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Mapping the distribution of contaminants identified by non-targeted screening of passively sampled urban air

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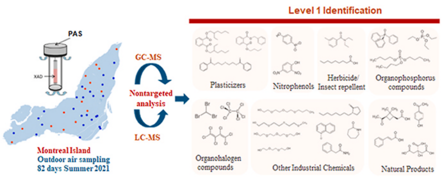
HIGHLIGHTS

- First application of non-targeted analysis using both LC- and GC-MS to outdoor urban air.
- Forty passive samplers deployed across the Island of Montreal, Canada in 2021.
- Many organic compounds were detected for the very first time in the atmosphere.
- Results indicate the impact of anthropogenic activities on spatial distribution.

GRAPHICAL ABSTRACT



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ABSTRACT

Air pollution is closely associated with increased lung cancer incidence and mortality. Because many semi-volatile industrial chemicals, pesticides and combustion by-products are endocrine-disrupting or genotoxic, their mixtures in outdoor urban air, even at trace levels, could have cumulative effects. However, evidence for the impact of outdoor air pollution on human health remains limited, partly because its composition is poorly characterized. Non-targeted analysis (NTA) based on the combination of liquid (LC) and gas (GC) chromatographic separation with high resolution mass spectrometry (MS), allows for the comprehensive analysis of contaminants in environmental samples. Here, we present the first application of an NTA approach using both LC- and GC-MS to characterize the chemical mixture in outdoor urban air by analyzing forty passive samplers deployed for 82 days during summer 2021 across the Island of Montreal, Canada. The confirmed 25 molecular features included nitrophenols, pesticides/repellents, plasticizers, organophosphorus compounds, organohalogen compounds, other industrial chemicals, and natural products. Triethylene glycol monomethyl ether, triethylene glycol monobutyl ether, n-octyl-pyrrolidone, quinoline n-oxide, 4-hydroxy-acetophenone, citric acid, 2-phenyl acetamide, and hexachloroethane were detected for the very first time in the atmosphere. Previously reported in atmospheric particles, 4-nitrophenol, 2,4-dinitrophenol, tri- and tetraethylene glycol, nonanoic acid, diethylene glycol dibenzoate, caprolactam, phenylacrylic acid, pinonic acid and triphenylphosphine oxide were also detected in the outdoor atmospheric gas phase. The spatial grouping of data between residential and public areas

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emphasizes the impact of anthropogenic activities on atmospheric vapor composition. This study facilitates the assessment of airborne exposure to chemical mixtures and its effects on human health.

1. Introduction

Ambient (outdoor) air pollution is a leading cause of death and disease globally. Exposure to air pollution is recognized to be closely associated with increased lung cancer incidence and mortality (Turner et al., 2020). Air quality monitoring typically measures a limited number of well-known air pollutants, e.g. ground-level ozone, particular matter including $PM_{2.5}$ and PM_{10}, carbon monoxide, sulfur dioxide and nitrogen dioxide. The analysis of organic vapors is often limited to the volatile organic compounds implicated in ozone formation. The intense production and usage of chemicals that is associated with rapid industrialization and urbanization accelerates the emissions of volatile and semi-volatile organic compounds into the atmosphere, escalating the level of global air pollution. Many of the emitted industrial chemicals, pesticides and combustion by-products have been classified as endocrine disrupting or genotoxic, and their mixtures in urban air, even at trace levels, could have cumulative adverse effects on human health (Sjoestroem et al., 2024; Minuti et al., 2024; Street et al., 2024). A thorough characterization of the urban atmosphere would enhance the assessment of the risk posed by air pollution. However, due to the large number of compounds present, the chemical composition of the atmospheric gas phase still remains poorly characterized, and the presence of contaminants with potential health hazards have yet to be characterized.

High resolution mass spectrometry (MS), when coupled with gas chromatographic (GC) and liquid chromatographic (LC) separations, is now capable of collecting data for thousands of compounds in complex matrices within a single run. Post-acquisition data treatment allows for the quantification of known target compounds as well as the untargeted identification of unknown compounds covering a wide polarity range. Non-targeted analysis (NTA) has been widely used on various environmental (water, soil, atmosphere, etc.) and food matrices (Liu et al., 2021; Zheng et al., 2024; Tian et al., 2024; Jiang et al., 2014). NTA studies of atmospheric samples so far mainly focused on the hydrocarbons and persistent pollutants in atmospheric particles (Jiang et al., 2014; Kuang et al., 2018; Pereira et al., 2021; Papazian et al., 2022; Ning et al., 2024; Noblet et al., 2024). Recently, Cheng et al. reviewed the application of suspect screening and non-targeted approaches for discovering emerging organic pollutants in the atmosphere, mainly in fine particulate matter ($PM_{2.5}$) (Cheng et al., 2023). Relatively few applications of NTA have been reported for contaminant discovery in the outdoor gas phase (Zhang et al., 2010; Röhler et al., 2020a, 2020b; Hashimoto et al., 2022).

