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Article

High-Resolution Mass Spectrometry Screening of Quaternary Ammonium Compounds (QACs) in Dust from Homes and Various Microenvironments in South China

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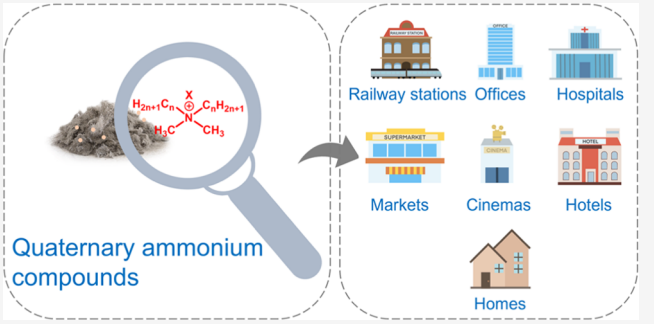
ABSTRACT: Despite their ubiquitous use, information regarding the presence of quaternary ammonium compounds (QACs) in various microenvironments remains scarce and only a small subset of QACs has been monitored using targeted chemical analysis. In this study, a total of 111 dust samples were collected from homes and various public settings in South China during the COVID-19 pandemic and were analyzed for traditional and emerging QACs using high-resolution mass spectrometry. The total traditional QAC concentrations in residential dust ($\sum_{traditional}$ QAC, sum of 18 traditional QACs) ranged from 13.8 to 150 μg/g with a median concentration of 42.2 μg/g. Twenty-eight emerging QACs were identified in these samples, and the composition of $\sum_{emerging}$ QAC (sum of emerging QACs) to $\sum$QAC (sum of traditional and emerging QACs) ranged from 19 to 42% across various microenvironments, indicating the widespread existence of emerging QACs in indoor environments. Additionally, dust samples from cinemas exhibited higher $\sum$QAC concentrations compared to homes (medians 65.9 μg/g vs 58.3 μg/g, respectively), indicating heavier emission sources of QACs in these places. Interestingly, significantly higher $\sum$QAC concentrations were observed in dust from the rooms with carpets than those without (medians 65.6 μg/g vs 32.6 μg/g, $p < 0.05$, respectively). Overall, this study sheds light on the ubiquitous occurrence of QACs in indoor environments in South China.



KEYWORDS: *quaternary ammonium compounds (QACs), emerging contaminants, indoor environments, dust, textiles, high-resolution mass spectrometry*

INTRODUCTION

Quaternary ammonium compounds (QACs) make up a group of cationic substances with at least one long hydrophobic hydrocarbon chain connected to a positively charged nitrogen atom. QACs are widely used as active constituents in antimicrobials, surfactants, preservatives, antistatics, fabric softeners, and dispersants.[1−3] Given their effectiveness in deactivating the SARS-CoV-2 coronavirus and their use as favorable substitutes for triclosan and triclocarban, QAC disinfectants saw heavy utilization during the COVID-19 pandemic. The extensive use of QACs has led to their ubiquitous presence in wastewater sludge, surface waters, sediments, and soils,[4−10] and elevated QAC levels in these environments were also observed during the pandemic.[11−13] Moreover, recent biomonitoring studies indicate that QACs can bioaccumulate in human tissues (e.g., blood and breast milk),[14,15] and consequently, potential health effects may occur in the human body, including immune, developmental, and reproductive toxicity as well as disruptions to metabolic functions (e.g., lipid homeostasis).[16−19] Thus, there is growing concern about human exposure to QACs, given their recognition as a class of emerging contaminants.[20]

Indoor dust is commonly recognized as an important route for human exposure to various semivolatile contaminants.[21] Due to their low volatility, QACs are easily adsorbed to solid airborne particles and dust, subsequently accumulating in indoor environments.[22] Recent studies found that QACs were frequently detected in residential dust collected from North America and Europe with median concentrations of 36.3−58.9 and 14.73 μg/g, respectively.[22,23] Apart from North America and Europe, China's mainland, with its vast population, was greatly impacted by the pandemic. Although information regarding production volumes and the occurrence of QACs in dust from

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China is unavailable, more than 200 brands and 300 disinfecting products labeled with QACs are currently on sale in the Chinese consumer market based on the search results of QAC disinfecting products on JD.com. Additionally, QAC levels in sediment collected from China in 2013 were comparable to or higher than those from North America and Europe,[24] providing indirect evidence that indoor contamination of QACs is prevalent in China as well. Thus, it is crucial to determine the QAC dust concentrations in residential homes collected from China, extending the scope beyond North America and Europe.

Disinfecting practices are suggested to greatly influence QAC levels in residential dust.[22] Aside from households, intense disinfection procedures are recommended for care facilities, schools, and other high-risk areas during the pandemic,[20,25] a number of which serve populations most vulnerable to these exposures. Furthermore, distinct patterns of environmental contaminants could occur in homes and public spaces and suggest the presence of specific indoor sources of these contaminants, such as per- and polyfluoroalkyl substances (PFAS) and organophosphate flame retardants (OPFRs).[26,27] However, limited information is available on the occurrence of QACs in different microenvironments.

The category of QACs covers a vast spectrum of chemicals, but only a minor fraction of QACs has been monitored via targeted chemical analysis.[20] The most extensively studied QAC groups include benzylalkyldimethylammonium compounds (BACs, with C8−C18 alkylated chains), dialkyldimethylammonium compounds (DADMACs, with C8−C18 alkylated chains), and alkyltrimethylammonium compounds (ATMACs, with C8−C18 alkylated chains),[14,15,22] whereas a broad range of QACs has been documented in other literature and consumer products.[23,28,29] For example, QACs used in cleaning and disinfecting products tend to have shorter alkyl chain lengths (C8−C16) than those used in personal care products, which can have alkyl chains as long as 22 carbons.[20] In addition, C20- and C22-ATMACs are mainly used as active ingredients in antistatic/softening agents in hair conditioners and hair care products, stabilizers, and preservatives in air fresheners.[20] Regarding other emerging QAC analogues, mixed C14:16-, C14:18-, C16:18-, and C18:20-DADMACs were found in municipal sewage sludge, and these compounds constituted up to 40% of total DADMAC concentrations.[30] However, there is still a dearth of research on the identification, distribution, and fate of other emerging QAC analogues in indoor environments.

The target and suspect screening strategy based on a high-resolution mass spectrometer (HRMS) has been utilized to identify unknown chemicals successfully.[23,31−33] Here, we aim to identify emerging QACs, specifically those outside the range of 18 well-known QACs (consisting of C8−C18-BACs, C8−C18-DADMACs, and C8−C18-ATMACs) using HRMS, and further (semi)quantitate traditional and emerging QACs in indoor dust collected from homes and different public settings, including railway stations, hotels, hospitals, markets, cinemas, and offices. The objectives of this study are (1) to identify emerging QACs in indoor dust and quantify their contribution to the total QAC concentration; (2) to compare the dust concentrations of QACs measured in the current study and those reported in previous studies; and (3) to investigate the distributions of traditional and emerging QACs in indoor dust across various microenvironments.

