineteen synthetic antioxidants (SAs) commonly used in lubricants, personal care products, or consumer goods were also detected widely dispersed in all settings (DF=2–87%; Figure S9). This category includes 10 parent antioxidants and 9 TPs. Most of them correlated significantly ($p < 0.05$), pointing to common sources and/or the use of multiple products containing SAs such as plastics or other elastomeric products [48] (Table S7). Exceptions were *m*-tert-Butylphenol (3-tBP; 58%), which is an SA byproduct [49] or an industrial intermediate of complex antioxidants (i.e. Irgafos), and other compounds with a rather different chemical structure (e.g. 4,4'-di-tert-octyldiphenylamine, DODPA; 43%). The latter was the most abundant amino antioxidant in residential dust from Canada, although its concentrations were much lower than those of phenolic antioxidants [50]. Residential environments exhibited the highest DFs and NIRs for SAs ($p < 0.05$), showing high intensities of the parent butylhydroxytoluene (BHT) and some of its TPs (e.g. BHT-quinone, BHT-quinol), as well as Irganox/Irgafos degradation products like 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione or *tris*(2,4-di-tert-butylphenyl) phosphate (AO168=O). The latter was more frequently detected at homes (DF=86%) than in occupational (45%) and educational environments (19%). These two compounds have caused a recent emerging concern due to their significant presence in the environment and indoor dust [10,16,51]. The compositional profiles showed a different behavior between settings (Fig. 3). While residential dust was enriched in these complex TPs, high schools showed higher relative contributions of parent BHT-related compounds. A more heterogeneous behavior is observed at offices and kindergartens. The phosphite antioxidant, Irganox 1076 (DF=38%) and the phenolic antioxidant Irgafos 168 (DF=2%) are used as plastic stabilizers and are ubiquitous contaminants in indoor environments [10,30,51]. The prevalence of TPs over parent Irgafos 168 suggests prolonged accumulation and aging in domestic settings which is consistent with the higher concentrations of TPs found in literature [10]. Additionally, BHT is a low molecular weight and highly volatile compound that tends to migrate from the original material and is pervasive in dust [3], including in Spain [23,52], where it eventually degrades. To evaluate this BHT degradation across different indoor environments, individual TFs were calculated for its six primary TPs. Individual comparison of TFs of each individual compound was carried out to qualitatively compare distribution differences observed in Fig. 3. Although interpreted with caution due to their compound-specific nature and potential alternative sources, these TFs provide useful and practical qualitative insights into indoor