Passive air samplers (PASs), without requirement for a power source and equipped with low-cost sorbents, have been applied for sampling volatile and semi-volatile chemicals in the atmosphere (Wania and Shunthirasingham, 2020). Major sorbents used in PASs include polyurethane foam (Shoeib and Harner, 2002), and XAD resin (Wania et al., 2003). During long deployments, gaseous compounds continuously diffuse to, and sorb onto, these sorbents, from which they are then extracted and analyzed. It has been reported that the stability of absorbed compounds during storage of XAD were higher than on PUF (Chuang et al., 1987). A recent study also reported that even during extended ozone exposure, no degradation of PAHs absorbed to the XAD-resin was observed (Li et al., 2024). Given the volatility of compounds in the atmospheric gas phase, NTA studies identifying new atmospheric pollutants, including organophosphorus flame retardants, and unsubstituted, alkylated and heterocyclic polycyclic aromatic compounds, have predominantly relied on GC-MS (Röhler et al., 2020a, 2020b; Hashimoto et al., 2022; Yang et al., 2020; Zhang et al., 2020a). By focusing on polar, but still semi-volatile, compounds, LC-MS can provide information that is complementary to the results obtained with GC-MS. To date, studies using LC-MS for the NTA of atmospheric samples are scarce (Papazian et al., 2022; Froment et al., 2025). Only one study reported the use of both GC-MS and LC-MS in the NTA of indoor PAS extracts with most compounds remaining tentatively identified (Papazian et al., 2023). Two other studies focused solely on the targeted screening of air pollutants in outdoor PAS samples using GC-MS and/or LC-MS (Zaller et al., 2022, 2023).

This study aimed to investigate chemical mixtures in outdoor air by combining PASs and NTA. The objectives were to (i) design a workflow for the NTA of air sampling extracts that incorporates both LC-MS and GC-MS, (ii) demonstrate the capacity of this workflow to identify new compounds in outdoor air through suspect and non-targeted screening, and (iii) assess the spatial variability of the chemical mixtures at the scale of a city using PASs deployed across the Island of Montreal. To our knowledge, this is the first study that applies both GC-MS and LC-MS in the NTA of outdoor air, thereby providing a new perspective on chemical mixtures in the urban atmosphere.

2. Materials and methods

2.1. Chemicals

Details of spiked mass-labeled internal standards and authentic standards are listed in the supporting information (SI). All chemicals were stored at −20 °C in the dark.

2.2. Sampling preparation

The NTA Study Reporting Tool was used in the sample preparation and data acquisition/analysis as described in the supporting information (Peter et al., 2021; BP4NTA, 2022). The study relied on PASs of the type described in elsewhere (Wania et al., 2003), which consists of a cylindrical stainless-steel shelter with a lid on top and an opening at bottom, in which cylindrical sorbent-filled stainless steel mesh containers are suspended. Air exchange in the shelter is through the bottom opening as well as a number of small holes in the top of the shelter. To prepare the mesh containers, approximately 20 g of pre-cleaned XAD-2 resin (20/60 mesh, 350 m^2/g surface area, 9 nm pore diameter, Supelco, purchased from Sigma-Aldrich, Burlington, MA, United States) was filled into each pre-cleaned container with both ends plugged with a small amount of clean glass wool. The resin-filled containers were placed in an amber glass jar, dried under nitrogen flow, and sealed in a metal shipping tubes before use (Wania et al., 2003).

The PASs were deployed at 40 sites on the Island of Montreal, Canada (364.74 km^2), from the middle of July to the first week of October in 2021, for a period of 82 days to collect volatile and semi-volatile organic compounds from the outdoor atmosphere. Deployment sites were in residential areas (n = 25) and public parks (n = 15) based on acceptance of surveyed residents and municipal permission, all distributed to represent the entire territory (see map in Fig. 1). Numbers from 3 to 50 and from 101 to 115 were assigned randomly to sites in residential and public areas, respectively. The PASs were attached to an existing structure or a pole at around 1–1.5 m above the ground. At each site, two resin-filled stainless steel mesh containers were removed from the shipping tubes and hung on a hook attached to the inside of the shelter lid. Upon collection, the mesh cylinders were transferred back into the shipping tubes closed with a silicone cap and sealed with Teflon tape for transport and storage at −80 °C until extraction. In order to quantify sampling precision, duplicate samplers were deployed at sites 3 and 107 using separate structures or poles. During the PASs' deployment, three