MATERIALS AND METHODS

Chemicals and Reagents. The detailed information, including full names, abbreviations, formulas, CAS numbers, vendors, and purities of native standards, is listed in Table S1. Three mass-labeled internal standards, including benzyldimethyldodecylammonium-d_7 chloride (d_7-C12-BAC), denzyldimethyltetradecylammonium-d_7 chloride (d_7-C14-BAC), and decyltrimethylammonium-d_9 bromide (d_9-C10-ATMAC), were purchased from Toronto Research Chemicals (Toronto, ON, Canada). All solvents applied in the present study were of HPLC grade or higher.

Sample Collection and Pretreatment. A total of 111 dust samples were collected in homes (n = 17), railway stations (n = 12), hotels (n = 18), hospitals (n = 18), markets (n = 20), cinemas (n = 12), and offices (n = 14) in Shenzhen City, China, during July−September 2022. The chosen public places are based on previous investigations, which revealed that typical public places implemented more rigorous disinfecting practices to prevent the spread of the pandemic.[34,35] It is noteworthy that the COVID-19 pandemic-related restrictions and extensive disinfection activities are still ongoing in this area. Shenzhen City (22°55′N, 114°09′E) has an annual average temperature of 22.4 °C. In addition to the sample locations, a summary of housing characteristics, including information on site volumes, ventilation, sampling areas, and floor types, for public places and homes is given in Table S2. The samples were obtained using a precleaned nylon sock (with a pore size of 25 μm) connected to a commercial vacuum cleaner (Dyson, V8 Fluffy Extra).[36−40] To minimize background contamination, nylon socks were sequentially extracted with ultrapure water and methanol in ultrasonics twice and then air-dried before use. All collected samples were wrapped with aluminum foil, sealed in a polypropylene (PP) bag, transported to the laboratory, and stored at −20 °C for further chemical analysis. Information about flooring types was collected at the time of sampling.

The pretreatment method used in this research was based on the protocols established in our prior study.[22] Briefly, approximately 100 mg of dust sieved through a 500 μm mesh size sieve was weighed in a 15 mL polypropylene tube, spiked with surrogate standards (d_7-C12-BAC and d_9-C10-ATMAC), and extracted with 4 mL of acetonitrile for 30 min using sonication under room temperature. The extraction procedure was repeated twice. The combined extracts were concentrated to ∼1 mL of acetonitrile and spiked with d_7-C14-BAC before instrumental analysis.

Instrumental Analysis. Chemical analysis was performed on an Agilent 1290 Infinity ultrahigh-performance liquid chromatograph system coupled to an Agilent 6546 quadrupole time-of-flight mass spectrometer (UPLC-QTOF-MS, Santa Clara, CA). Sample separation was conducted by a C18 column (ACQUITY UPLC BEH C18, 1.7 μm, 2.1 × 50 mm, Waters, Ireland), and the column temperature was kept at 30 °C. The mobile phase consisted of water (A) and acetonitrile (B), both containing 0.1% formic acid with a flow rate of 0.4 mL/min. The injection volume was 5 μL. The gradient was linearly programmed as follows: 0−0.5 min, 10% B; 0.5−6 min, 100% B; 6−10 min, 100% B; 10−10.5 min, 10% B; 10.5−14.5 min, 10% B. The mass spectrometer was equipped with an electrospray ionization (ESI) source operating in positive ion mode. The details of the MS parameters were as follows: nebulizer, 25 psi; gas flow, 10 L/min; sheath gas temperature, 300 °C; capillary voltage, 2800 V; and sheath gas flow, 11 L/min.

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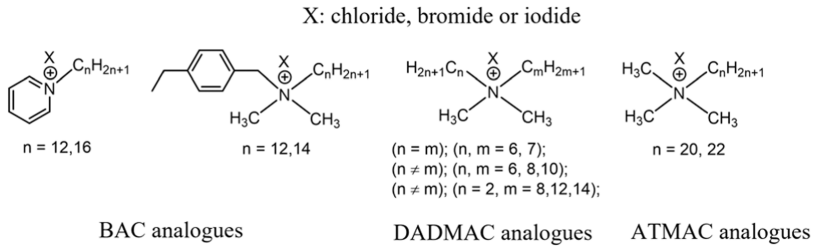

Figure 1. Chemical structures of representative emerging QACs, including BAC analogues, DADMAC analogues, and ATMAC analogues identified in the dust samples.

Prior to each batch analysis, the QTOF was calibrated with the reference standards of m/z 121.0508 and 922.0098, which were periodically used to adjust the mass accuracy.

Full scan and iterative data-dependent acquisition (DDA) modes were selected with the parameters described below. For full scan mode, a full MS^1 scan was acquired with a scan rate of 2 spectra/s. Full MS^1 scan data was acquired in the range of 50−1000 m/z with a resolving power of 40,000 (at m/z 121.0508) and a mass accuracy of <5 ppm. For the iterative DDA mode, the acquisition rates of MS^1 and MS^2 were 6 and 5 spectra/s, respectively. A narrow isolation width (~1.3 m/z) was used. The active exclusion was enabled for exclusion after one spectrum and release after 0.3 min. The mass error tolerance of iterative MS^2 was 10 ppm, and the retention time exclusion tolerance was ±0.1 min. Two precursor ions were selected for CID fragmentation per scan cycle. Four iterative injections were performed and collected in the range of 30−1000 m/z with collision energies (CEs) at 10, 20, and 40 eV. The representative structures and chromatograms of QACs with authentic standards are presented in Figures 1 and S1, respectively.

Target and Suspect Screening of QACs. In this study, an integrated workflow of target and suspect screening of QACs was applied in the current research (Figure S2) based on previous studies with a minor modification.[32,41] The core framework of the Personal Compound Database and Library (PCDL) program based on a target and suspect screening strategy produced two chemical databases: (1) an in-house database with accurate mass and retention times (RTs) for routine monitoring 18 QACs and (2) a larger QAC homologue data was compiled from Web of Science and PubChem.[24,30,42] The suspect screening workflow is composed of four main steps: (i) the mixture dust sample (QC), individual dust sample, and procedural blank samples were injected in the same batch along with target screening, which was analyzed by HRMS in full MS^1 scan and MS^2 scans modes. (ii) After subtracting the background signals from procedural blanks, features were further extracted with Agilent Mass Hunter Qualitative Analysis software (version B.10.1) by applying the Find by Formula (FBF) workflow. Briefly, compounds that had their primary adducts identified by a chromatographic peak and that exhibited an acceptable match in the isotope score (including an exact mass deviation of monoisotopic m/z, abundance deviation, and exact mass difference of isotopes vs theoretical pattern) of >70 were selected. (iii) The relatively high response of the chromatographic peak was compared among individual dust samples. (iv) For further definitive confirmation of suspect chemicals, commercial standards were obtained to tentatively identify these chemicals based on fragmentation patterns and RTs of suspect QACs with high responses (peak area >10,000).

In terms of annotating QACs in the present study, we employed the annotation rules proposed by Schymanski et al.,[43] where level S1 annotations represent confirmed chemicals with commercial standards, level S2 annotations represent tentative identification with characteristic MS/MS fragment ions, and level S3 annotations have some diagnostic evidence based on existing literature or open sources.