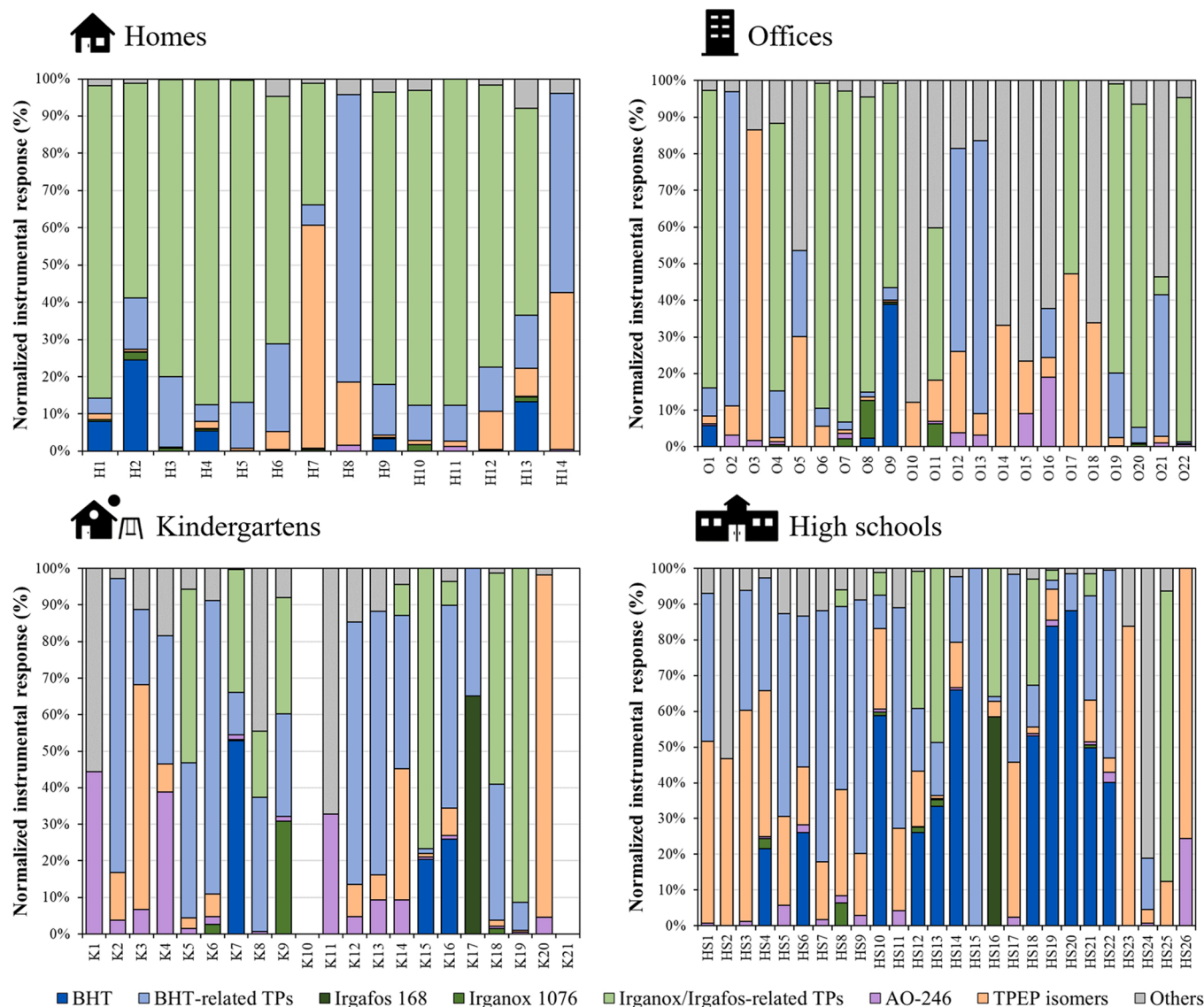


Fig. 3. Composition profile (NIR, %) of antioxidants annotated in indoor dust samples.

chemical transformation. Significant differences were observed in the degradation of BHT-Q, DB4NP, DB6NP, and DTBHA across the studied facilities ($p < 0.05$). For instance, a consistent trend was observed in dust from high schools and offices that exhibited significantly lower TFs for BHT-Q and DB4NP compared to kindergartens and homes. Specifically, the nitrated derivatives (DB4NP and DB6NP) which can be formed from BHT in lubricants [53] or from textiles [54], showed the most pronounced differentiation among settings, potentially reflecting higher rates of atmospheric nitration or longer residence times in residential dust. The lower ratios observed in high schools and offices appear to align with a higher prevalence of the parent BHT, which may be attributed to more frequent cleaning schedules preventing environmental degradation or the presence of fresh emission sources. In contrast, higher TFs in residential settings suggest that BHT undergoes extensive oxidative and nitrative transformation over time, supporting the hypothesis that monitoring TPs could help to assess antioxidant distribution in indoor environments.

3.2.7. Polymer surface curing and coating compounds

Six additional compounds used in polymer surface curing and coatings comprised PIs and PFAS. PIs have been used for years, but there is growing awareness of their fate and toxicity related to endocrine

disrupting effects, carcinogenicity, and neuro- or cytotoxicity [55]. In this study, 4-methylbenzophenone (4-MBP), 4-phenylbenzophenone (PBZ), and Irgacure 651 (PI 651) showed DFs of 82%, 35%, and 58%, respectively, with benzophenone analogues prevailing in non-educational settings ($p < 0.05$). Additionally, volatile and semi-volatile PFAS were screened in the analyzed samples through the NTS workflow incorporating a specific HRMS-mass spectral library that contains GC-EI mass spectra of 158 perfluorinated compounds. Among them, only N-Ethyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide (CAS 1691-99-2; N-EtFOSE; IC=2, Figure S10B) was sporadically detected in all environments (DFs=4–10%). Two additional features with very close elution (RT=5.6–5.8 min) and virtually identical mass spectra were tentatively annotated as its structural analogues (IC=3; Figure S10). While their mass spectra showed an accurate match with the library mass spectrum, the extensive in-source fragmentation characteristic of EI prevented the detection of the molecular ion, thus limiting the confirmation of their exact isomeric structures. These three isomers were detected simultaneously in kindergartens and exhibited prominent NIRs in the reference material SRM 2585 (Table S5), further supporting their identity and relevance in indoor environments. Indeed, indoor dust has recently been recognized as a reservoir for volatile PFAS [56], where the methylated analog N-MeFOSE was the predominant