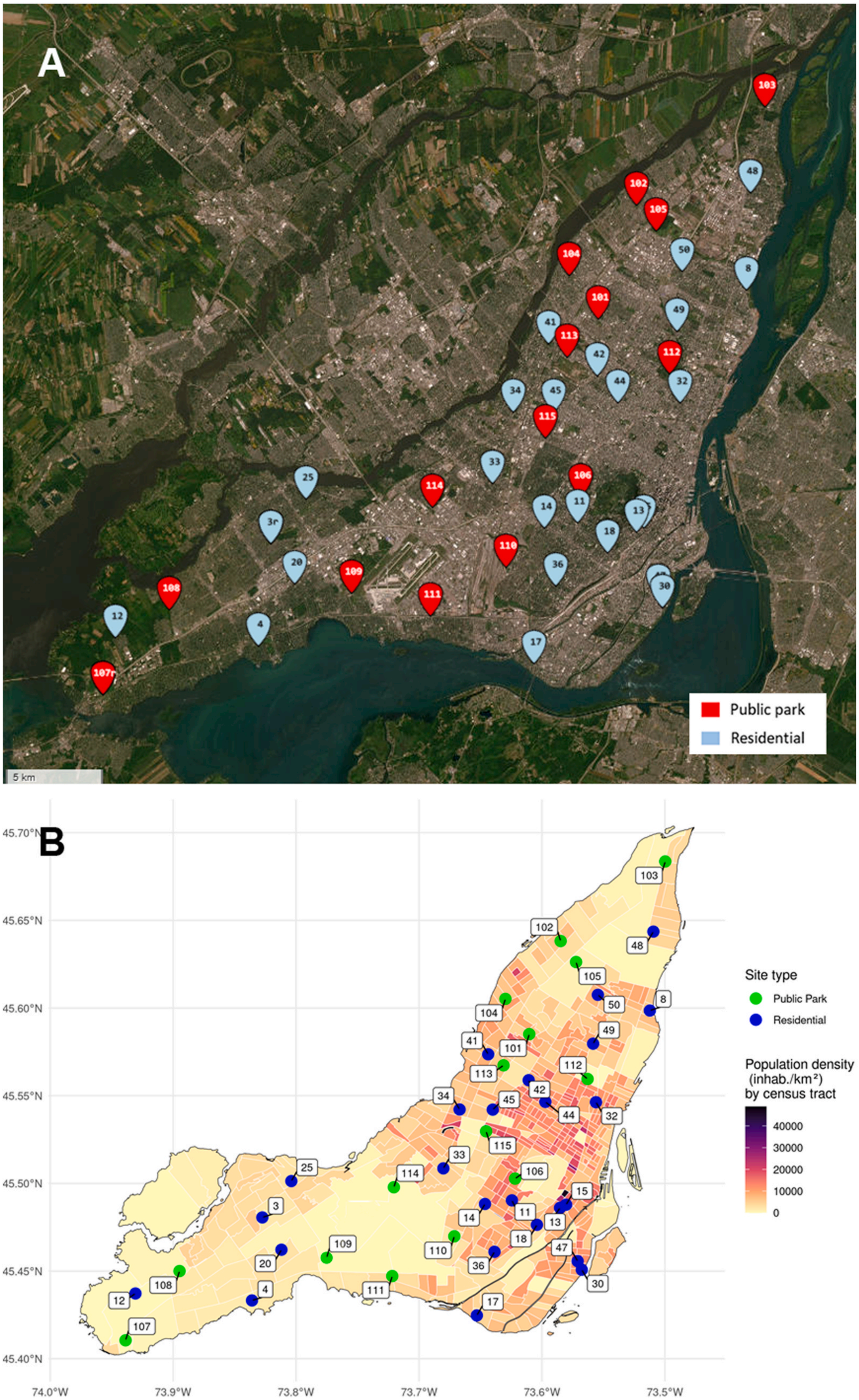

Fig. 1. Maps showing the 40 deployment sites of passive air samplers across the Island of Montreal. (A: satellite view-For copyright of the base map: Source: Esri, Maxar, Earthstar Geographics, and the GIS User Community; B: 2021 Census of Population, Statistics Canada).

field blank were deployed at designated sampling locations (2 at site 3, and 1 at site 115), with the resin-filled mesh cylinders only exposed to the surrounding air during the initial installation or final collection stages. Field blanks remained sealed and stored at the sites at room temperature during sampling period before collection.

2.3. Sample extraction

Two groups of internal standard mixtures for both GC (50 μL of 400 ng/mL, Table S1) and LC (50 μL of 1000 ng/mL) (Table S1) were spiked onto the XAD-resin, followed by accelerated solvent extraction (Dionex ASE 300) with a mixture of acetone/hexane (1:1 v/v) at 75 °C for 3 static cycles (6 min/cycle). Each extract was separated into two aliquots destined for GC-MS and LC-MS analysis. Both aliquots were concentrated to 1 mL via rotary evaporation and furthered reduced to 0.5 mL under nitrogen flow. For LC-MS analysis, the concentrated extract was transferred into a HPLC vial, dried under nitrogen, reconstituted into 1 mL methanol, spiked with 25 μL of an internal injection standard solution (1000 ng/mL, Table S1), and diluted 10-fold in methanol. For GC-MS analysis, 450 μL iso-octane and 50 μL of GC internal injection standards (400 ng/mL, Table S1) were added to the extract, which was concentrated to 0.5 mL. Because extracts from sites 11 and 32 were lost during sample preparation, only samples from 38 sites were subjected to GC-MS analysis.

2.4. Instrumental analysis

LC-MS samples were analyzed on an Agilent 1290 Infinity II LC system coupled to a 6545 Q-TOF-MS (Agilent Technologies, Santa Clara, USA) via full-MS scan, targeted MS/MS as well as the automated iterative-exclusion Auto MS/MS acquisition (Koelmel et al., 2017). The GC fraction of the extracts were analyzed using an Agilent 7250B GC-TOF-MS system (Agilent Technologies, Santa Clara, USA). Details of instrumentation parameters is provided in Text S1 (SI).

2.5. Quality assurance and quality control

The field blank PASs were used to assess any potential contamination introduced by manual sampler handling, shipping, and storage. Glass containers were thoroughly cleaned, oven baked at 325 °C for 4 h, and rinsed with hexane and acetone before and after each use. Along with the extraction of resin from the 40 sites, including two replicates and three field blanks, five procedural blanks were prepared following the same extraction method using the same resin without exposure to field air.