(Semi-)Quantification of Traditional and Emerging QACs in Dust Samples. Both traditional and emerging QACs were quantified by LC-QTOF-MS operated in full scan mode. In detail, the quantification of target compounds was performed using $[M]^+$ quasi-molecular ion within a mass window of 10 ppm. Quantification of QACs with authentic standards was performed by isotope dilution using calibration curves with concentrations ranging from 1 to 200 ng/mL. The semi-quantification of emerging QACs without standards was carried out using the calibration curves of QACs with similar structures (Table S3). A semiquantification approach has been applied in the analysis of emerging contaminants, such as PFAS and OPEs.[33,44−47] Correlation coefficients in linearity tests were all >0.99, and samples with concentrations that surpassed the linearity ranges were diluted until they reached levels within the concentration ranges of the calibration curves.

Quality Control and Quality Assurance (QA/QC). One procedural blank was included in each batch of 15 samples, and two field blanks were collected by using precleaned nylon socks briefly opened during sampling. Procedure blanks (n = 6) and matrix spike recovery samples (n = 6) were analyzed across the pretreatment progress. The absolute recoveries ranged from 97 to 124, 71 to 116, and 98 to 126%, for BACs, DADMACs, and ATMACs, respectively, with the exceptions of C18-DADMAC (137%) and C8-ATMAC (149%). These unusually high recoveries were likely due to the unavailability of isotopically labeled standards of DADMACs and ATMACs, which could have impacted the accuracy of these measurements. The surrogate recoveries were 106 ± 2.3 and 118 ± 0.9% for d_7-C12-BAC and d_9-C10-ATMAC, respectively. All reported concentrations were subtracted from the average procedural blank concentrations but were not surrogate recovery corrected. If compounds were not observed in the procedural blanks, MDL was set as 3 times the signal-to-noise (S/N) based on the lowest calibration point. The details on matrix spike recoveries, field blanks, and procedural blanks are presented in Tables S3 and S4.

Data Analysis. The difference of the individual QAC and the concentration of total QACs among diverse microenvironments were examined using detection frequencies and median values. The individual contribution of each analyte to the total concentration was calculated based on the ratio of the median concentration of that analyte to the median of the total concentration. Because the QAC concentrations were not normally distributed, the data set was log-transformed to correct for skewed distributions. Consequently, the log-transformed data set was verified through the skewness−kurtosis normality

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test. Pearson correlation analysis was used to examine the correlations of the log-transformed concentration of QACs in dust samples. The analysis of variance (ANOVA) was performed to explore the difference in QAC concentrations. All descriptive statistics were computed by using Microsoft Excel. Plots were generated by using Origin and R Studio.

RESULTS AND DISCUSSION

Identification of Emerging QACs in Dust Samples. Overall, 18 traditional QACs, including C8−18 BACs, C8−18 DADMACs, and C8−18 ATMACs, were found in dust samples, and 28 emerging QACs were identified (Figures S3−S5). Among the newly identified QACs, 16 were confirmed with commercially available standards (level S1), 11 matched reference MS/MS fragment ions (level S2), and 1 was tentatively identified through characteristic MS/MS fragmentations (level S3). Of these emerging QACs identified, only 13 have been reported in the environments,[9,13,23,24,30,42,48,49] demonstrating the effectiveness of the QAC screening strategy applied in the present study. The newly identified QACs were divided into three groups based on their structural similarity to traditional QACs, including 9 BAC analogues, 10 DADMAC analogues, and 9 ATMAC analogues (Figures 1 and S3−S5). A comprehensive list of common subclasses of QACs and their associated usage is provided in Table S5. Of these, 7 are utilized as disinfectants, 3 are employed as antistatic agents and preservatives, and the remaining 18 are designated for various other applications.

BAC Analogues. Five BAC analogues, including benzethonium chloride (BEC), benzyltriethylammonium bromide (BTEAC), benzyltributylammonium chloride (BTBAC), benzyltrimethylammonium bromide (BTMAC), cetylpyridinium chloride (CPC), and domiphen bromide (DMPC), were identified with authentic standards (level S1). The rest of the BACs, including laurylpyridinium, C12ADEAC, and C14ADEAC, were identified as level S2.

On the basis of the molecular ion at m/z 248.2373, two consecutive peaks were observed in the extracted ion chromatograms (peaks 1−2, Figure S6). Peak 1 (RT 3.29 min) was identified as C8-BAC with an authentic standard. Peak 2 with m/z = 248.2376 ($C_{17}H_{30}N^+$, 1.29 ppm) generated a characteristic fragment ion of m/z = 80.0494 ($C_5H_6N^+$, −1.44 ppm), as identified by the presence of pyridinium in the structure. The presence of pyridinium also resulted from the characteristic fragment generated by an authentic standard of CPC (peak 4, Figure S7), indicating that peak 2 undergoes a similar fragmentation pathway to that of CPC. Therefore, peak 2 was tentatively identified as laurylpyridinium with the quasi-molecular ion of $C_{17}H_{30}N^+$ differing by a unit of C_4H_8 ($\Delta m/z$ = 56.0621) with that of CPC ($C_{21}H_{38}N^+$, 2.95 ppm). Peak 5 and Peak 7, two respective isomers of C14-BAC and C16-BAC, were found at retention times of 5.21 and 5.98 min, respectively (Figures S8 and S9). Peak 5 with m/z 332.3291 ($C_{23}H_{42}N^+$, −2.03 ppm) was tentatively identified as C12ADEAC based on the characteristic fragment ions m/z 212.2367 ($C_{14}H_{30}N^+$, −0.61 ppm) and m/z 119.0851 ($C_9H_{11}^+$, −0.46 ppm) that resulted from the presence of 4-ethyltoluene in the structure. Similarly, peak 7 was deduced to be C14ADEAC because of the same characteristic fragment ion m/z 119.0851 with that of C12ADEAC and a different unit of C_2H_4 ($\Delta m/z$ = 28.0313) in their precursor ion. To the best of our knowledge, this is the first report of BTEAC, BTBAC, BTMAC, laurylpyridinium, and ethylbenzylalkyldimethylammonium compounds (C12ADEAC and C14ADEAC) in indoor environments.

DADMAC Analogues. A total of 10 DADMAC analogues were identified based on their similar structures to DADMACs. Diallyldimethylammonium chloride (DDA), C2:12-DADMAC, and C8:10-DADMAC were confirmed with authentic standards as level S1. Six DADMACs, including C2:8-DADMAC, C6-DADMAC, C4:10-DADMAC, C6:8-DADMAC, C2:14-DADMAC, and C10:12-DADMAC, were identified as level S2, while C7-DADMAC was tentatively identified as level S3.