compound. Dust samples were also screened for N-MeFOSE, although it was not detected. However, this compound and two possible structural isomers were observed in the reference material (Table S5). The detection of MeFOSE and EtFOSE in the current study highlights the importance of GC-HRMS as a complementary and orthogonal platform to standard LC-HRMS methods, which are generally used for ionic PFAS (e.g. PFOA, PFOS), but are less suitable to detect neutral precursors like FOSE-derivatives in the same matrices.

3.2.8. Other compounds

Nearly 20% of the characterized compounds corresponded to organic compounds indicative of indoor lifestyle sources. This group included fragrances and synthetic musks used in cosmetics or cleaning products such as acetyltetramethyltetralin (AETT), galaxolide, musk ketone, and butylphenyl methylpropional (BMHCA, lilial) and its TP lysmerol. Most of them were frequently found (DFs > 70%), in line with recent studies [3,8,21,23,30], despite of EU restrictions based on their bioaccumulation potential and/or toxicity (e.g. endocrine disruption, neuro or reproductive toxicity) [57–61]. Similarly, cosmetic additives like UV filters, such as salicylates, benzophenones, benzoates, and cinnamates or the thickening agent vitamin E acetate (VEA) were widespread in indoor dust. Although VEA gained notoriety as a diluent in e-cigarettes linked to severe lung injury [62], its near-universal detection in this study (DF = 98%) suggests the predominance of non-vaping sources. Given that no participants reported vaping habits, its prevalence may arise from use in cosmetics, such as skin creams or sunscreens, where it acts as an antioxidant and moisturizer [62]. On the contrary, a behavioral trend related to tobacco was observed for nicotine (DF = 28%) and its two TPs, myosmine (20%) and cotinine (2%), which were generally not detected in kindergartens.

3.3. Differences between environments and type of dust

A PCA was carried out to explore contamination profiles across

indoor dust collected in different environments (Fig. 4 and Table S8). The observed partial score overlaps and cumulative variance reflect the inherent heterogeneity of indoor dust; as a complex matrix influenced by multiple overlapping emission sources and numerous features, dust profiles naturally exhibit transitional and partial patterns rather than isolated clusters. The first principal component (PC1) was primarily defined by a cluster of PAHs/PASHs, which partially distinguished residential and occupational settings from educational environments, particularly high schools. This suggests that while common hypothesized combustion-derived processes such as urban traffic infiltration and heating in both settings, alongside domestic cooking in residences significantly influence the chemical variance in homes and offices, high schools appear less impacted by these plausible specific sources [1,3]. PC2 was characterized by high loadings of PCPs, including fragrances or preservatives (e.g. 2-methoxynaphthalene, alpha-cyclohexylidene benzeneacetonitrile, amyl salicylate, ethyl 4-ethoxybenzoate, n-hexyl salicylate), alongside APs (i.e. 2,2,4-trimethyl-1,3-pentanediol diisobutyrate; TXIB). This factor separated most of the kindergartens and homes from the other sites. In kindergartens, the prominence of TXIB is likely linked to specialized building materials and applications, such as resilient flooring, surface coatings, sealants, adhesives, paints, and school supplies [63], differentiating their profile from older high school installations. The higher load of PCPs suggests the specific use of hygiene and personal care products. The presence of these compounds is of particular concern in kindergartens, as children in early developmental stages might experience higher contact rates with indoor dust via ingestion and dermal transfer.

PC3 seems associated with structurally related styrenated phenols (i.e. bis(1-phenylethyl)-phenol and tris(1-phenylethyl)-phenol isomers), which were particularly prevalent in residential dust. Styrenated phenols are high production chemicals used both as secondary polymer antioxidants (mainly in rubber) and as industrial intermediates in the manufacturing of surfactants. Currently, they are listed under the ECHA's Endocrine Disruptors Assessment List [64], with some isomers

