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Measured Concentrations of Consumer Product Chemicals in California House Dust: Implications for Sources, Exposure, and Toxicity Potential

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Abstract

Household dust is a reservoir of various consumer product chemicals. Thus, characterizing comprehensive chemical profiles of house dust may help improve our understanding of residential chemical exposure. We have previously developed a method for detecting a broad spectrum of chemicals in dust by applying a combination of target, suspect screening, and non-target methods with mass spectrometry preceded by liquid chromatography and gas chromatography. Building upon a previous study that detected 271 compounds in 38 dust samples, we presented concentrations of 144 compounds that were confirmed and quantified by standards in the same set of samples. Ten compounds were measured with median concentrations greater than 10,000 ng/g of dust: cis-hexadec-6-enoic acid, squalene, cholesterol, vitamin E, bis(2-ethylhexyl) phthalate, dioctyl terephthalate, linoleic acid, tricaprylin, tris(1-chloroisopropyl) phosphate, and oxybenzone. We also reviewed *in vitro* toxicity screening data to identify compounds that were not previously detected in indoor dust but have potential for adverse health effects. Among 119 newly detected compounds, 13 had endocrine disrupting potential and 7 had neurotoxic potential. Toxicity screening data were not available for eight biocides, which may adversely affect health. Our results strive to provide more comprehensive chemical profiles of house dust and identified information gaps for future health studies.

Keywords

concentration; dust; in vitro bioactivity assays; non-target; suspect screening; target

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Conflict of interest

The authors declare that they have no competing interest.

Appendix A. Supporting Information

Supplementary data associated with this article can be found in the online version at.

1. Introduction

Thousands of chemicals are currently used in consumer products. Many of the consumer product chemicals have not been studied for exposure potential in the indoor environment where people in developed countries spend most of their time.¹ The most studied chemical classes in the indoor environment include pesticides, flame retardants, plasticizers, polycyclic aromatic hydrocarbons (PAHs), and per- and polyfluoroalkyl substances (PFAS). ^{2, 3} Because of potential health concerns over exposures to some of these chemical classes, a large number of alternative chemicals are being introduced into consumer products every year, following legislative activities or advocacy campaigns.^{4–6} However, exposure and toxicity information needed to evaluate potential human health effects are limited for the alternative chemicals that were not previously measured in indoor environmental media.⁷

Chemical concentrations in indoor environmental media including air, airborne particles, and settled floor dust have been used to characterize residential exposure to indoor contaminants. ^{2, 8–10} Many consumer product chemicals of current and emerging health concerns are semivolatile organic compounds (SVOCs).² When released from their original sources, SVOCs are redistributed over time and primarily partitioned to dust and other indoor surfaces.^{3, 11, 12} When dust concentrations are known but other media concentrations are not measured, partitioning models among dust, gas-phase, and airborne particles can be used to characterize residential chemical exposure.^{2, 10} Thus, there have been growing efforts in detecting and quantifying SVOCs in house dust.³ However, a complete picture of the chemical fingerprint of dust (i.e., identity and quantity of all chemicals present) is missing, because most previous studies analyzed *known* chemical classes via a targeted analytical method.^{2, 13–17} Therefore, development of advanced environmental monitoring methods has emerged as a prominent topic in indoor environmental research in order to detect both *known* chemical classes and those that were previously not targeted for detection in dust.

Advances in high-resolution mass spectrometry make it possible not only to detect known compounds for which reference standards are available (targets), but also to detect expected compounds using existing databases, libraries, or software matching algorithms (suspects) and even to identify previously unknown compounds (non-targets) through careful examination of high-resolution mass spectra.^{18, 19} To date, four studies have applied suspect screening and non-target methods to dust samples. Hilton et al.²⁰ first applied a non-target method to one household dust sample obtained from the National Institute of Standards and Technology (NIST) using two-dimensional gas chromatography time-of-flight mass spectrometry (GC×GC-TOF/MS). Ouyang et al.²¹ carried out a non-target analysis for one household dust sample collected in Sweden using two-dimensional liquid chromatography (LC×LC)-TOF/MS. Rager et al.²² applied suspect screening and non-target methods to 50 household dust samples collected in the U.S. from 2005 to 2006 using LC-TOF/MS. A comparative study of a non-target analysis was conducted in a composite house dust sample as part of a collaborative effort using LC-MS and GC-MS.²³ The methods used in the four studies are useful for identifying previously unknown and even unexpected chemicals in dust, but none of them presented concentrations that were confirmed and quantified by standards.

As part of an effort to evaluate a large number of environmental chemicals for potential health effects efficiently, the U.S. Environmental Protection Agency (EPA)'s Toxicity Forecaster (ToxCast) program utilizes hundreds of *in vitro* high-throughput screening (HTS) assays to support prediction of *in vivo* toxicities.²⁴ In a parallel effort to screen a larger of number of chemicals based on exposure, several high-throughput (HT) methods including exposure models were developed to characterize and quantify exposures.^{10, 25–28} As indoor dust is a reservoir for SVOCs released indoors and can provide reasonable surrogates for characterizing exposures, we have previously developed a method for detecting a broad spectrum of chemicals in dust by applying a combination of target, suspect screening, and non-target methods using both LC-quadrupole time-of-flight (QTOF)/MS and GC-QTOF/MS.¹⁸ Building upon this previous publication,¹⁸ this current study presents chemical concentrations that were quantified in the same set of dust samples for target, suspect and selected nontarget compounds. In addition, we investigated whether the compounds detected in our samples had either endocrine-disrupting or neurotoxic potential, and discussed possible applications of our findings to future health studies.

2. Materials and Methods

2.1. Overview and scope of this study

The aim of this study is to inform key data gaps for assessing potential health effects for consumer product chemicals by integrating our measured dust concentrations with existing exposure and toxicity potential data. Our previously published study comprehensively characterized compounds found in house dust samples, detecting diverse and numerous consumer product chemicals. The present study extends those findings by quantifying concentrations, assessing household level variability, and considering potential exposure and toxicity of the compounds detected. Five steps were taken toward achieving the overall aim. First, we classified detected chemicals by their chemical class (e.g., phthalate) and their common use category (e.g., plasticizer). Second, we compiled information on chemical analysis techniques used to detect the compounds, including analytical instrument (LC or GC) and method (target, suspect screening, or non-target), the limit of detection (LOD), and information on whether identities were confirmed and concentrations were quantified by standards. Third, we summarized results from the chemical analysis, including the number of samples in which a compound was detected, information on whether a compound was newly detected in our house dust, and summary statistics of measured concentrations. Fourth, we added information on whether each detected compound has endocrine disrupting or neurotoxic potential based on in vitro HTS assays. Fifth, we indicated whether the compounds detected in our dust have been biomonitored in the U.S. National Health and Nutrition Examination Survey (NHANES).29