Peak 9 with a m/z of 186.2217 ($C_{12}H_{28}N^+$, 0.21 ppm) was eluted at 3.22 min (Figure S10). In the MS^2 spectrum, the fragment at m/z 74.0965 ($C_4H_{12}N^+$, 0.89 ppm) indicated the presence of ethyldimethylamine in the structure. Thus, peak 9 was identified as C2:8-DADMAC. Peak 10 (RT: 3.89 min) with m/z 214.2528 was generated with formula $C_{14}H_{32}N^+$ with a mass error of −0.75 ppm (Figure S11). The MS^2 fragment patterns (m/z 71.0853 [$C_5H_{11}^+$, −2.98 ppm] and m/z 57.0696 [$C_4H_9^+$, −4.99 ppm]) were also observed in those of C8−C18 DADMACs, and thus, peak 10 was identified as C6-DADMAC based on the increment of retention times with longer alkyl chains of DADMAC homologues (C8-DADMAC: 4.41 min). Peak 13 was identified as C2:12-DADMAC using its commercial standard (Figure S12). Unexpectedly, three isomers (peaks 11, 12, and 14) were observed along with C2:12-DADMAC in extracted ion chromatograms (EICs) of m/z 242.2842 and different MS^2 fragment patterns were found for the three peaks (Figure S12). Peak 11 (RT: 3.3 min) with a m/z of 242.2841 ($C_{16}H_{36}N^+$, −0.13 ppm) was confirmed as C4:10-DADMAC on the basis of the characteristic fragment ions at *a* m/z 186.2215 ($C_{12}H_{28}N^+$, −0.1 ppm) and a m/z of 142.1593 ($C_9H_{20}N^+$, 0.27 ppm). Similarly, peak 12 (RT: 3.66 min) with m/z 242.2835 ($C_{16}H_{36}N^+$, −0.69 ppm) was diagnosed using m/z 158.1908 ($C_{10}H_{24}N^+$, 0.48 ppm) and m/z 130.1595 ($C_8H_{20}N^+$, 0.51 ppm) and identified as C6:8-DADMAC. Peak 14 (RT: 4.34 min) with m/z 242.2805 ($C_{16}H_{36}N^+$, −3.68 ppm) resulted in fragment ions of m/z 71.0859 ($C_5H_{11}^+$, 0.33 ppm) and m/z 57.0706 ($C_4H_9^+$, 0.71 ppm), similar to the fragmentation patterns observed for C6−C18 DADMACs. Thus, peak 14 was tentatively identified as C7-DADMAC. Two isomeric peaks were observed at m/z 270.3155 and peak 15 was confirmed as C8-DADMAC with an authentic standard (Figure S13). Peak 16 exhibited a characteristic fragment ion at m/z 74.0961 ($C_4H_{12}N^+$, −3.81 ppm), indicating the presence of ethyldimethylamine in the structure analogue to that of C2:12-DADMAC (Figures S12 and S13). Therefore, peak 16 was identified as C2:14-DADMAC based on a mass difference of C_2H_4 ($\Delta m/z$ = 28.0313) in their molecular ions. In addition, peak 17 (RT: 6.03 min) with m/z 354.4091 generated with formula $C_{24}H_{52}N^+$ with a mass error of −0.84 ppm and was confirmed as C10:12-DADMAC based on the characteristic fragment ions at m/z 214.2533 ($C_{14}H_{32}N^+$, 1.72 ppm) and m/z 186.2227 ($C_{12}H_{28}N^+$, 5.8 ppm) (Figure S14). Interestingly, DADMACs with mixed chain lengths (C ≥ 8) were also identified in indoor dust,[23] sludge, and estuarine sediment,[8,9,30,48] while this is the first report on the identification of DADMACs with shorter chain lengths (C < 8) in dust samples, including DDA, C2:8-DADMAC, C4:10-DADMAC, C6:8-DADMAC, and C7-DADMAC.

ATMAC Analogues. A total of 9 homologues were identified as ATMAC analogues. Seven ATMAC analogues, including (3-carboxypropyl)trimethylammonium chloride (CPAC), (5-bromopentyl)trimethylammonium bromide (BPTMAC), s-

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Table 1. Confidence Levels (CLs), Detection Frequencies (DF, %), and Median Concentrations (μg/g) of Traditional QACs in Indoor Dust Collected from Homes, Railway Stations, Hotels, Hospitals, Markets, Cinemas, and Offices

		homes (n = 17)		railway stations (n = 12)		hotels (n = 18)		hospitals (n = 18)		markets (n = 20)		cinemas (n = 12)		offices (n = 14)	
compounds	CL	DF	median	DF	median	DF	median	DF	median	DF	median	DF	median	DF	median
traditional QACs															
C8-BAC	S1	71	0.0738	92	0.0418	72	0.0830	72	0.0331	90	0.0160	100	0.123	79	0.0483
C10-BAC	S1	94	0.121	100	0.0414	89	0.0372	100	0.0846	95	0.0625	100	0.203	86	0.0593
C12-BAC	S1	100	16.6	100	7.56	100	6.42	100	8.31	100	7.93	100	16.7	100	8.96
C14-BAC	S1	100	5.94	100	2.85	100	1.90	100	2.90	100	3.86	100	6.30	100	2.26
C16-BAC	S1	100	1.08	100	0.307	100	0.204	100	0.180	100	0.635	100	0.835	100	0.298
C18-BAC	S1	100	0.184	100	0.117	100	0.134	100	0.114	100	0.114	100	0.243	100	0.255
∑BAC		100	27.0	100	10.9	100	8.82	100	12.1	100	13.2	100	25.0	100	12.5
C8-DADMAC	S1	100	0.353	100	1.38	100	0.594	100	0.626	100	1.61	100	3.30	93	0.219
C10-DADMAC	S1	100	0.323	100	0.762	100	0.444	100	1.68	100	0.729	100	2.48	93	0.466
C12-DADMAC	S1	82	0.0434	58	0.00804	44	<MDL	67	0.0135	45	<MDL	92	0.0209	93	0.0126
C14-DADMAC	S1	76	0.0335	50	0.0045	33	<MDL	56	0.0124	40	<MDL	75	0.0263	79	0.0114
C16-DADMAC	S1	100	0.466	100	0.126	100	0.414	100	0.330	100	0.297	100	0.672	100	0.374
C18-DADMAC	S1	24	<MDL	33	<MDL	28	<MDL	22	<MDL	55	0.519	0		29	<MDL
∑DADMAC		100	2.30	100	2.35	100	2.00	100	3.10	100	3.47	100	6.16	100	1.36
C8-ATMAC	S1	100	0.0273	100	0.0716	100	0.0344	100	0.0431	100	0.0278	100	0.0413	100	0.0413
C10-ATMAC	S1	71	0.0256	92	0.0624	83	0.0311	100	0.189	100	0.0529	100	0.131	93	0.178
C12-ATMAC	S1	100	0.605	100	0.992	100	0.940	100	1.56	100	0.469	100	1.62	100	0.434
C14-ATMAC	S1	100	0.181	100	0.261	94	0.217	100	0.251	100	0.116	100	0.356	93	0.119
C16-ATMAC	S1	100	2.37	100	2.29	100	2.42	100	2.42	100	2.01	100	4.18	100	2.32
C18-ATMAC	S1	100	3.71	100	2.22	100	2.50	100	2.21	100	2.40	100	4.77	100	2.04
∑ATMAC		100	9.13	100	6.52	100	7.45	100	7.74	100	5.53	100	11.4	100	6.20
$\sum_{traditional}$ QACs		100	42.2	100	19.4	100	19.3	100	24.7	100	23.6	100	44.5	100	20.4