Twenty-four deuterated or ^{13}C labeled internal standards (16 for LC-MS and 8 for GC-MS) were spiked onto the resin samples at a constant concentration before extraction, and the peak area of each internal standard in the extracts were compared with the values from the solvent standard solution to evaluate the apparent recoveries. Five deuterated or ^{13}C-labeled instrumental internal standards (4 for LC-MS and 1 for GC-MS) were spiked in each sample at a constant concentration at the end sample preparation to evaluate instrument performance during data collection (Table S1). A pooled quality control sample (QC, mixing 10 μL of each sample including five procedure blanks and three field blanks) was re-injected every 10 field samples across the LC-MS data acquisition, which was used in post-data processing and MF filtering. In GC-MS, an instrument performance check standard (Nonpolar Column Test Mix, Supelco) was injected every 10 samples to evaluate peak shape, mass accuracy, sensitivity variation and retention time shift throughout the sequence.

2.6. Non-targeted screening by LC-MS

Non-targeted screening of MS-full scan data was performed using Agilent MassHunter Profinder B.10.00. MFs were extracted for a batch of files including procedural blanks, field blanks and pooled QC sample by the "Batch recursive feature extraction". The sequential filtration of initial molecular features based on criteria in the order of (I) detection frequency and relative standard deviation of features in five pooled QC data, (II) method detection limit (mean plus 3 times of standard deviation) calculated using blanks, and (III) peak area and peak height thresholds (Details in Text S3 (SI)). Principal components analysis (PCA) and clustering were performed on the initial MFs to check the grouping of the dataset using Mass Profiler Professional 15.1 (MPP, Agilent Technologies). The MS/MS spectra were subjected for comparison with either MS/MS special mass spectra in Agilent personal compound database and libraries (*PCDL*) (pesticide *PCDL*, water screening *PCDL* and extractable & leachable *PCDL*) and open-source library from mass bank or for structure prediction using SIRIUS (Dührkop et al., 2019), if the parent ions remained in the final molecular features (FMFs) lists. 20 MFs of interest with matched MS/MS spectra or with high matching score from SIRIUS were subjected to confirmation based on retention times and fragmentation pattern of authentic standards.

2.7. Non-targeted screening by GC-Q-TOF-MS

Agilent Mass Hunter Unknowns Analysis 10.0 was used for the GC-TOF-MS data processing. The SureMass MF detection was applied to peaks with intensity >10,000 and shape quality score >50. The extracted MFs were searched against the NIST 2020 mass spectral library and MFs with match factor >50 % were tentatively annotated. The identification of six MFs was confirmed with authentic standards, using retention times and fragmentation patterns.

2.8. Quantitative analysis

The 25 confirmed compounds were semi-quantified in the PAS extracts, in the case of the GC-MS using MassHunter Quantitative Analysis 10.0 (TOF version, Agilent Technologies). Quantified amounts (ng/sampler) were converted into volumetric air concentrations (ng/m^3) using a generic sampling rate of 0.6 m^3 day^{-1} over 82 deployment days (Table 1). (Wania et al., 2003; Li et al., 2023)

3. Results and discussion

3.1. Performance of sample extraction methods

LC-MS full scan analyses were conducted in both ion modes and included 56 injections (2 solvent standards, 45 field samples including field blanks, 5 procedural blanks, and 1 pooled QC sample injected 5 times). The five replicate injections of the pooled QC sample confirmed satisfactory instrument performance throughout the sequence (Table S2). The 4 instrumental internal standards and 13 out of 16 pre-spiked internal standards exhibited reproducible signal intensities (RSD within 3 %–11 %) and stable retention times (RT shifted within 0.02–0.10 min). The apparent recoveries of 13 out of 16 mass-labeled surrogates were from 30 to 110 % with median at 74 % (Table S2). More description of the extraction method's performance is given in Text S2 (SI). Overall, we find that the extraction method for the resin was effective for the majority of compounds, except for certain compound families, such as the bisphenols, which were not detectable in extracts. Since mass-labeled bisphenols' standards were detected in pure solvent but not detectable after spiking in extracted matrix at the same concentration, it indicated that the loss of bisphenol signals were due to strong matrix suppression (data not shown).

During the GC-Q-TOF-MS analysis, the mass error of 8 compounds in the GC instrument performance check standard was less than 2.51 ppm, and sensitivity variations were lower than 10 % (Table S3). Retention time variation of the 8 compounds was less than 0.006 min with no peak tailing observed throughout the sequence (Table S3). Recoveries of ^{13}C$_{12}$-labeled PCB congeners 52, 101, 118, 138, 153, and 180 were 79

Table 1
Compounds confirmed in passive air sampler extracts at identification level 1 by LC-MS and GC-MS. Semi-quantitative concentrations obtained using single standard solution and subtracting average value within procedural and field blanks. Detection frequency was counted for responses higher than maximum (mean + 3σ) value within procedural and field blanks. Rank in LC-MS is based on average peak area of 660 FMFs (ESI+) or 788 FMFs (ESI-) at 40 sites. For GC-MS, rank is based on average peak area of 329 FMFs at 38 sites.