Note that we did not compare our measured concentrations to those reported in other peerreviewed studies but focused on summarizing our concentrations by chemical class or use category. Other studies have already ascertained that differences in concentrations among studies may result from different sampling methods as well as geographic and temporal variation in chemical use.^{2, 30} In addition, we did not describe sample collection, dust extraction and analytical methods in detail in the current study because the details are

available in the previous study.¹⁸ The whole analytical method and workflow were completely validated, results of quality assurance (QA) and quality control (QC) for each of the analytical approaches were provided, and strengths and weaknesses of the various approaches and analytical instruments were discussed previously.¹⁸ Thus, we briefly described sampling and analytical methods to the extent necessary for others to quickly extract key information regarding environmental monitoring, such as sample size, sampling method, period and location, and type of analytical instruments. Results of *in vitro* HTS assays presented in this study do not necessarily represent *in vivo* toxicities. Factors influencing toxicity such as pharmacokinetics and metabolism, early-life susceptibility, and genetic variability are not addressed by ToxCast.^{24, 31} Thus, toxicity potentials presented in this study need to be interpreted with caution. Other limitations of using *in vitro* HTS assays for predicting *in vivo* response are discussed elsewhere.³¹

2.2. Sampling and analytical methods

We recruited 38 families in Northern California from May 2015 to August 2016. From each household, we collected one dust sample from an approximate 2 m² area in the main living room using a high-volume small surface sampler (HVS3), following a standard protocol.³² Dust samples were sieved and 100 mg aliquots were sonication-extracted with hexane/ acetone (3:1 v/v) and acetone (100%). The extracts were then analyzed by both LC-QTOF/MS and GC-QTOF/MS with methods that were able to analyze compounds from various compound classes with widely differing chemical properties (e.g., molecular size, logP). In addition to the classical target analysis using reference standards and isotope-labelled internal standards, additional suspect screening and non-target analysis were performed. In order to unambiguously confirm the identity of suspected and non-targeted compounds, additional reference standards were purchased if they were available. Details of quantification methods are available elsewhere.¹⁸

2.3. Selection of target compounds

For the targeted method, we selected 76 chemicals for GC analysis and 56 chemicals for LC analysis (see Supporting Information [SI], Table S1). The targeted compounds included personal care products (PCPs; antimicrobial compounds, fragrance ingredients, parabens, ultraviolet [UV] filters), markers of human inputs (skin oils, metabolites), flame retardants (polybrominated diphenyl ethers [PBDEs], organophosphate flame retardants [OP-FRs], and other FRs), pesticides (insecticides, fungicides, herbicides), and a variety of other compounds widely detected in homes (phenols, phthalates, other plasticizers, PAHs, PFAS, and surfactants). The selection criteria included one (or multiple) indicator compounds from substance classes identified in our previous study⁷ or compounds present in products listed in the U.S. EPA's Consumer Product Chemical Profiles database (CPCPdb).³³

2.3. Chemical use categorization

Chemicals identified in the current study were classified into the most common and primary use category to understand the distribution of measured compounds by use category. For most compounds, we relied on "product" or "use" categorization available in databases such as CPCPdb and the U.S. National Library of Medicine's Household Product Database (https://householdproducts.nlm.nih.gov/index.htm) to find the most common and primary

use category of the compounds associated with at least one consumer product. For compounds with multiple uses, we also relied on web searches to find common uses. Multiple-use compounds were assigned to a primary use category and their secondary or tertiary use categories were further discussed in Results and Discussion. Thus, use categorization may be imprecise. For compounds that are consumed via dietary sources and also formulated in cosmetic products (e.g., linoleic acid, palmitic acid, cholesterol, fatty acids),³⁴ it is likely that emissions from cooking are their dominant source to residential floor dust. Therefore, we preferentially assigned their primary use category to food sources. We further discussed this in Results and Discussion.

2.4. Data sources of endocrine-disrupting potential or neurotoxic potential

Many chemicals present in consumer products exhibit endocrine-disrupting potential³⁵ or neurotoxic potential.³⁶ To determine whether the compounds detected in our samples have either endocrine-disrupting or neurotoxic potential, we used in vitro HTS assays, most of which are included in the U.S. EPA's ToxCast program. For endocrine-disrupting potential, we evaluated four main processes, including androgen, estrogen, thyroid, and steroidogenic. For androgen, we utilized androgen receptor (AR) pathway activity integrated from 11 ARrelated in vitro HTS ToxCast assays and considered compounds with area under the curve (AUC) of 0.1 to be active in at least one AR pathway assay (active, inactive).³⁷ For estrogen, we utilized estrogen receptor (ER) interaction scores integrated from 13 ER-related *in vitro* ToxCast assays and considered compounds with an AUC score of 0.1 to be active in at least one ER pathway assay (active, inactive).³⁸ For thyroid, we utilized the results from the *in vitro* Amplex UltraRed thyroperoxidase or thyroid peroxidase (AUR-TPO) assay³⁹ and a thyroid-specific in vitro HTS ToxCast assay.⁴⁰ Because decreased TPO activity reduces thyroid hormone synthesis, compounds that elicited a 20% reduction in maximal TPO activity were considered to inhibit TPO (active, inactive).³⁹ We also identified compounds that exhibited thyroid receptor activity measured by the *in vitro* ToxCast assay (active, inactive).⁴⁰ For steroidogenesis, we utilized results from a method that considered 10 steroid hormones, including progestogens, glucocorticoids, androgens, and estrogens using an *in vitro* HTS assay with H295R human adrenocortical carcinoma cells.⁴¹ Among 2,060 evaluated compounds, we considered compounds that altered at least 4 steroid hormones at the maximum tolerated concentration to be active (or inactive), the same criteria used in Karmaus et al.⁴¹ For a neurotoxic indicator, we utilized microelectrode array hits as a measure of neural network activity in vitro (yes, no).42 A summary of toxicological endpoint data is provided in Table S2.

2.5. Statistical analysis

Statistical analyses were performed using Microsoft Excel 2018. For concentrations between the limit of quantification (LOQ) and the LOD, we assigned a value of the LOQ divided by 2. For concentrations below the LOD, we assigned a value of the LOD divided by the square root of 2.⁴³ For compounds detected in more than 50% of the samples, we summarized measured median concentrations by five levels (<500, 500–1,000, 1,000–5,000, 5,000–10,000, >10,000 ng/g of dust) to investigate which compound classes were measured and present at high concentrations. We also computed coefficients of variation (CV) to examine the variability of concentrations in dust across homes.