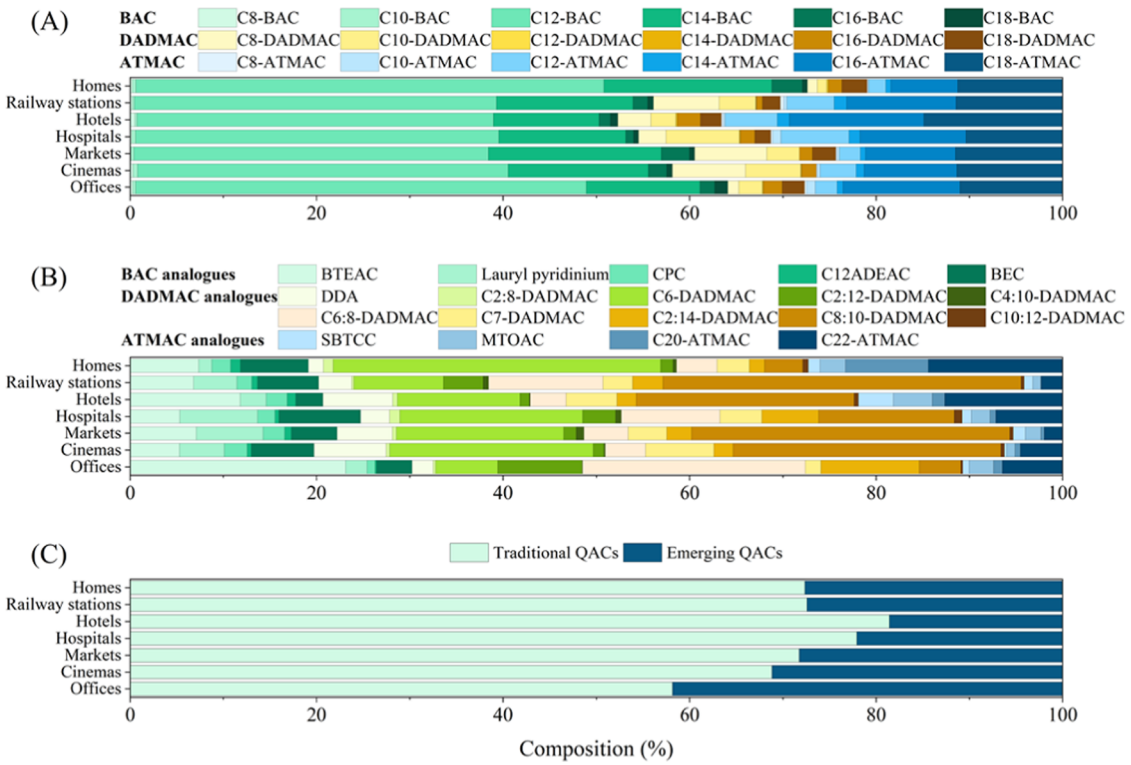

Figure 2. Composition of QACs measured in different microenvironments: (A) the contributions of individual traditional QACs to $\sum_{traditional}$ QAC concentrations; (B) the contributions of individual emerging QACs to $\sum_{emerging}$ QAC concentrations; and (C) the contributions of $\sum_{traditional}$ QACs and $\sum_{emerging}$ QACs to ∑QAC concentrations.

butyrylthiocholine iodide (SBTCC), tetrapropylammonium bromide (TPABC), methyltrioctylammonium chloride (MTOAC), tributylmethylammonium bromide (TMABC), and tetraheptylammonium bromide (THAC), were identified with authentic standards (level S1), while C20-ATMAC and C22-ATMAC were identified as level S2.

Peak 18 and peak 20, two respective ATMAC homologues with different chain lengths, were found at retention times of

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Table 2. Confidence Levels (CLs), Detection Frequencies (DF, %), and Median Concentrations (μg/g) of Emerging QACs in Indoor Dust Collected from Homes, Railway Stations, Hotels, Hospitals, Markets, Cinemas, and Offices

		homes		railway stations		hotels		hospitals		markets		cinemas		offices	
compounds	CL	DF	median	DF	median	DF	median	DF	median	DF	median	DF	median	DF	median
emerging QACs															
BTEAC	S1	94	0.500	100	0.391	100	0.402	100	0.264	100	0.471	100	0.850	100	1.80
BTBAC	S1	24	<MDL	100	0.00869	72	0.00361	39	<MDL	15	<MDL	67	0.0363	86	0.0669
BTMAC	S1	29	<MDL	50	0.0809	50	0.0862	61	0.108	75	0.204	83	0.454	79	0.180
laurylpyridinium[a]	S2	100	0.0952	100	0.268	94	0.0953	100	0.417	100	0.473	100	0.778	93	0.179
CPC	S1	94	0.138	100	0.0918	83	0.0764	100	0.0932	100	0.153	100	0.394	93	0.067
C12ADEAC[a]	S2	71	0.0716	92	0.0357	78	0.0316	100	0.0217	90	0.0469	100	0.0723	71	0.0124
C14ADEAC[a]	S2	47	<MDL	67	0.0602	61	0.0135	44	<MDL	85	0.0234	92	0.0367	36	<MDL
DMPC	S1	18	<MDL	50	0.0110	33	<MDL	56	0.00631	45	<MDL	92	0.0248	50	0.00462
BEC	S1	94	0.494	100	0.377	94	0.100	100	0.436	100	0.327	100	1.08	93	0.294
∑BAC analogues		100	1.50	100	1.67	100	0.872	100	1.70	100	1.89	100	3.71	100	4.23
DDA	S1	88	0.428	100	0.204	83	0.255	100	0.155	95	0.392	100	1.25	79	0.176
C2:8-DADMAC[a]	S2	100	0.0717	100	0.0130	89	0.0177	100	0.0545	100	0.0286	100	0.0614	93	0.0211
C6-DADMAC[a]	S2	100	2.39	100	0.553	94	0.448	100	0.977	100	1.19	100	3.52	93	0.520
C2:12-DADMAC	S1	100	0.0908	100	0.245	94	0.0339	100	0.176	100	0.0887	100	0.187	93	0.703
C4:10-DADMAC[a]	S2	82	0.0253	83	0.0323	67	0.00261	72	0.0301	75	0.0556	100	0.022	71	0.00247
C6:8-DADMAC[a]	S2	100	0.297	100	0.706	83	0.132	100	0.527	100	0.313	100	0.694	100	1.86
C7-DADMAC[a]	S3	100	0.235	100	0.182	94	0.186	72	0.224	100	0.275	100	1.18	57	0.132
C2:14-DADMAC[a]	S2	100	0.111	100	0.187	100	0.0708	100	0.305	100	0.178	100	0.332	100	0.818
C8:10-DADMAC	S1	100	0.244	100	2.21	100	0.798	100	0.724	100	2.26	100	4.63	93	0.349
C10:12-DADMAC[a]	S2	94	0.0418	100	0.0197	94	0.0156	100	0.0427	100	0.0247	100	0.0620	100	0.0160
∑DADMAC analogues		100	6.07	100	4.59	100	1.90	100	3.93	100	6.13	100	14.4	100	4.60
CPAC	S1	47	<MDL	33	<MDL	39	<MDL	6	<MDL	55	0.212	75	0.212	50	0.0649
BPTMAC	S1	12	<MDL	0		0		0		5	<MDL	17	<MDL	0	
SBTCC	S1	88	0.0862	75	0.0529	78	0.128	94	0.0487	80	0.0859	75	0.0367	71	0.0534
TPABC	S1	6	<MDL	0		6	<MDL	0		5	<MDL	0		57	0.0335
TMABC	S1	24	<MDL	100	0.0274	100	0.0211	22	<MDL	40	<MDL	83	0.0347	14	<MDL
MTOAC	S1	71	0.185	83	0.0473	89	0.142	89	0.0995	90	0.110	92	0.144	79	0.202
C20-ATMAC[a]	S2	82	0.603	8	<MDL	67	0.0461	78	0.0306	45	<MDL	92	0.0932	86	0.0729
C22-ATMAC[a]	S2	88	0.981	92	0.133	83	0.431	100	0.358	100	0.132	100	0.733	93	0.504
THAC	S1	0		0		0		0		0		0		7	<MDL
∑ATMAC analogues		100	2.60	100	0.343	100	0.599	100	0.653	100	0.439	100	1.35	100	0.882
$\sum_{\text{emerging}}$ QACs		100	16.1	100	7.3	100	4.41	100	7.00	100	9.31	100	20.2	100	14.7
∑QACs		100	58.3	100	28.4	100	23.7	100	34.2	100	34.2	100	65.9	100	44.2