Compound name	Usage type or source[a]	Formula	Quantifier *m/z*	RT (min)	Frequency (# site/40 or 38 sites)	Concentration range (ng/m^3) min-max (mean)	Site with highest conc.	Rank (avg peak area)	First report of occurrence in
LC-MS (ESI+)									
Triethylene glycol monobutyl ether	OIC	$C_{10}H_{22}O_4$	207.1592	4.95	40	0.19–8.3 (1.2)	44	86	outdoor air
Triethylene glycol monomethyl ether	OIC	$C_7H_{16}O_4$	165.1121	3.58	40	0.21–14 (2.0)	44	121	outdoor air
Triethylene glycol	Pls; OIC	$C_6H_{14}O_4$	151.0966	3.15	20	2.1–8.3 (3.0)	112	130	outdoor gas phase
Tetraethylene glycol	Pls; OIC	$C_8H_{18}O_5$	195.1231	3.35	1	11 (N/A)	113	48	outdoor gas phase
TBP	OPC	$C_{12}H_{27}O_4P$	267.1725	6.17	8	7.0–12 (8.7)	44	98	
DEHP	Pls	$C_{24}H_{38}O_4$	391.2849	8	22	28-1120 (158)	47	11	
BBP	Pls	$C_{19}H_{20}O_4$	313.1441	6.12	2	88-113 (100)	106	328	
Diethylene glycol dibenzoate	Pls; OIC	$C_{18}H_{18}O_5$	315.1253	5.91	3	447-548 (507)	107-r	286	outdoor gas phase
Quinoline n-oxide	OIC	C_9H_7NO	146.0601	3.87	35	0.48–6.1 (1.6)	108	403	outdoor air
DEET	OIC	$C_{12}H_{17}NO$	192.1385	5.44	28	0.58–6.7 (1.4)	112	39	
Caprolactam	OIC	$C_6H_{11}NO$	114.0916	3.9	4	18-34 (24)	47	20	outdoor gas phase
N-octyl pyrrolidone	OIC	$C_{12}H_{23}NO$	198.1858	6.05	3	2.1–5.4 (4.0)	11	457	outdoor air
2-phenyl acetamide	OIC,Nat	C_8H_9NO	136.0757	4.22	11	8.0–17 (11)	50	143	outdoor air
LC-MS (ESI-)									
4-Nitrophenol	BrC P OIC	$C_6H_5NO_3$	138.0196	4.8	39	4.4–26 (13)	11	4	outdoor gas phase
2,4-Dinitrophenol	BrC; P; OIC	$C_6H_4N_2O_5$	183.0046	4.15	6	0.25–0.54 (0.40)	14	596	outdoor gas phase
Nonanoic acid	P; Nat	$C_9H_{18}O_2$	157.1233	5.47	13	16-35 (22.71)	44	14	outdoor gas phase
4-Hydroxy-acetophenone	Nat	$C_8H_8O_2$	135.0452	4.4	39	2.4–22 (9.6)	44	28	outdoor air
Phenylacrylic acid	Nat	$C_9H_8O_2$	147.0451	4.05	8	250-314 (280)	50	17	outdoor gas phase
Pinonic acid	Nat	$C_{10}H_{16}O_3$	183.1034	3.63	40	6.9–416 (58)	110	27	outdoor gas phase
Citric acid	Nat	$C_6H_8O_7$	191.0204	1.37	2	225-276 (250)	105	158	outdoor air
GC-MS									
Triphenylphosphine oxide (TPPO)	OPC	$C_{18}H_{15}OP$	227.0773	18.78	36	0.10–0.29 (0.18)	103	328	outdoor gas phase
Triethyl phosphate	OPC	$C_6H_{15}O_4P$	98.9842	8.60	31	1.0–8.4 (2.2)	44	316	
Bromoform	OHC	$CHBr_3$	172.8417	2.39	32	0.69–3.9 (2.1)	4	208	
Hexachloroethane	OHC	C_2Cl_6	200.8404	6.81	37	0.25–1.0 (0.52)	44	288	outdoor air
Hexachlorobutadiene	OHC	C_4Cl_6	224.8405	9.52	37	0.70–4.0 (1.9)	44	258	
DEET	OIC	$C_{12}H_{17}NO$	191.131	13.0	29	0.50–3.0 (1.1)	112	189	

b: "outdoor air" indicates no previous report of detection in either atmospheric gas or particle phases. "outdoor gaseous phase" indicates only previous reported in the outdoor particle phase.

[a] BrC = brown carbon; P = pesticides; Pls = plasticizers; Nat = natural products; OIC = other industrial chemicals; OPC = organophosphorus compound; OHC = organohalogen compound.

%, 96 %, 112 %, 99 %, 104 % and 108 %, respectively, confirming effective extraction (Table S3).

3.2. Non-targeted analysis

3.2.1. Sequential data filtration and data grouping

Recursive MF extraction was performed in both ion modes for the LC-MS dataset consisting of field samples, all blanks and the pooled QC. The initial extraction obtained 7676 and 5612 MFs in ESI+ and ESI- modes, respectively. Principal component analysis (PCA) of the all MFs illustrated good grouping and separation among procedural blanks, field blanks, pooled QC and field samples, indicating satisfactory data quality (Fig. S1A and S1B). In both ion modes, the 5 procedural blanks were fully separated from the other three groups. Hierarchical clustering of FMF in procedural blanks, field blanks and pooled QCs (Fig. S2) also demonstrated satisfactory sample preparation and data acquisition. The peak areas of the all MFs in the two replicates from site 3 and 107 are highly correlated and aligned along 1:1 line (correlation coefficients 0.9838 ± 0.0036 for site 3 and 0.9734 ± 0.0034 for site 107 in both ion modes) (Fig. S3). In a dendrogram of all MFs, close proximity of data obtained in both ion modes for duplicate PASs deployed at sites 3 (Fig. S2) implied strong similarity and similar FMF distribution between replicates. Duplicate samples at site 107 were slightly separated on the clustering plot in both ion modes (Fig. S2). The initial MFs were filtered sequentially to retain key filtered MFs (FMFs) using three criteria: detection frequency and precision in pooled QC, method detection limits based on blanks, and peak area and height relevant to peak shape (More details in Text S4 and Table S4). The final list contained 660 and 788 MFs for ESI+ and ESI-, respectively. Within the FMFs, 211 and 153 MFs were detected with detection frequency≥ 50 % in ESI+ and ESI-, respectively (Table S4). 34 MFs in ESI+ and 24 MFs in ESI- were detected in all 40 sites (Table S4).