3. Results

3.1. Measured dust concentrations

A total of 276 compounds were detected in our dust samples in which 5 additional compounds were later detected after a previous study was published.¹⁸ For 14 compounds, identification was not possible and only molecular formula (e.g., C₄H₇FO) could be assigned. Table S2 summarizes information of analytical methods, results from the analysis, exposure and toxicity potential for 262 detected compounds that could be identified with structure and formula. Additional summary for all 262 compounds detected in our dust is provided in the Supporting Information (see Data S1 for overall description and Table S3 for summary by chemical class and analytical instruments/methods). Overall, a large number of UV filters, phthalates, and OP-FRs were detected in our dust samples and median concentrations for some of them were above 10,000 ng/g of dust (Figure 1). Ten compounds were measured with median concentrations greater than 10,000 ng/g of dust: cis-hexadec-6enoic acid, squalene, cholesterol, vitamin E, linoleic acid, tricaprylin, bis(2-ethylhexyl) phthalate [DEHP], dioctyl terephthalate [DOTP], tris(1-chloroisopropyl) phosphate [TCIPP], and one UV filter (oxybenzone). Cis-hexadec-6-enoic acid, squalene, cholesterol and vitamin E comprise or are found in skin surface lipids.⁴⁴ Linoleic acid, cholesterol, and tricaprylin are widely used in cosmetics and personal care products. However, it is likely that emissions from cooking may significantly contribute to the measured dust levels of linoleic acid, cholesterol, and vitamin E.34 Consumer products (e.g., electronics, plastic products, shower curtains), building materials (e.g., vinyl flooring), and furniture (e.g., couches) are well-known emission sources of DEHP, DOTP, or TCIPP in the indoor environment. High concentrations of other chemical classes (e.g., skin oils, cosmetic ingredients, UV filters) detected in the current study highlight that humans and their activities, and possibly pets, play a role as sources of SVOCs in the indoor environment. Fungicides, PBDEs, PFAS, and pharmaceuticals were also abundant in our samples, but most were measured at concentrations below 500 ng/g of dust.

In the present study, 119 compounds were identified and/or quantified for the first time in household dust (Figure S1). Some of these compounds were previously measured in U.S. wastewater samples via target analysis but had not been measured in indoor dust. The majority of these compounds was detected via LC non-target (45%) and LC suspect (31%) approaches (see inset of Figure S1). These newly measured compounds mainly comprised surfactants (n = 25), pharmaceuticals (n = 19), compounds with unknown use information (n = 17), and human metabolites (n = 12), because of the polarity of these compounds. We also identified 6 phenols (some are also used as biocides) and 11 biocides (4 insecticides, 7 fungicides) in dust for the first time mostly via GC target and/or LC target analyses.

Overall, dust concentrations varied by almost three orders of magnitude across household samples and by almost four orders of magnitude across compounds (Figure 2). PFAS were measured at the lowest concentrations and had relatively large variability in concentrations. DEHP was shown to have the smallest variability (coefficient of variation, CV = 0.35) across the samples. Except for tri-n-butyl phosphate (TNBP), OP-FRs were measured at higher concentrations than PBDEs, and bisphenol S (BPS) was measured at higher concentrations

than bisphenol A (BPA). This is consistent with recent changes in consumer use due to changes in product formulation and regulations affecting PBDEs and BPA. Variability metrics for all compounds including CVs are available in Table S2.

Below, we summarized our measured dust concentrations along with other exposure and toxicity potential information by four categories: (1) chemical classes other than biocides that have received considerable public attention in indoor dust (e.g., phthalates, PBDEs, OP-FRs, PFAS), (2) biocides (e.g., insecticides, fungicides), (3) compounds in PCPs (e.g., fragrance ingredients, UV filters), and (4) chemical classes whose dust concentrations are of less concern for environmental exposure calculations (e.g., food additives, skin oils).

3.2. Chemical classes of current and emerging concerns in indoor dust

3.2.1. Phthalates and other plasticizers—Among 7 target phthalates, benzyl butyl phthalate (BBP), DEHP, di-isobutyl phthalate (DiBP), and di-n-butyl phthalate (DnBP) were detected in all of our samples. Median concentrations of these four phthalates were above 3,000 ng/g of dust (Table 1). Diethyl phthalate (DEP) and dimethyl phthalate (DMP) were detected in 79% and 71% of the samples, respectively, at relatively low concentrations (medians were below 1,000 ng/g of dust). Di-n-octyl phthalate (DOP), a target compound of the current study, was not detected in our dust, whereas it was detected in 100% of other California house dust samples collected in 2006.²

We detected 6 non-phthalate plasticizers and two were newly detected in our dust (dioctyl terephthalate (DOTP), 1,3-diphenylguanidine, toluene-2-sulfonamide, and diethylene glycol dibenzoate). Note that 1,3-diphenylguanidine is primarily used in various solid items including rubber footwear and automobile tires. The four compounds were widely detected in our samples (34 out of 38 samples). The latter two were detected via suspect screening and non-target methods, respectively. The median concentration of DOTP, a direct replacement for DEHP, was as high as DEHP. Among the four newly detected compounds, 1,3-diphenylguanidine has both endocrine and neurotoxic potential, but has not been biomonitored in NHANES.

3.2.2. Bisphenols and bisphenol analogues (hereafter referred as

'bisphenols')—BPA and BPS were detected in all of our samples, and two bisphenol analogues that can serve as replacements for BPA were measured in our dust samples via a target method, including bisphenol A bis (2,3-dihydroxypropyl) ether [BADGE.2H2O] and bisphenol A (3-chloro-2-hydroxypropyl) (2,3-dihydroxypropyl) ether [BADGE-HCI-H2O]. Bisphenol AF (BPAF) was also detected in our samples via a suspect screening method. We confirmed that BPAF has both endocrine and neurotoxic potential, but has not been biomonitored in NHANES. BADGE.2H2O and BADGE-HCI-H2O were not tested for endocrine-disrupting and neurotoxic potential using *in vitro* HTS assays and have not been biomonitored in NHANES.

3.2.3. PBDEs, OP-FRs, and other FRs—Seven PBDEs were detected and quantified in our samples via a target method and they have been biomonitored in NHANES. Although *in vitro* toxicity screening data were not available for all PBDEs, other adverse health effects of PBDEs have been summarized elsewhere.⁴⁵ BDE-209 has been widely detected in other

California house dust.^{46, 47} However, we could not have detected BDE-209 in our samples because our GC method was not designed to measure compounds with such low volatility.