[a]Semiquantifications based on their respective calibration curves of similar chemical structure analogues were applied due to their unavailable commercial standards.

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6.82 and 7.11 min, respectively (Figures S15 and S16). Peak 18 with m/z = 340.3928 ($C_{23}H_{50}N^+$, −2.75 ppm) was tentatively identified as C20-ATMAC based on the characteristic fragment ion m/z = 60.0805 ($C_3H_{10}N^+$, −4.97 ppm), indicating the existence of trimethylammonium. Similarly, peak 19 and peak 20 were generated from m/z 368.4251 with the formula of $C_{25}H_{54}N^+$. Peak 19 was identified with a standard of MTOAC, while its isomer, peak 20, was deduced to be C22-ATMAC due to the same characteristic fragment ion m/z 60.0808 ($C_3H_{10}N^+$, −0.22 ppm) with that of C20-ATMAC and a different unit of C_2H_4 ($\Delta m/z$ = 28.0313) in their precursor ion. Of the identified ATMAC homologues, C20-ATMAC and C22-ATMAC have been reported in the European dust and municipal sewage sludge in China.[23,30] Nonetheless, this is the first report on the identification of CPAC, BPTMAC, SBTCC, MTOAC, TMABC, and THAC in indoor environments.

Traditional QACs in Dust from Homes. Concentrations and detection frequencies (DFs) of traditional QACs are summarized in Table 1. All traditional QACs were detected in 71−100% of the dust samples, except for C18-DADMAC (DF: 24%). The infrequent detection of C18-DADMAC can potentially be attributed to the varying formulations of disinfectants, fabric softeners, and other personal care products used in China. The total traditional QAC concentrations ($\sum_{traditional}$ QAC, sum of 18 traditional QACs) ranged from 13.8 to 150 μg/g at a median concentration of 42.2 μg/g, similar to those reported in residential dust collected from the United States (36.3−58.9 μg/g)[22] and almost 3 times higher than those reported in indoor dust from Europe (14.73 μg/g).[23] This can be attributed to the fact that several QACs, including C12- to C18-BACs and others, are currently under evaluation in the European Union before these chemicals can be approved to be active ingredients in the market.[23] Compared with other emerging contaminants previously reported in home dust from South China, the median concentration of $\sum_{traditional}$ QAC measured in the current study was comparable to that for phthalate monoesters (45.4 μg/g),[36] higher than that for liquid-crystal monomers (18.5 μg/g)[50] and organophosphate esters (10.6 μg/g).[51] These results suggest that QACs are ubiquitous in indoor environments and may cause health risks to humans.

BACs were the most abundant QAC group (Figure 2), contributing 70.3% to $\sum_{traditional}$ QAC concentrations, followed by ATMACs (23.7%) and DADMACs (6.00%). This pattern was different from that reported in indoor dust collected from the United States (56, 26, and 18% for BACs, DADMACs, and ATMACs, respectively) and Europe (45.7, 26.8, and 27.5% for BACs, DADMACs, and ATMACs, respectively).[22,23] The observed lower proportion of DADMACs in our study, compared to samples from the United States and Europe, may be linked to their decreased utilization in products, such as disinfectants and fabric softeners. In addition, this trend could be partially explained by the industry's shift toward the production of shorter chain DADMACs as alternatives due to the phase-out of long-chain ditallowdimethylammonium cations in the 1990s.[52,53]

Specifically, C12- and C14-BACs and C16- and C18-ATMACs were the predominant QAC congeners, and these four compounds comprised nearly 90% of $\sum_{traditional}$ QAC concentrations, likely as a result of their high production volumes and wide applications in the market from China (e.g., cleaning products, hair conditioners, and hair care products).[20,52]

Emerging QACs in Dust from Homes. Twenty-eight emerging QACs, including 9 BAC analogues, 10 DADMAC analogues, and 9 ATMAC analogues, were identified in the current study. Overall, the total concentrations of emerging QACs ($\sum_{emerging}$ QAC, sum of 28 emerging QACs) in residential dust ranged from 2.09 to 46.9 μg/g with a median of 16.1 μg/g, approximately 2 times lower than those of traditional QACs (42.2 μg/g; Table 2). It should be noted that DADMAC analogues are detected in 82−100% of the samples and constitute the major group of emerging QACs. The median DADMAC analogue concentration was 6.07 μg/g, which was 2 times higher than those of ATMAC analogues (median 2.60 μg/g) and almost 4 times higher than those of BAC analogues (median 1.50 μg/g).