Among a total of 11,450 MFs extracted from all samples analyzed by GC-MS, 9386 had a peak intensity greater than the MDL in at least one of the samples, with the MDL defined by the mean plus three times the standard deviation of all blanks. 9126 MFs had intensities greater than 10^5 in at least one sample. Notably, 329 MFs were detected in over 50 % of the analyzed samples and 66 MFs detected in all samples. Figure S1

(E, F) show the PCA of all 11,450 MFs derived from the GC-MS data. Intensities of MFs below the MDL were replaced with MDL/ $\sqrt{2}$ for the PCA (Baccarelli et al., 2005). Similar to the LC-MS data, PCA of GC-MS data separated procedural and field blanks from exposed samples (PC1 in the PCA score plot, Fig. S1E).

3.2.2. Spatial distribution of MFs

The inspection of the PCA revealed a grouping of LC-MS data in ESI + based on the type of site (Fig. S1C, grouping into residential site or park area indicated using confidence ellipse). In ESI- mode, the public park sites were more spread out compared to the more tightly clustered residential sites (Fig. S1D). Hierarchical clustering of MFs in ESI + data showed nested groupings with separation of many residential sites from public parks (Fig. S2A); while in ESI- data, higher ranking clusters merged with lower clusters from both site types, indicating a low degree of separation (Fig. S2B).

In the score plot of the PCA performed on the GC-MS data, PC2 differentiated sites in residential areas and parks (Fig. S1E and S1F). MFs contributing the most to this separation include C_9H_{20} (ID#870 and ID#872) and C_9H_{18} (ID#853). There are 1141 and 398 possible structures associated with these MFs but based on the annotations and locations with elevated concentrations, they are likely lube oil and auto fluids additives. (https://pubchem.ncbi.nlm.nih.gov/compound/31285#section=Use-and-Manufacturing; https://pubchem.ncbi.nlm.nih.gov/compound/8141#section = Use-and-Manufacturing.) The MFs located on the right of the loading plot have little presence in blanks and do not contribute to separating residential areas and parks in the PCA, meaning they do not have much of a spatial trend. Typical MFs in this region are ID#144, 451 and 808, tentatively identified as undecane (or other isomers), tris(trimethylsilyl)-hydroxymandelic acid and methyl salicylate. Undecane is a biogenic VOC and also widely used in personal care products, (https://pubchem.ncbi.nlm.nih.gov/compound/Undecane#section = Use-and-Manufacturing.) while methyl salicylate (Le Grand et al., 2005) has natural sources such as coniferous plants