Ten OP-FRs, including 7 target compounds, were detected in our dust samples. Five OP-FRs were ubiquitous (>97%) in our samples. Overall, median concentrations of OP-FRs were higher than those of PBDEs by one order of magnitude. Even though tris(2-butoxyethyl) phosphate (TBOEP) was ubiquitous (>97%) in our samples and measured at high concentrations (median was 7,445 ng/g of dust), it has not been biomonitored in NHANES. Octyl diphenyl phosphate was newly detected in our dust via suspect screening. Four OP-FRs have either endocrine-disrupting or neurotoxic potential, but *in vitro* toxicity screening data were not available for tris(4-butyl-phenyl) phosphate (TBPP) and octyl diphenyl phosphate.

In addition to PBDEs and OP-FRs, we detected five compounds that are used as flame retardants. Three compounds were detected in a few samples (<4) via a target method. Melamine and 3,3',5,5'-Tetrabromobisphenol A (TBBPA) were detected in 17 and 36 samples, respectively, via suspect screening. TBBPA has both endocrine-disrupting potential and neurotoxic potential, but has not been biomonitored in NHANES. Because melamine was detected in almost half of our samples and has been detected in urine specimens of children who consumed milk products,⁴⁸ toxicity testing and biomonitoring are recommended for this compound.

3.2.4. PFAS—A total of 15 PFAS were detected in our dust, including 10 target compounds. We newly detected 3-(perfluorooctyl)propyl iodide in our dust (37 out of 38 samples) via a non-target method. Compared to other chemical classes, PFAS median concentrations were relatively low (<12 ng/g of dust). Eleven PFAS have been biomonitored in NHANES and seven of them were tested for endocrine-disrupting and neurotoxic potential using *in vitro* HTS assays.

3.2.5. Phenols—Among 15 targeted phenols, only 7 phenols were detected in our samples where trichlorophenols and cresols were detected with multiple isomers. Four phenols were newly detected in our dust via a target method, but in only one sample. We additionally detected 2,4-dinitrophenol via suspect screening. Overall, due to the low detection frequency, median concentrations were computed only for phenol and cresols (580 and 250 ng/g of dust, respectively). None of the 8 detected phenols was biomonitored in NHANES and only three phenols were tested for toxicity using *in vitro* HTS assays. Cresols were detected with multiple isomers (o-, m-, p-) in 34 out of 38 samples and thus are recommended to be included in future biomonitoring and *in vitro* toxicity screening testing.

3.2.6. PAHs—Among 12 targeted PAHs, 8 PAHs were detected in our samples. Because structures of dibenzo(a,h)anthracene and indeno(1,2,3-cd)pyrene were too close to discriminate one from the other, results were reported together in Table 1. Except for phenanthrene, 7 other PAHs were detected in fewer than 50% of our samples. Four PAHs were or have been biomonitored in NHANES. *In vitro* toxicity screening testing data for endocrine-disrupting potential or neurotoxic potential were not available for three PAHs, but other toxic endpoints are available from *in vitro* HTS assays.⁴⁹

3.3. Biocides

3.3.1. Insecticides—We detected 22 insecticides mostly via a target method (Table 2). Four insecticides were newly detected in our samples, but in fewer than 25% of our samples. Permethrin was measured at the highest median concentration (1,922 ng/g of dust), but the 95th percentile concentration of other four insecticides (imidacloprid, etofenprox, cypermethrin, tetrachlorvinphos) was higher than that of permethrin. In addition to common insecticides used to control pests indoors, other potential indoor sources of fipronil, imidacloprid, pyriproxifen and permethrin may be associated with their use as topical flea control agents for dogs and cats. About 53% of the participating homes had at least one indoor cat or dog. Fipronil products have been shown to persist on pets for over 28 days⁵⁰ and this is likely true for other active ingredients based on the relatively low frequency of application required for these products. These active ingredients will accumulate in dust as pets shed treated fur and skin cells. The less frequent detection of some of the insecticides in this study, coupled with their relatively high coefficients of variation (see Table S2), likely reflects the fact that pet ownership and indoor insecticide applications are not as ubiquitous as other indoor product uses. Compared to toxicity testing data (n = 16), biomonitoring data are limited (n = 9). For fipronil-sulfone, fipronil, fipronil-desulfinyl, and fipronil-sulfide that were detected in around or greater than 50% of the samples, both toxicity testing and biomonitoring are recommended.

3.3.2. Fungicides—A total of 15 fungicides were detected, 11 of them via suspect screening or non-target methods. Seven fungicides were newly detected in our dust. Eight fungicides mostly detected via suspect screening or non-target methods had a detection frequency above 50%, indicating widespread use of fungicides in the indoor environment. Except for didecyldimethylammonium chloride (DDAC; median concentration = 2,859 ng/g of dust), measured median concentrations of fungicides were low compared to insecticides. In addition to a fungicidal use, DDAC is used as an antibacterial agent and has wide indoor applications where it is used on walls, floors, tables, toilets and fixtures.⁵¹ Of the 15 detected fungicides, 13 fungicides were previously tested for either endocrine-disrupting potential or neurotoxic potential. Except for pentachlorophenol, none of the 14 detected fungicides has been biomonitored in NHANES. Among the compounds that were newly detected and have both endocrine-disrupting and neurotoxic potential, two fungicides (DDAC, fludioxonil) were commonly detected (>70%) in our samples; two other fungicides (azoxystrobin, difenoconazole) were detected infrequently (29% and 5%, respectively). Thus, fungicides with a high detection frequency are recommended to be included in future biomonitoring studies.

3.3.3. Herbicides—Five herbicides were detected in our dust via a target method. A detection frequency was below 50% for 4 out of 5 herbicides. Given the detection frequency, they might be attributable to applications in agricultural fields or gardens. Except for 2,4-dichlorophenoxyacetic acid, none of them was biomonitored in NHANES. Propanil and pendimethalin showed both endocrine-disrupting potential and neurotoxic potential, and diuron showed endocrine-disrupting potential from the *in vitro* testing. Thus, they might need to be included in future biomonitoring studies.

3.4. Compounds in personal care products

We detected parabens, fragrance ingredients, UV filters, cosmetic ingredients, and those with other personal care uses in our dust (Table 3). Overall, they were widely detected, and median concentrations were on the order of 1,000 to 10,000 ng/g of dust for 11 compounds. For users of products containing these compounds, direct dermal uptake is likely to be a primary exposure route. However, for non-users, such as young children who spend most of their time on the floors and have high dust ingestion rates, dust may be an important exposure medium for these compounds.⁵² Eight compounds in PCPs were newly detected in our dust and four compounds are cosmetic ingredients. Among newly detected compounds, toxicity testing and biomonitoring are recommended for dexpanthenol because it was detected in all samples with a median of 1,311 ng/g of dust. There are only 8 compounds that have been biomonitored in NHANES and that were tested for endocrine-disrupting and/or neurotoxic potential. However, we observed that there are many PCP compounds that may require biomonitoring and toxicity testing based on the detection frequency and high median concentrations.