Five out of nine BAC analogues were detected in >50% of the samples. Specifically, BTEAC, utilized as a catalyst in antibacterial agent synthesis,[54] was found in 94% of the samples with a median concentration of 0.500 μg/g. The occurrence of this emerging QAC in indoor environments is possibly released from electrochemical devices, such as lithium batteries.[55] BEC was detected in 94% of all dust samples, ranking the second most abundant BAC analogues with a median concentration of 0.494 μg/g. Both BEC and BACs serve as antimicrobials in a variety of personal care products, such as hand soaps, sanitizers, and wipes.[11,20,56] Following the FDA's 2016 ban on 19 active ingredients, including triclosan and triclocarban, it has been documented that BEC and BACs were increasingly used as replacement antimicrobial agents in over-the-counter hand and body wash products.[57,58] Moreover, BEC could exhibit comparable toxicity to triclosan, causing effects such as hatching delay, embryonic mortality, and neurotoxicity in zebrafish embryos.[59] The ubiquitous occurrence of this compound in dust and its potential toxicities warrant additional human exposure research focused on BEC. Laurylpyridinium and CPC, the isomers of C8- and C12-BACs, are reported to be ingredients in antimicrobial mouthwashes and toothpaste.[60] These two compounds were found in 100 and 94% of the samples and were detected with median concentrations of 0.0952 and 0.138 μg/g, respectively. Their levels were slightly higher than that of C8-BAC but 2 magnitudes lower than that of C12-BAC. C12ADEAC and C14ADEAC, the isomers of C14- and C16-BACs, respectively, were used as ingredients in disinfectants[13] and were detected with lower detection frequencies (71 and 47%, respectively) and concentrations (0.0716 μg/g and <MDL, respectively) than those of C14- and C16-BACs. DMPC, commonly applied in drugs,[61] was only detected in 18% of the samples.

Notably, C6-DADMAC was the most abundant DADMAC analogue (median of 2.39 μg/g; DF: 100%) and comprised 35.1% of $\sum_{emerging}$ QAC concentrations. The level of C6-DADMAC was significantly higher than other C8−C18 DADMACs that were frequently reported (<MDL to 0.466 μg/g). C7-DADMAC, an intermediate in the production of porogen dielectric thin films,[62] was detected in all of the samples with a median concentration of 0.235 μg/g. Interestingly, Belova et al. also found odd numbers of chain lengths of BACs (e.g., C11-BAC and C13-BAC) in the dust samples.[23] In addition, mixed DADMACs were constantly observed in dust along with paired DADMACs that had been frequently reported.[23] Two mixed DADMACs with long alkyl chains, C8:10- and C10:12-DADMAC, were detected in 100 and 94% of the samples with median concentrations of 0.244 and 0.0418 μg/g, respectively. The level of C8:10-DADMAC was also reported in dust

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collected from Europe (0.02 μg/g)[23] but 10 times lower than that determined in the current study. Interestingly, mixed DADMACs with shorter alkyl chains, including C2:8-DADMAC, C2:12-DADMAC, C4:10-DADMAC, C6:8-DADMAC, and C2:14-DADMAC, were frequently detected in the current study (DF: 82−100%) and their median concentrations were 0.0717, 0.0908, 0.0253, 0.297, and 0.111 μg/g, respectively. To the best of our knowledge, this is the report on the occurrence of these mixed DADMACs with shorter alkyl chains, their presence is likely attributed to biodegradation processes.[9] The ubiquitous detections of mixed and paired DADMACs in dust can be tracked back to their manufacturing procedures when fatty acids serve as feedstock.[63] Since fatty acids encompass a diverse array of alkyl-chain-substituted mixtures, it is possible that mixed DADMACs may inadvertently manifest as byproducts alongside their paired DADMAC counterparts during the ensuing stages of catalytic hydrogenation and the quaternization synthesis processes.[64] Notably, previously identified long-chain DADMACs with mixed alkyl chain lengths in sludge samples as well as a series of TPABC homologues and various ionic liquids in wastewater effluent samples[9,30] were not identified in the present study, possibly due to the different environmental matrices.

Regarding ATMAC analogues, 4 out of 9 ATMAC analogues were detected in >50% of the samples, including C20- and C22-ATMACs, MTOAC, and SBTCC. Owing to their excellent antistatic properties, C20- and C22-ATMACs were commonly used as ingredients in hair conditioners and hair care products.[65] The levels of C20- and C22-ATMACs in dust (medians 0.603 and 0.981 μg/g, respectively) are comparable to those measured in dust collected from Europe (0.18 and 1.45 μg/g, respectively),[30] further implying their ubiquitous sources in indoor environments. MTOAC and SBTCC were observed at a median concentration of 0.185 and 0.0862 μg/g, respectively. However, the usage of these two compounds is scant, and more efforts are needed to clarify their potential sources. Relatively low detection frequencies (<50%) and concentrations were found for CPAC, BPTMAC, TPABC, TMBAC, and THAC, which are not included in the further discussion. The frequent detections of BAC, DADMAC, and ATMAC analogues highlight the importance of measuring these compounds in different indoor environments.

Traditional and Emerging QACs in Dust from Various Microenvironments. Each QAC detected in residential dust was also found in other public settings with comparable detection frequencies. Overall, the highest ∑QAC concentrations (sum of traditional and emerging QACs) in dust were observed in cinemas (median 65.9 μg/g), followed by homes (58.3 μg/g), offices (44.2 μg/g), markets (34.2 μg/g), hospitals (34.2 μg/g), railway stations (28.4 μg/g), and hotels (23.7 μg/g; Figure 3). This trend persisted when examining the dust concentrations for traditional and emerging QACs in these microenvironments (Figure S17). The elevated QAC concentrations in cinemas are likely due to the intensified disinfection practices and the presence of potential sources of QACs in cinemas, such as carpets, curtains, and seating materials, which contribute to these higher concentrations.[20,52,66] In general, the composition of $\sum_{emerging}$ QAC (sum of emerging QACs) to ∑QAC (sum of traditional and emerging QACs) ranged from 19 to 42% across various microenvironments, indicating the widespread existence of emerging QACs in indoor environments (Figure 2). To investigate the potential effects of housing characteristics on the QAC levels among various public settings,

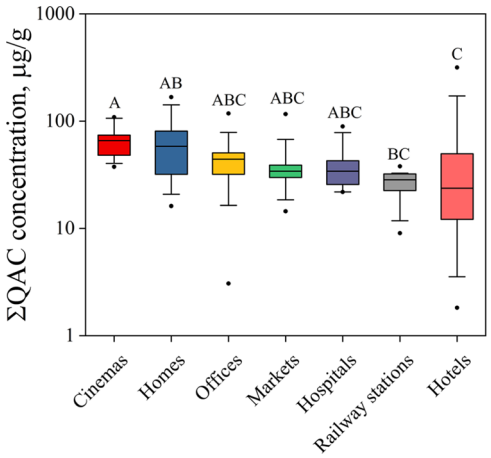

Figure 3. Total concentrations of QACs detected in the dust samples collected from various microenvironments (μg/g). Concentrations are shown as box plots, representing the 25th and 75th percentiles; black lines represent the median; whiskers represent the 10th and 90th percentiles; and dots represent the 5th and 95th percentiles. The letters represent the results of the one-way analysis of variance (ANOVA); the concentrations are ranked from the highest to lowest in alphabetic order, and concentrations sharing the same letter are not statistically different at $p < 0.05$.

we grouped the samples based on ventilation conditions and volumes inside buildings. As presented in Figure S18, it was noteworthy that relatively lower QAC concentrations were observed in samples from more well-ventilated (combination of natural and forced ventilation and forced, medians of 30.6 and 34.8 μg/g, respectively) than those from less well-ventilated (natural ventilation, 47.6 μg/g). Moreover, the relatively lower QAC concentrations were observed in samples from large volumes inside buildings (median 34.8 μg/g) than those of small volumes inside buildings (42.8 μg/g).