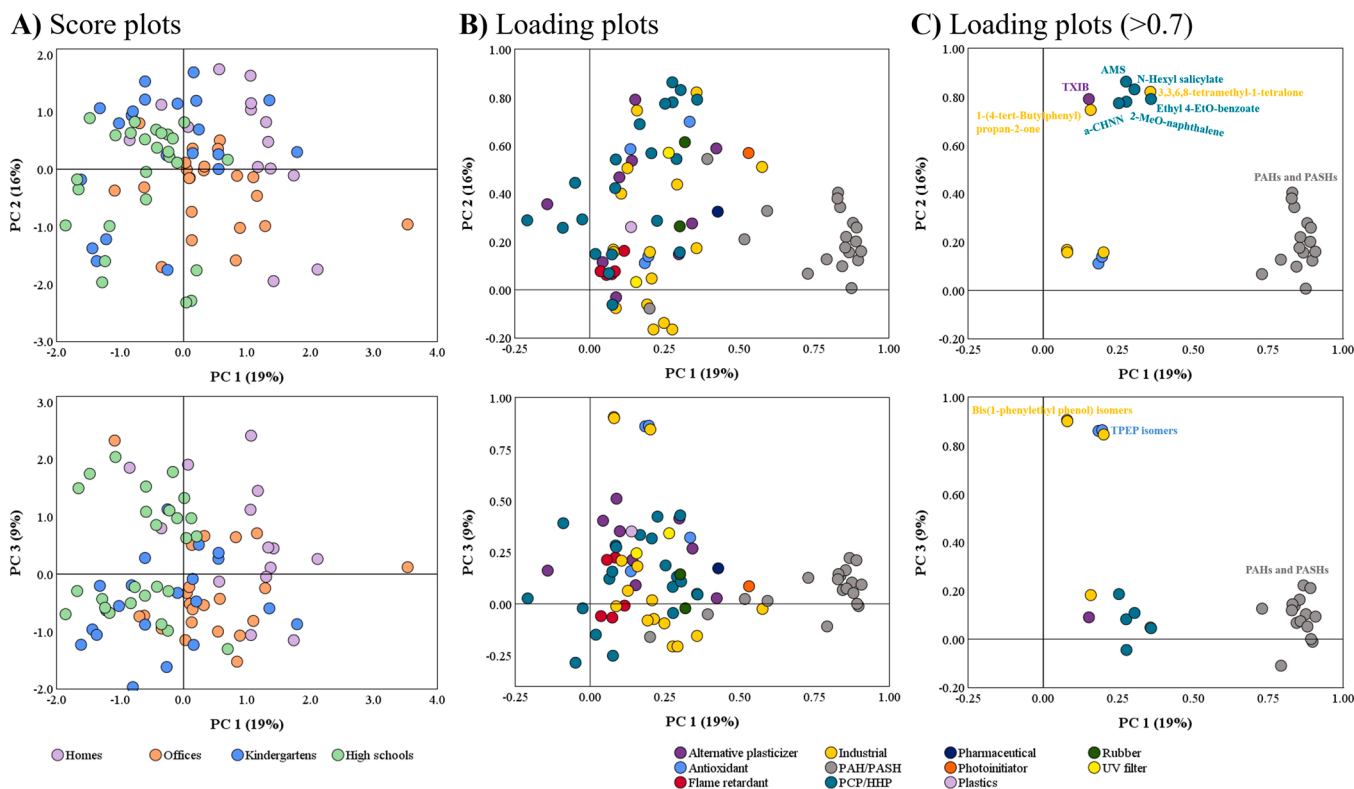


Fig. 4. PC1, PC2, and PC3 from PCA depicting (A) score plots, (B) loading plots and (C) simplified loading plot (only compounds with weights higher than 0.7 are shown) for each environment and highlighting the compound use.

reported to be persistent, bioaccumulative, and toxic [65]. These compounds showed notably lower scores in kindergartens compared to the other environments. Given that styrenated phenols are additives in older rubber and polymer formulations, their lower prevalence in kindergartens might reflect more frequent furniture renovation or the use of more modern building materials, as building age and material replacement practices are known to substantially drive pollutant concentrations and profiles across indoor environments, including preschool facilities [11, 66]. Finally, although the contribution of PC4 to the total variance was lower, it was uniquely defined by high loadings of legacy PCBs (Figure S11), with offices exhibiting the highest positive scores. This may suggest that aging administrative building infrastructure or old electrical equipment may act as background sources of legacy contaminants, even though they have been banned for decades [1,27].