3.5. Chemical classes whose dust concentrations are of less concern for environmental exposure calculations

In our samples, we detected 10 food additives, 5 sweeteners,11 food sources, 29 pharmaceuticals, 3 skin oils, 14 human metabolites, 31 surfactants, and 17 compounds whose use is not known (Table S2). Most of them were detected via suspect screening or non-target methods. These compound classes were not of interest in identifying or measuring dust concentrations in previous indoor environmental monitoring studies. Thus, their presence was rarely reported in the literature and 87 out of 119 newly detected compounds fell in this category. Among the compounds classified in this category, only 18 compounds were tested for endocrine-disrupting and/or neurotoxic potential. We found that sorbic acid (food additive), ketoconazole (pharmaceutical), nicotine (pharmaceutical), linoleic acid (food sources), linolenic acid (food sources), and genistein (food sources) have endocrine-disrupting and/or neurotoxic potential. Exposure to genistein occurs primarily through foods made with soybeans and soy protein.⁵³ Biomonitoring is recommended for linoleic acid because it was detected in all samples at a high median concentration (34,308 ng/g of dust) and has endocrine-disrupting potential.

4. Discussion

Results from this study provided more comprehensive chemical profiles of house dust. We detected a total of 276 compounds in our dust samples and quantified concentrations of 144 compounds using standards. In addition to the compounds that were previously measured in indoor dust, we tried to identify overlooked compounds that were not previously measured in dust but were shown to have potential for adverse health effects from the HTS toxicity testing. We were also able to expand the list of compounds present in indoor dust by applying both LC-MS and GC-MS with three analytical approaches. For example, 75% of the newly measured chemicals were observed via LC non-target or LC suspect approaches (see Figure S1). The newly measured compounds in our study mainly comprised surfactants, pharmaceuticals, and human metabolites. Because of the polarity of these compounds, we

were able to detect a large number of compounds via LC-MS. Another reason we could extend the list of compounds present in indoor dust is that our samples were recently collected (2015–2016). Compared to Rager et al.²² who investigated non-targeted compounds using LC-MS in U.S household dust samples collected from 2005 to 2006, we were able to newly detect four replacement plasticizers (e.g., acetyl tributyl citrate, DOTP) in our samples, reflecting currently used products.

Our study showed that indoor dust contains chemicals from various consumer product uses and also supported the idea that dust can serve as a marker of use. For example, most of the food additives and sweeteners detected in our dust are used in processed foods or drinks. Thus, the presence of food additives or sweeteners in dust indicates that they exist outside their intended use, which is to be consumed via direct food intake. Cholesterol (found in skin and emitted during cooking) and skin oils were ubiquitously measured in Danish homes and daycare centers.⁴⁴ In addition to these compounds, we observed cosmetic ingredients and vitamin E with median concentrations greater than 10,000 ng/g. In a separate study in which we analyzed skin wipe samples,⁵⁴ 11 compounds (triethyl citrate, butylated hydroxytoluene, cholesta-3,5-diene, vitamin E, cholesterol, tridecanoic acid, arachidonic acid, palmidrol, palmitic acid, pentadecanoic acid, linolenic acid) were detected, and they were also detected in our dust samples. This indicates that human activities, including cooking, cosmetic use, skin sloughing, dropping food residue or debris unintentionally on floors, could be sources of these compounds. Moreover, because we analyzed recently collected dust samples, we observed that relatively new chemicals (e.g., OP-FRs, BPS) were measured at higher concentrations than those for controversial or banned chemicals in consumer products (e.g., PBDEs, BPA). This reflects the dynamic nature of consumer product formulations, especially given heightened consumer awareness and concerns about the safety of product ingredients.

Compiling existing exposure and toxicity potential data of our detected compounds allowed us to inform key data gaps for assessing potential health effects for previously overlooked chemicals. For example, we found that *in vitro* HTS toxicity data were not available for some of the detected plasticizers, bisphenols, and biocides, which may adversely affect human health. Of most interest are one plasticizer (toluene-2-sulfonamide), two bisphenols (BADGE.2H2O, BADGE-HCl-H2O), and eight biocides and biocide transformation products (fipronil-desulfinyl, fipronil-sulfide, fipronil-sulfone, chlorantraniprole, cypermethrin, cyfluthrin, 4-hydroxychlorothalonil, physcion). Because most of these compounds were ubiquitous in our samples and may have toxicity potential, they are recommended to be included in future *in vitro* toxicity screening.

In conclusion, following the identification of a broad spectrum of chemicals from a previous study,¹⁸ this study integrated their measured dust concentrations with existing exposure and toxicity information to inform key data gaps for assessing potential health effects for consumer product chemicals. We found that 13 newly detected compounds may potentially disrupt endocrine systems and/or be neurotoxic based on *in vitro* bioactivity assays. These results expand our knowledge of chemicals present in indoor residential environments where vulnerable populations, especially young children, spend most of their time on the floors.⁵⁶ Consequently, we expect that our findings may trigger further environmental health research

regarding previously overlooked compounds. Many of the pharmaceuticals and PCPs newly detected in our dust have been extensively studied in various aquatic environments, including drinking water, wastewater, surface water, and groundwater⁵⁵ because they may pose a threat to the ecosystem and/or human health. Given that people spend most of their time indoors,⁵⁶ more studies are needed to examine the presence of these compounds in residential dust and to investigate potential health effects associated with indoor non-dietary exposure routes. Additional studies are also recommended to confirm the presence of compounds that were less frequently detected in the current study and not yet confirmed by standards.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

Acknowledgments

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Practical Implications:

Our dust samples contain chemicals from various consumer product uses, including cleaning and personal care products, furniture, plastics, and pesticides. This supports the idea that dust can serve as a marker of use. We expect that this comprehensive investigation of chemicals present in dust will form the basis for future work to develop new hypotheses of adverse health effects due to exposures to previously overlooked compounds.

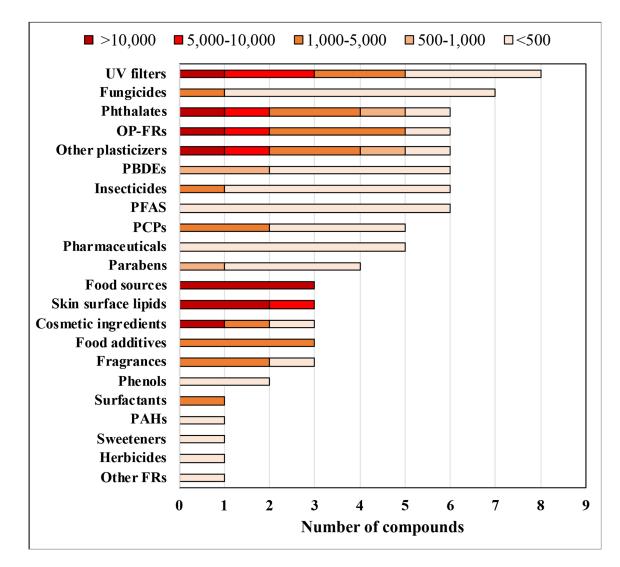


Figure 1.