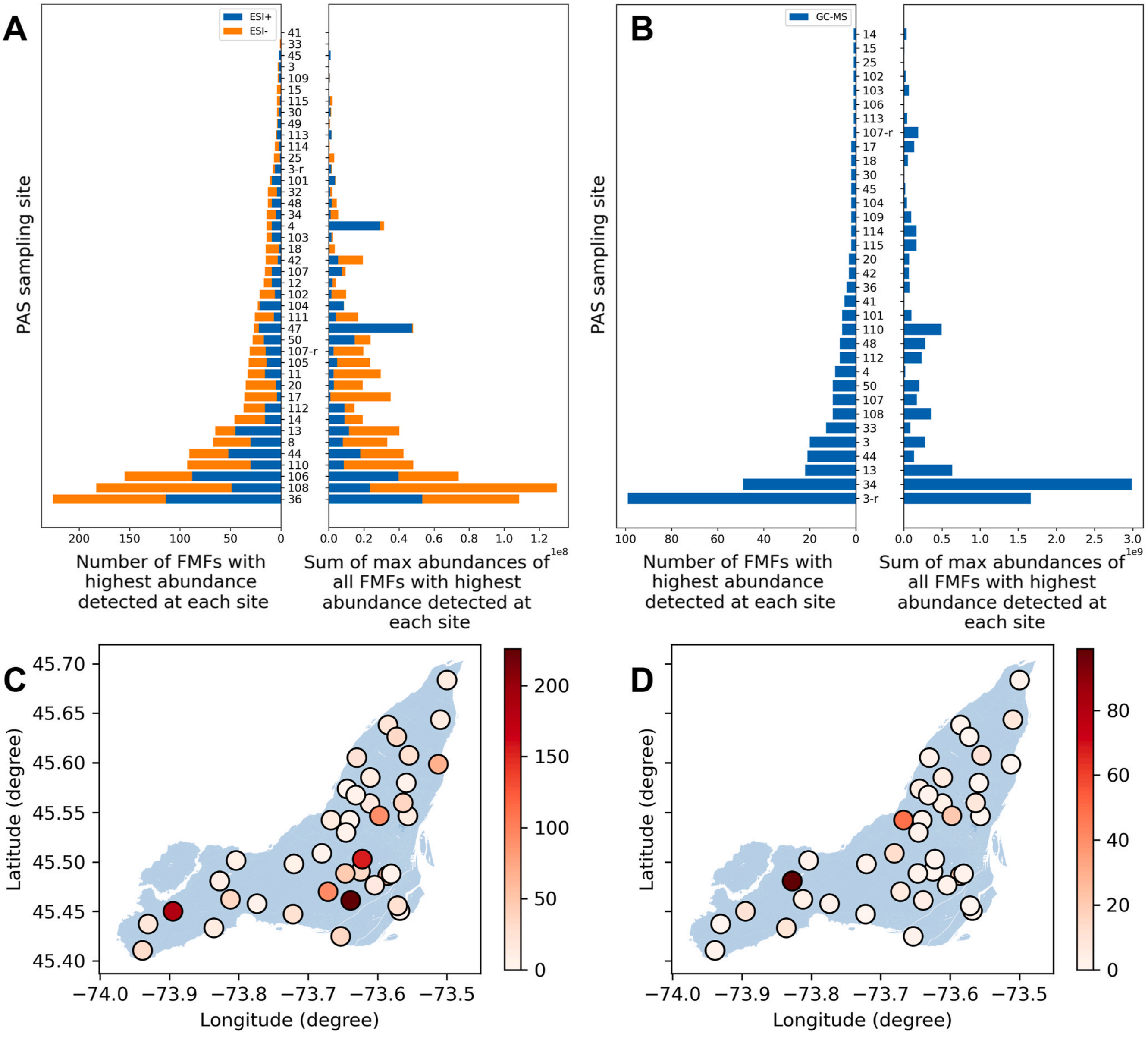

Fig. 2. Occurrence distribution (left) and cumulative distribution (right) of the highest abundances of all filtered molecular features (FMFs) across all the sampling sites: Panel A for the FMFs detected by LC-MS (662 FMFs in ESI+ in blue and 788 FMFs in ESI- in orange); Panel B for the 329 FMFs detected by GC-MS. In panel A and B, the sampling sites were arranged by increasing occurrence number of the highest abundances of FMFs detected at a site. Map of occurrence frequency for the highest abundances of Filtered MFs in LC-MS data (C) and GC-MS (D): color bar corresponded to the number of FMFs with highest abundance detected at each site.

and is also used in household cleaning products. (https://pubchem.ncbi.nlm.nih.gov/compound/Methyl-Salicylate#section = Use-and-Manufacturing.) Multiple sources of both natural and anthropogenic origin likely contribute to the absence of a clear spatial pattern. MFs located in the lower right of the loading plot (including ID#682 ($C_6H_{10}O$), #1486 ($C_{11}H_{24}O$), and #1914 ($C_8H_{16}O$)) are abundant in parks but not at residential sites. These MFs are likely oxidation products of biogenic emissions. For example, $C_6H_{10}O$ is likely an oxidation product of cyclohexene, a proxy for biogenic monoterpenes in secondary organic aerosol studies (Räty et al., 2021).

The number of FMFs detected in an extract and the sum of their abundance can be interpreted as the overall 'chemical load' accumulated in a PAS. When comparing both these metrics for the 660 (ESI+) and 788 (ESI-) LC-MS FMFs between different sites (Fig. 2A), we find that the highest response of each FMF were frequently detected at sites 36, 106, 110, 44 or 108 in both ion modes, while none of the highest response of each FMF was observed at sites 41 or 15 (both ESI+ and ESI-), or 33 (ESI+). Interestingly, when the same two metrics were calculated for the 329 GC-MS FMFs (Fig. 2B), the sites with the highest response (sites 3, 34, 13, 44, 33) were different from those identified by LC-MS (Fig. 2A). Sites 41 and 33 with the least number of the most abundant FMFs in the LC-MS data showed a high detection frequency for the most abundant FMFs in the GC-MS data. Site 15 showed a low number of the most abundant FMFs in both LC-MS and GC-MS. These results highlight the complementarity of LC-MS and GC-MS analyses.

The present observations support that PASs can record spatial patterns in the collected chemical mixtures. The outdoor air contains chemical mixtures influenced by long-range atmospheric transport, local sources and possible sources specific to the deployment sites (vegetation, traffic etc.) (Wania and Shunthirasingham, 2020; Zaller et al., 2022; Qu et al., 2019; Zhao et al., 2023; Zhan et al., 2024). For example, the abundance of pesticides in ambient air has been demonstrated to be strongly related to the surrounding agricultural use (Zaller et al., 2022; Zhao et al., 2023) and pesticides found in National Parks (eastern Austria) surrounded mainly by forest and grassland indicated the possibility of the long range transport of volatile pesticides (Zaller et al., 2022). Zhan et al., relying on the same PAS as was used here, identified a small number of commonly occurring spatial patterns of organic contaminants in outdoor air, indicative of similar sources and atmospheric dispersion behavior (Zhan et al., 2024). These include patterns dominated by point sources (associated with industrial facilities and activities, sewage treatment plant, etc.), and patterns correlated with population density or proximity to large water bodies. Melymuk et al. identified potential sources of urban air pollutants by combining PAS data with land use regression analysis (Melymuk et al., 2013). Others have correlated PAS-derived concentrations with spatially resolved data on population density (Westgate et al., 2010; McDonough et al., 2014). Further investigations should be conducted to explore spatial patterns in the data from the current study.