In an assessment of the proportions of individual QAC to ∑QAC concentrations across different settings, homes exhibited greater proportions of C12- and C14-BACs (51.6 and 18.5%, respectively) as compared to cinemas (39.8% and 15.0%, respectively). Conversely, cinemas had a more pronounced presence of C8- and C10-DADMACs at 7.87 and 5.91%, while these compounds represented only 1.1 and 1.0% in homes, respectively (Figure 2). One possible explanation is the predominant use of BACs as antibacterial agents in hand soaps and sanitizers within households. On the other hand, DADMACs, serving as antistatic agents, are integrated extensively into textile items, especially in cinemas, including carpets, drapes, and seating materials.[20] As ATMACs with long alkyl chains were widely used in personal care products (e.g., hair care products),[67] higher median concentrations of C20- and C22-ATMACs (0.603 and 0.981 μg/g, respectively) were detected in homes than in other microenvironments (<MDL to 0.0932 μg/g and 0.132−0.733 μg/g, respectively).

In the light of textiles serving as a potential source for other environmental contaminants (i.e., PFASs) in indoor environments,[68−70] we grouped the dust samples based on noncarpet rooms and carpet rooms. ∑QAC concentrations in dust collected in carpet-covered rooms were significantly higher than those in noncarpet indoor environments (65.6 μg/g vs 32.6 μg/g, $p < 0.05$, Figure S19), suggesting that carpets may be a potential source of QACs in indoor environments. While interpreting these results, it is important to exercise caution due

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to the lack of collected information about the specific disinfecting practices and cleaning processes of carpets in this study. However, there is a substantial body of evidence, indicating that QACs have been incorporated into textiles to mitigate static and enhance fabric feel due to their cationic nature.[66,71] Among them, DADMACs have gained prominence as antistatic agents in fabric softeners.[52,66] Over the years, extensive research revealed that QACs, particularly those with elongated alkyl chains, possess the capability to impart antimicrobial properties to textiles.[72,73] This discovery has expanded their applications, making them highly suitable for various textiles, including carpets, medical fabrics, and activewear.[74] A case in point is benzalkonium chloride (C8−C18 BACs), which has been effectively employed to neutralize dust mites, their allergens, and fungi prevalent in carpets.[75] Given these findings, further research is needed to explore the influence of textiles on the QAC levels in indoor environments.

Correlations and Potential Sources. To further explore potential sources of QACs in indoor environments, heatmaps and cluster analysis were performed with Pearson correlations for analytes found in more than 50% of the samples (Figure S20). As a result, concentrations of C2:8-DADMAC, C6-DADMAC, C8-DADMAC, C8:10-DADMAC, C10-DADMAC, and C10:12-DADMAC exhibited significant positive correlations with C12-BAC, C14-BAC, and C16-BAC, with correlation coefficients ranging from 0.519 to 0.818 ($p < 0.01$). This trend can be attributed to the prevalent use of C12-, C14-, and C16-BACs, as well as C8- and C10-DADMACs, as primary constituents in disinfectants,[22] whereas other mixed DADMAC homologues may function as impurities in such products. Moreover, a positive correlation was observed for C12-DADMAC and C14-DADMAC (r: 0.566; $p < 0.01$), indicating a common source for these two compounds. As documented, longer chain DADMACs often serve as key components in fabric softeners over disinfectants due to their antistatic properties.[11,52] In a separate correlation set, C12 through C18-ATMAC showed a high mutual correlation (r: 0.394−0.878; $p < 0.01$), implying their distinct applications apart from BACs and DADMACs. Notably, ATMACs are primary constituents in stabilizers and preservatives present in air fresheners, conditioners, and hair care solutions.[20] Their octanol−air partitioning coefficients ($\log K_{OA}$ 8.17−11.8) stand below those of BACs and DADMACs (11.0−18.2), suggesting a propensity of ATMACs to partition into the air.[14] Furthermore, C2:12-DADMAC, C2:14-DADMAC, and C6:8-DADMAC were positively correlated (r: 0.702−0.753; $p < 0.01$). Research indicates that these mixed DADMACs may originate from personal care products,[10] leading to their ubiquitous occurrence in indoor environments. While BEC and BACs are employed as antimicrobials in a variety of sanitizing products like hand soaps, sanitizers, and wipes, there was no observed correlation between these compounds in this analysis (r: 0.044−0.169; $p > 0.05$), suggesting that there is a significant source of BEC that has been overlooked. Intriguingly, a significant positive correlation was found between BEC and CPC ($r = 0.428$, $p < 0.01$), which is commonly used in cosmetics and personal care items. These findings point to the necessity for further investigation to uncover the sources of these newly recognized QACs (e.g., BEC) in indoor environments.

Environmental Implications. In this study, semiquantification was conducted for those emerging QACs without commercial standards and the absence of internal standards for DADMACs and ATMACs, which may introduce uncertainties in the quantification results of these compounds. In addition, the scope of the samples was geographically constrained and limited in terms of the sampling time frame during the COVID-19 pandemic. As a result, more research is needed to conduct and validate the seasonal levels of QACs across diverse microenvironments. This study also notes a lack of specific information regarding the disinfection and cleaning processes of carpets. The conclusion that carpets act as a potential source of QACs in indoor environments should be considered with caution. Although a series of emerging QACs were identified in the dust, some emerging QAC homologues (e.g., long-chain DADMACs) were not identified in the present study. The absence of these compounds in our results could be attributed to the low MS signal of these chemicals and our use of a specific acquisition mode in our instrument, which may have hindered the capture of the necessary MS^2 data for their identification. Therefore, more appropriate acquisition mode (e.g., data independent acquisition mode) and nontargeted analysis workflow (e.g., characteristic fragments, neutral losses), as well as advanced analytical technologies (e.g., ion mobility mass spectroscope), are needed to better characterize more potential QAC analogues in further research.

Nonetheless, this research has successfully identified an array of emerging QACs in dust, with some detected at concentrations nearing ppm levels. Given the rising production and market applications of QACs, future research should endeavor to detect an even broader range of these compounds in environmental samples. Particularly, C12ADEAC, C14ADEAC, CPC, laurylpyridinium, and shorter chain DADMACs (C < 8) were identified in dust for the first time. Their detections underscore the importance of biomonitoring and rigorous toxicity studies to elucidate potential impacts on human health. In addition, this research marks the first time QACs have been studied in this context within China, expanding the knowledge base beyond North America and Europe. It is also worth noting that elevated concentrations of QACs were found in dust sourced from cinemas and carpeted areas. This suggests textiles, such as carpets, curtains, and seating materials, might be potential emission sources of QACs in indoor environments.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.est.3c09942.

Detailed information on chemicals and reagents, housing characteristics, and instrumental methods, surrogate and matrix spike recoveries, MDLs and blank concentrations, functions and usage, workflow of target and suspect screening, chemical structures, chromatograms, and MS/MS spectra of emerging QACs, traditional and emerging QACs in dust across various microenvironments, dust concentrations of QACs from carpet and noncarpet indoor environments, and correlation heatmaps (PDF)

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Notes

The authors declare no competing financial interest.

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