Summary of median concentrations (ng/g of dust) for 87 compounds (target + suspect + non-target) detected in more than 50% of samples.

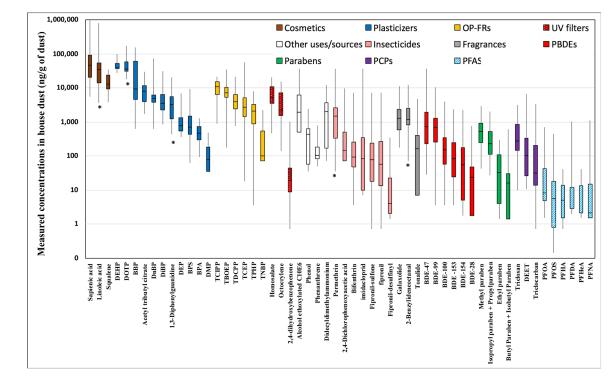


Figure 2.

Distributions of dust concentrations (ng/g of dust) for 56 target compounds detected in more than 50% of samples.

Two skin oils (Sapienic acid, squalene) and linoleic acid (used in cosmetics and emitted during cooking) were grouped into 'cosmetics' in this figure. Compounds with asterisk (*) indicate the first measurement in household dust. This figure excludes two phenols (tetrachlorophenols, cresol) that were detected in most samples (above LOD) but that were below LOQ. See Table 1 for identification of abbreviations.

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Table 1.

Summary of chemical classes that were detected in our dust samples (n = 38) and have been receiving considerable public attention

Chemical		Abbreviation	Instrument ^I	Method ²		Standard ³	# detections	New detection ⁴	Median conc. (ng/g of	95 th percentile (ng/g of	Endocrine ⁵	Neurotoxic ⁶	NHANES ⁷
class	Compound Name		c	E	_		ç		dust)	dust)	-	-	-
	Benzyl butyl phthalate	BBP	פ	-	Ŋ	-	38		9181	134/64	I	I	_
	Bis(2-ethylhexyl) phthalate	DEHP	G	Т	50	1	38		39124	77532	0	0	1
Phthalates	Di-isobutyl phthalate	DiBP	G	Т	100	1	38		3465	25917	0	1	1
or Ai	Di-n-butyl phthalate	DnBP	G	Т	100	1	38		4974	15983	1	1	1
<i>r</i> . Au	Diethyl phthalate	DEP	G	Т	500	1	30		996	4184	0	0	1
ithor	Dimethyl phthalate	DMP	IJ	Т	50	1	27		103	388	0	0	1
manus	Bis(2-ethylhexyl) adipate	DEHA	G	F	5000	1	15			17522	0	0	
cript:	Acetyl tributyl citrate	ATBC	G	Т	50	1	38		7969	27543	0	0	
J.Her Other	Dioctyl terephthalate	DOTP	G	Т	50	1	38	1	35678	115606	0	0	
pla	1,3-Diphenylguanidine		Г	Т	30	1	38	1	3218	9659	1	1	
in PN	Toluene-2-sulfonamide		Г	s^{8}	<100	1	38	1	1922	6313			
AC 202	Diethylene glycol dibenzoate		G	6 ^N			34	1			0	0	
1 Jar	Bisphenol A	BPA	L	Т	50	1	38		461	1043	1	1	1
nuarv	Bisphenol S	BPS	Г	Т	55	1	38		691	5225	1		1
	Bisphenol A bis (2,3- dihydroxypropyl) ether	BADGE. 2H2O	L	Т	1000	1	16			11237			
propuentos	Bisphenol A (3- chloro-2- hydroxypropyl) (2,3- dihydroxypropyl) ether	BADGE- HCI-H2O	L	Т	125	1	L			2205			
	Bisphenol AF	BPAF	L	S	1	1	3				1	1	
	2,4,4'- Tribromodiphenyl ether	BDE-28	G	Т	2.5	1	26		38	363			1
PBDEs	2,2',4,4' - Tetrabromodiphenyl ether	BDE-47	ũ	Т	1.0	1	38		720	6878			1

Chemical class	Compound Name	Abbreviation	Instrument ^I	Method ²	LOD (ng/g of dust)	Standard ³	# detections	New detection ⁴	Median conc. (ng/g of dust)	95 th percentile (ng/g of dust)	Endocrine ⁵	Neurotoxic ⁶	NHANES ⁷
	2,2',4',5- Pentabromodiphenyl ether	BDE-99	Ð	Ц	5.0	-	36		721	5090			1
	2,2',4,4',5,5'- Hexabromodiphenyl ether	BDE -153	ŋ	Т	5.0	1	31		111	1033			1
Indoo	2,2',4,4',5,6'- Hexabromodiphenyl ether	BDE-154	Ð	Т	2.5	1	31		88	872			1
or Air. Au	2,2',4,4',6- Pentabromodiphenyl ether	BDE-100	Ð	Т	5.0	1	35		165	1394			1
thor manu	2,2',3,4,4',5',6- Heptabromodiphenyl ether	BDE-183	Ð	Ц	50	1	7			215			1
Iscrit	Tri-n-butyl phosphate	TNBP	IJ	г	100	1	19		100	2024	0	1	1
ot; av	Triphenyl phosphate	TPHP	G	т	5.0	1	37		2105	7120	1	1	1
ailable	Tris(1-chloroisopropyl) phosphate	TCIPP	Ð	Т	50	1	38		10666	20407	0		1
in PM0	Tris(4-butyl-phenyl) phosphate	TBPP	Ð	Т	25	1	14			217			
	Tris(2-butoxyethyl) phosphate	TBOEP	Ð	Т	250	1	37		7445	14159	0		
SH-dO January	Tris(1,3-dichloro-2- propyl) phosphate	TDCPP	Ð	Т	50	1	38		3955	15338	1	1	1
/ 01.	Tris(2-chloroethyl) phosphate	TCEP	G	Т	25	1	37		2810	20946	0	0	1
	Triethyl phosphate	TEP	Г	s^{g}	<100	1	8			154	0		
	Tricresyl phosphate	TCP	Г	S	25	1	8			8529	1		1
	Octyl diphenyl phosphate		L	S			3	1					
Other FRs	Bis(2- ethylhexyl)-2,3,4,5- tetrabromophthalate	BEH-TEBP	Ð	Т	1000	1	3			13761	0		
	2,4-Dibromophenol		Ð	Ч	20	1	2			50			