Complementary to PCA, HCA was performed on the selected marker compounds as an exploratory grouping tool to visualize site-specific co-occurrence patterns across the different studied microenvironments [7]. The dendrogram categorized individual samples into two primary nodes (cluster 1 and 2) based on their contamination profiles (visualized across the heatmap in Fig. 5 where a monochromatic blue scale was used to represent normalized abundance). Cluster 2 represented samples with low contaminant loads exhibiting lighter blue tones, all of which belonged to educational settings. In contrast, cluster 1 comprised the more complex environments, further segregating into four sub-clusters with distinct chemical composition and potential exposure scenarios. Sub-cluster 1.1, predominantly composed of educational samples, displayed a branched chemical fingerprint preferentially dominated by PCP/HHPs and styrenated phenols, visible as distinct darker blue bands, in accordance with PC2 and PC3. Sub-cluster 1.2 was composed almost entirely of offices with elevated levels of PCBs (i.e. PC4) indicated by prominent dark blue zones and relatively low antioxidant and other industrial compounds content. Finally, sub-clusters 1.3 and 1.4 captured those environments with higher complexity, encompassing most of the household samples. These were branched into a combustion-impacted group (sub-cluster 1.3), showing a distinct dark blue hot-spot for PAHs/PASHs and other settings (sub-cluster 1.4) with more heterogeneous contamination patterns.

Regarding occupational environments, two types of samples were

compared: floor dust and elevated-surface settled dust accumulated on elevated surfaces. This comparison revealed higher median values in elevated-surface settled dust for both, the number of compounds and NIRs, although statistically significant differences were only observed for the latter case (Mann-Whitney). This finding is consistent with previous studies that reported higher concentrations in elevated-surface settled dust [67], likely influenced by several factors such as infrequent cleaning, proximal sources, or dust aging [2]. When comparing each location separately, only high schools presented differences ($p < 0.05$). In this environment, up to 39 compounds exhibited statistical differences or were uniquely detected in one type of dust, reflecting distinct emission sources and/or transport dynamics (Table S9; Figure S12). Elevated-surface settled dust showed particularly higher levels of APs (e.g. TOTM, ATBC, DEHM) and SAs (e.g. 2,4,6-TPEP, AO-246). Low vapor pressures and high Koc/Koa of these compounds may suggest preferential accumulation in elevated-surface settled dust due to source proximity (i.e. electronics or polymer-based furniture) and less frequent cleaning, which facilitates dust enrichment and aging. On the other hand, floor dust revealed greater variability, probably more influenced by physical transport, more intensive cleaning and external factors. For instance, the heaviest PAHs, such as benzopyrenes, benzoanthracenes, and benzofluoranthenes, were preferentially accumulated in floor dust, while lighter analogues did not show statistical differences between different dust types. This suggests that outdoor sources (e.g. traffic) and lower volatility could be the main drivers for the accumulation of heavier PAHs in floor dust. In addition, the unique detection in this matrix, high particle affinity, and the low volatility of the flame retardant 2-isopropylphenyl diphenyl phosphate (2IPPDPP) would link its presence to proximal sources for this compound. Its use in plastics and flooring applications makes direct abrasion of these materials a plausible source [68]. Interestingly, the detection of myosmine (30%, DF) and nicotine (15%) reflects different dynamics, suggesting a more favorable oxidative degradation on the floor or non-tobacco contributions such as dietary sources or soil tracked from outdoors [69]. Consequently, our results could reflect that elevated-surface settled dust provides a more stable profile of long-term indoor emissions, whereas floor dust captures greater variability driven by outdoor-to-indoor transport and physical disturbance [2].