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Chemical class	Compound Name	Abbreviation	Instrument ^I	Method ²	LOD (ng/g of dust)	Standard ³	# detections	New detection ⁴	Median conc. (ng/g of dust)	95 th percentile (ng/g of dust)	Endocrine ⁵	Neurotoxic ⁶	NHANES ⁷
	1,2-bis(2,4,6- tribromophenoxy) ethane	BTBPE	U	Т	100	1	1						
	3,3',5,5'- Tetrabromobisphenol A	TBBPA	Г	s ⁸	<100	1	36		18	91	1	1	
	Melamine		L	s ⁸	<100	1	17			3162			
PFAS	N-ethyl perfluorooctane sulfonamide ethanol	MeFOSE	Г	Т	8.0	1	9			90			1
	Perfluorobutane sulfonate	PFBS	Г	Т	2.0	1	6			23			-
	Perfluorohexane sulfonate	PFHxS	г	Н	1.0	1	16			21			-
	Perfluorooctane sulfonate	PFOS	Г	Ŧ	0.2	1	36		6	221	1	1	
	Perfluorodecanoic acid	PFDA	Г	Т	4.0	1	21		11	76	1	0	1
	Perfluoroheptanoic acid	PFHpA	Г	Т	3.0	1	23		6	39	0	0	-
	Perfluorohexanoic acid	PFHxA	Г	Т	1.0	1	35		9	30	0	0	1
	Perfluorononanoic acid	PFNA	L	Т	3.0	1	29		8	217	1	0	1
	Perfluorooctanoic acid	PFOA	Г	Т	3.0	1	34		10	138	0	0	1
	Perfluoropentanoic acid	PFPeA	г	Т	3.0	1	12			10			-
	Perfluoroundecanoic acid	PFUnDA	Г	8 ^S	<100	1	5			125	0	0	1
	6:2 polyfluoroalkyl phosphate diester	6:2diPAP	Г	$6^{\rm N}$		1	38						
	6:2diPAP/8:2diPAP		L	^в и		1	38						
	Fluorotelomer sulfonic acid	FTSA 6:2	Г	6^{N}		1	38						
	1h-Perfluoroheptane		Г	Ν			37	1					
Phenols	2-Chlorophenol		G	Т	50	1	1	1			1	0	
	2,6-Dichlorophenol		G	Т	100	1	1	1					

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Chemical class	Compound Name	Abbreviation	Instrument ¹	Method ²	LOD of dust)	Standard ³	# detections	New detection ⁴	Median conc. (ng/g of dust)	95 th percentile (ng/g of dust)	Endocrine ⁵	Neurotoxic ⁶	NHANES ⁷
	3,4,5-Trichlorophenol		G	Т	500	1	1	1					
	Trichlorophenols (2,3,4-; 2,3,5-; 2,3,6-; 2,4,5-; 2,4,6-) ¹⁰		G	Т	100	1	1	1					
	Phenol		G	Т	50	1	28		580	1669	1	0	
	Tetrachlorophenol		G	Т	250	1	19	1		250			
ndoor	Cresol (o-,m-,p) ^{10, 11}		G	Т	100	1	34	1	250	250			
Air. A	2,4-Dinitrophenol		Г	δ^{δ}	50000	1	L				0	1	
SHFA utho	Anthracene		G	Т	5.0	1	9			24			
r ma	Benzo(a)anthracene		G	Т	5.0	1	10			89	1	1	1
nusci	Benzo(g,h,i)perylene		G	Т	50	1	17			289			
ript;	Chrysene		G	Т	5.0	1	18			130			1
avail	Phenanthrene		G	Т	10	1	38		106	367	1	0	1
able in 1	Dibenzo(a,h)anthracene + Indeno(1,2,3- $\frac{1}{2}$												
PM	$cd)pyrene^{1\mathcal{L}}$		G	T	50	1	5			260	0		
C 20	Fluorene		Ð	L	10	1	1				0	0	1
21 Ja	12 1. Dime of analytical instruments used to detect connormals (G – ass chromatoreacht) 1 – licuid chromatoreacht)	etect compounds (G - and chromate	- 1 when	oudo binoi	(indeconder)							

Type of analytical instruments used to detect compounds (G = gas chromatography, L = liquid chromatography). $\int_{-1}^{10} Type$ of analytical methods used to detect compounds (T = target analysis, S = suspect screening, N = non-target analysis).

 \mathcal{J}_{C} Compounds confirmed by standards (1 = Yes, blank = No).

4)Compounds newly detected in our dust (1 = Yes, blank = No).

 S_{j} Compounds having endocrine-disrupting potential from *in vitro* high-throughput screening assays (1 = active, 0 = inactive, blank = not tested or data not available).

 \hat{O} Compounds having neurotoxic potential from *in vitro* high-throughput screening assays (1 = active, 0 = inactive, blank = not tested or data not available).

 γ Compounds biomonitored in NHANES (1 = Yes, blank = No).

 $g_{\rm D}$ betected by suspect screening or non-target methods first and quantified with standards later, thus concentrations are semi-quantitative.

 $g_{
m D}$ betected by suspect screening or non-target approach and quantified with standards later, but concentrations were not quantified.

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10) Detected with multiple isomers.

 II Detected in most samples (above LOD) but were below the limit of quantification (LOQ).

 12 Structures of these compounds were too close to discriminate one from the other.

<u>Abbreviations</u>: LOD, limit of detection; NHANES, National Health and Nutrition Examination Survey; PBDEs, polybrominated diphenyl ethers; OP-FRs, organophosphate flame retardants; PAHs, polycyclic aromatic hydrocarbons; PFAS, per- and polyfluoroalkyl substances

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Table 2.

Summary of biocides that were detected in our dust samples (n = 38)

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			Ī	Ì								
Chemical class	Compound Name	Instrument ¹	Method ²	LOD (ng/g of dust)	Standard ³	# detections	New detection ⁴	Median conc. (ng/g of dust)	95 th percentile (ng/g of dust)	Endocrine ⁵	Neurotoxic ⁶	NHANES ⁷
	Fipronil-sulfone	Г	Т	1.0	1	37		77	3004			
	Fipronil	Т	Т	1.0	1	37		62	5718	1	1	
	Permethrin	Ð	Т	50	1	34		1922	8151	1	0	1
	Imidacloprid	Г	Т	10	1	32		123	22455	0	0	1
	Bifenthrin	G	Т	5.0	1	31		140	3336	1	0	
	Fipronil-desulfinyl	Г	Т	2.0	-	28		11	248			
	Fipronil-sulfide	Г	Т	1.0	-	17			136			
	Novaluron	Г	Т	1.0	-	6	1		1826	1	0	
	Chlorpyrifos	IJ	Т	5.0	-	×			365	1	0	1
	Methoxyfenozide	Г	Т	2.0	1	7	1		204	1	0	
:	Propoxur	Г	Т	6.0	-	9			60	0	0	1
Insecticides	Chlorantraniprole	Г	Т	3.0	-	4	1		69			
	Pyriproxyfen	Т	Т	4.0	1	4			191	0	1	
	Deltamethrin	G	Т	500	1	4			6658	0		1
	Etofenprox	Ð	Т	10	1	4			38059	1	0	
	Cyhalothrin	Ð	Т	50	1	2			7449	0		1
	Cypermethrin	Ð	Т	500	1	2			24222			1
	1,3-benzothiazole	Т	Т	600	1	2	1		2714	0		
	Esfenvalerate	Ð	Т	250	1	1				0	1	
	Tetrachlorvinphos	Г	\mathbf{S}^{8}	<100	1	6			43222	1		1
	Cyfluthrin	Ð	N ⁹		1	1						1
	Piperonyl butoxide	Ð	Z			26				1	0	
	Boscalid	Г	Т	3.0	1	10			262	0	1	
Fungicides	Azoxystrobin	Г	Т	5.0	1	11	1		77	1	1	
	Difenoconazole	Г	Т	9.0	1	2	1		18	1	1	

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Chemical class	Compound Name	Instrument ¹	Method ²	LOD of dust)	Standard ³	# detections	New detection ⁴	Median conc. (ng/g of dust)	95 th percentile (ng/g of dust)	Endocrine ⁵	Neurotoxic ⁶	NHANES ⁷
	Didecyldimethylammonium chloride	L	Т	100	1	28	1	2859	10579	1	1	
	Pentachlorophenol	G	Т	1000	1	9			11511	1	0	1
	Carbendazim	L	S^8	<100	1	11			2568	1	0	
	Imazalil	L	S^8	<100	1	29		18	210	1	1	
	Octhilinone	L	S^8	<100	1	22		5	44	1	1	
	Propiconazole	Г	S^8	<100	1	31		34	194	1	1	
	Thiabendazole	Г	S^8	<100	1	22		54	713	0	0	
	Fludioxonil	Г	S^8	<100	1	22	1	12	61	1	1	
	Physcion	L	S^8	<100	1	38		177	866			
	4-hydroxychlorothalonil	L	N^9		1	38	1					
	Pyraclostrobin	L	S^9		1	L				0	1	
	Dichlorophen	L	S	250	1	1	1			1		
	3-Iodo-2-propynyl-N- butyLarbamate	L	S	50	1	16	1		385	1	1	
	2,4-Dichlorophenoxyacetic acid	L	Т	100	1	20		200	5057	0	0	1
	Propanil	L	Т	2.0	1	13			512	1	1	
Herbicides	Diuron	L	Т	15	1	11			1116	1	0	
	Pendimethalin	L	Т	150	1	5			591	1	1	
	Simazine	L	Т	3.0	1	1				0	0	

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Table 3.

Summary of compound classes that were detected in our dust samples (n = 38) and mainly used in dermal applications

	NHANES ⁷	1	1	1												1	1	1	-1				
	Neurotoxic ⁶	1	0	1	-	0									0		1	1	0				
	Endocrine ⁵	1	0	1		0		0	0		1				0	0	1	-	-1		0		
-	95 th percentile (ng/g of dust)	241	1559	235	1457	3950	5521	818	17398	13656	148	230	8037	26531	1326	64114	1144	1391	5536	13243	10628		
	Median conc. (ng/g of dust)	48	524	23	226	1194	1294	219	5233	2245	22	37	1450	7057	441	19170	33	275	154	1311	1280		
•	New detection ⁴					1														1	1	1	
	# detections	35	37	26	38	37	38	27	38	38	35	30	37	38	35	38	37	38	30	38	38	38	
, T	Standard ³	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1		
	LOD of dust)	2.0	60	2.0	2.0	100	5.0	10	25	25	1.0	<100	<100	n.d.	n.d.	n.d.	1.0	5.0	15	<100	n.d.		
	Method ²	Т	Т	Τ	F	Т	Т	Т	Т	Т	Т	S^8	S^8	^{8}N	^{8}N	^{8}N	Т	Т	Ŧ	S^8	^{8}N	z	;
	Instrument ¹	Г	Г	Т	Г	G	G	G	G	G	L	Т	Г	Ð	Ð	Ð	Т	L	Г	Т	Ð	L	
	Compound Name	Ethyl paraben	Methyl paraben	Butyl Paraben + Isobutyl Paraben ⁹	Isopropyl paraben + Propyl Paraben ⁹	2-Benzylideneoctanal	Galaxolide	Tonalide	Homosalate	Octocrylene	2,4- dihydroxybenzophenone	Benzophenone-4	Octyl methoxycinnamate	2-Ethylhexyl salicylate	Benzophenone	Benzophenone-3	Triclocarban	Triclosan	N,N-Diethyl-meta- toluamide (DEET)	Dexpanthenol	Benzyl Benzoate	Salnacedin	
	Chemical class			Parabens			Frag-rance					UV filters							Orher	personal		•	<u></u>

Chemical class	Compound Name	Instrument ¹	Method ²	LOD (ng/g of dust)	Standard ³	# detections	New detection ⁴	Median conc. (ng/g of dust)	95 th percentile (ng/g of dust)	Endocrine ⁵	Endocrine ⁵ Neurotoxic ⁶ NHANES ⁷	NHANES ⁷
	Ethyl N-acetyl-N-butyl-β- alaninate	L	S			4						
	Tricaprylin	G	N^8	n.d.	1	33		27882	75596			
	Isopropyl myristate	G	\mathbf{N}^{8}	n.d.	1	38	1	1836	8485	0		
	Lilial	G	N^8	n.d.	1	38	1	319	3557	0		
Cosmetics	Cholesteryl benzoate	G	N			38	1					
	Isopropyl palmitate	G	N			38						
	12-Hydroxystearic acid	L	N			38	1					
	Benzyl salicylate	Ð	N			38				0		
For 1 through 5	For 1 through 8 refer to footnote of Table 1	,										

For 1 through 8, refer to footnote of Table 1.

 $\boldsymbol{g}_{\rm Structures}$ of these compounds were too close to discriminate one from the other.

Abbreviations: n.d., not determined;

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