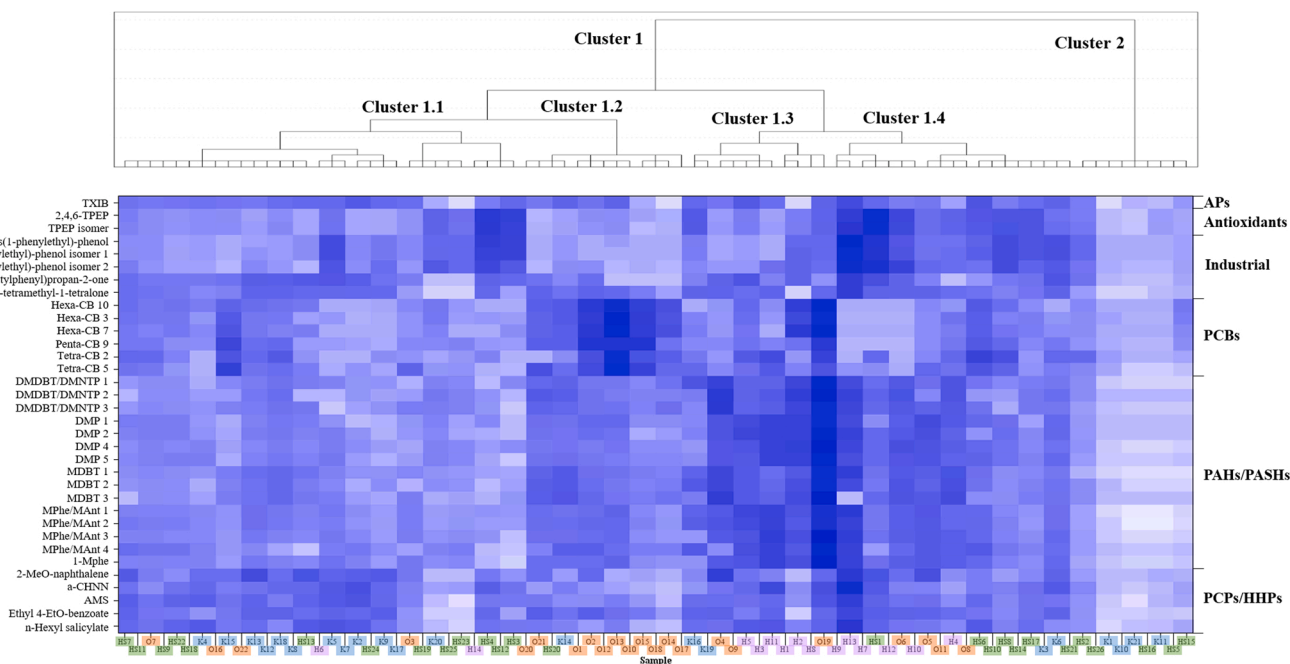


Fig. 5. HCA and heatmap across indoor microenvironments: homes (H, purple), offices (O, orange), kindergartens (K, blue), and high schools (HS, green). Color intensity reflects the normalized abundance of each compound, ranging from dark blue (high abundance) to light blue (low abundance).

4. Conclusions

This study evaluated the occurrence of POPs and emerging contaminants in indoor dust from four indoor micro-environments (homes, offices, kindergartens, and high schools) through a multi-tiered screening framework using a SS workflow complemented with NTS via GC-QTOF-HRMS. The proposed strategy characterized a wide variety of compounds belonging to different classes, such as plasticizers, antioxidants, FRs, industrial compounds, or PCPs and allowed to establish qualitative comparisons of chemical profiles.

Homes emerged as the most chemically complex environment, exhibiting the highest overall pollutant loads in terms of number of compounds and individual NIRs. Synthetic compounds related to plastics or other polymeric materials were the most ubiquitous and predominant pollutants in all environments. Among them, phthalate plasticizers and APs were more abundant in educational environments. The integration of multivariate analyses proved essential for deciphering these complex matrices, pinpointing contaminants hypothesized to arise from incomplete combustion products (i.e. PAHs) and legacy PCBs from old electronic equipment as key markers for residential and occupational exposure-relevant settings, while certain PCPs and plastic-related additives predominated in educational centers.

The broad profiling of indoor dust revealed a wide array of chemicals with diverse known and potential toxicological profiles. Consequently, indoor dust can serve as an environmental matrix for identifying potential indoor contaminant sources and prioritizing chemicals of exposure concern. However, dust chemical analysis alone cannot determine actual human exposure doses, dominant exposure pathways, or health risks. Further research is required to characterize concentration levels of prioritized compounds and perform integrated risk assessment.

CRedit authorship contribution statement

Silvia Royano: Writing – review & editing, Validation, Methodology, Investigation, Formal analysis, Data curation. **Juan Escobar-Arnanz:** Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation. **María Ángeles Martínez:** Writing – review & editing, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Adrián de la Torre:** Writing – review & editing, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Irene Navarro:** Writing – review & editing, Validation, Resources, Methodology, Investigation, Conceptualization. **Covadonga Alonso:** Writing – review & editing, Methodology, Investigation.

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. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.jhazmat.2026.143748](https://doi.org/10.1016/j.jhazmat.2026.143748).

Data Availability

Data will be made available on request.

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