3.2.3. Compound identification

For FMFs in LC-MS, after cross-checking spectra obtained from targeted MS/MS and iterative auto MS/MS via fragmentation comparison in *PCDL* as well as in mass bank and structure prediction using SIRIUS (Dührkop et al., 2019), several MFs with high matching score were selected for identity confirmation. By comparing retention time and fragmentation pattern with analytical standards, twenty tentatively identified MFs were confirmed at identification level 1 (Schymanski et al., 2014), including nitrophenols, pesticides/repellents, plasticizers, other industrial chemicals as well as natural products (Table 1, Fig. S4). Similarly, the identity of six MFs from the GC-MS analysis was confirmed by matching retention times and fragments in the mass spectra using analytical standards available in house (Table 1, Fig. S5). Specific groups of identified compounds that share specific use types and/or a particular spatial distribution (Figs. 3 and 4) are discussed below.

Nitrophenols. The major nitroaromatic substance detected in the outdoor gas phase was 4-nitrophenol (4-NP, present in 39 out of 40 sites, Fig. 3) with concentrations ranging from 4.4 to 26 ng/m^3 4-NP ranked 4th in terms of mean peak area across the 40 sites out of the 788 FMF (ESI-). 2,4-dinitrophenol (DNP) was also detected at 6 sites at relatively lower concentration (0.25–0.54 ng/m^3). The highest levels of 4-NP and DNP were detected at sites 11 and 14, respectively, both located in residential areas near the same highway. Nitrated phenols have been previously identified as major components of brown carbon in atmospheric particles on account of their relatively high concentrations (especially in urban area). 4-NP is one of the most abundant nitrated phenols in the atmosphere (Laskin et al., 2015; Tchieno and Tonle, 2018; Liang et al., 2020). They also find application in the production of pesticides, synthetic dyes, drugs and leathers. Primary sources for nitrated phenols in the atmosphere include anthropogenic emissions from vehicle exhaust, wood and biomass combustion, as well as decomposition and hydrolysis of pesticides (Zhang et al., 2010; Papazian et al., 2023; Laskin et al., 2015; Tchieno and Tonle, 2018). Amarandei et al. reported that wood and biomass burning is the major source of nitrophenols during wintertime, while traffic emissions and secondary formation is dominant during warmer periods (Tchieno and Tonle, 2018). The reported measured concentration of 4-NP in fine particle matters in outdoor air from various sites around the world range from <1 ng/m^3 to >70 ng/m^3 with seasonal variations, while DNP was detected at lower concentrations of up to 6 ng/m^3 (Pereira et al., 2021; Liang et al., 2020; Amarandei et al., 2023; Gu et al., 2022). Toxic nitrated phenols can harm plant growth and reduce crop output and have been associated with potential chronic adverse effects in humans (Tchieno and Tonle, 2018; Liang et al., 2020; Gu et al., 2022). While Papazian et al. tentatively identified several nitrophenols in indoor PAS extracts (Papazian et al., 2023), and Zachary et al. detected nitrophenol by the formula of $C_6H_5NO_3$ in wildfire plume using TOF chemical ionization MS (CIMS) without differentiating its isomer structure (Decker et al., 2021), we reported here to our knowledge the first direct identification of 4-NP and DNP in the outdoor ambient gas phase.

Herbicide/Insect Repellent. Nonanoic acid was detected at 13 out of 40 sites (16–35 ng/m^3, mean of 23 ng/m^3), mainly in the eastern and northern parts of the Island of Montreal. A naturally occurring medium chain fatty acid, nonanoic acid has also been used as an herbicide both as a stand-alone active constituent or in combination with other active components such as glyphosate (Wehtje et al., 2009). Based on a report of the European Food Safety Authority, nonanoic acid does not meet the criteria for endocrine disruption for humans and non-target organisms, while exposure to nonanoic acid leads to high acute oral and contact risk and/or chronic risk to honeybees (Alvarez et al., 2021). Nonanoic acid is also present in aerosols and has been reported as one of the most abundant fatty acids released from the exhaust of catalyst-equipped cars (Rogge et al., 1993). Aerosol concentrations of nonanoic acid (10–140 ng/m^3) and other fatty acids have been shown to increase significantly during a severe photochemical smog episode in Los Angeles, possibly arising from direct emissions from anthropogenic activities and formation by photochemical reaction of precursor compounds (Nolte et al., 1999). DEET was detected by both LC-MS and GC-MS with the abundance correlated between LC and GC data ($R^2 = 0.704$) across all sampling sites (40 in LC-MS and 38 in GC-MS, Fig. S6). According to the filtering criteria of abundance higher than the maximum MDL from procedural and field blanks, detection frequency of DEET was 28 out of 40 sites via LC-MS and 29 out of 38 sites from GC-MS, with 22 common sampling sites. Level of DEET ranged from 0.6 to 6.7 ng/m^3 (mean of 1.3 ng/m^3) and from 0.5 to 3.0 ng/m^3 (mean of 1.1 ng/m^3) based on LC-MS and GCM-MS semi-quantification, respectively. DEET is the most commonly used active ingredient in many insect repellent products. DEET is commonly detected in aquatic samples, such as drinking water, surface water, groundwater, wastewater, etc. (Kuch and Ballschmiter, 2001; Marques dos Santos et al., 2019; Arlos et al., 2023; Aronson et al., 2011), while reports of DEET in the atmosphere are scarce (Zaller et al., 2023; Ramírez et al., 2010; Balducci et al., 2012; Wang et al., 2022).

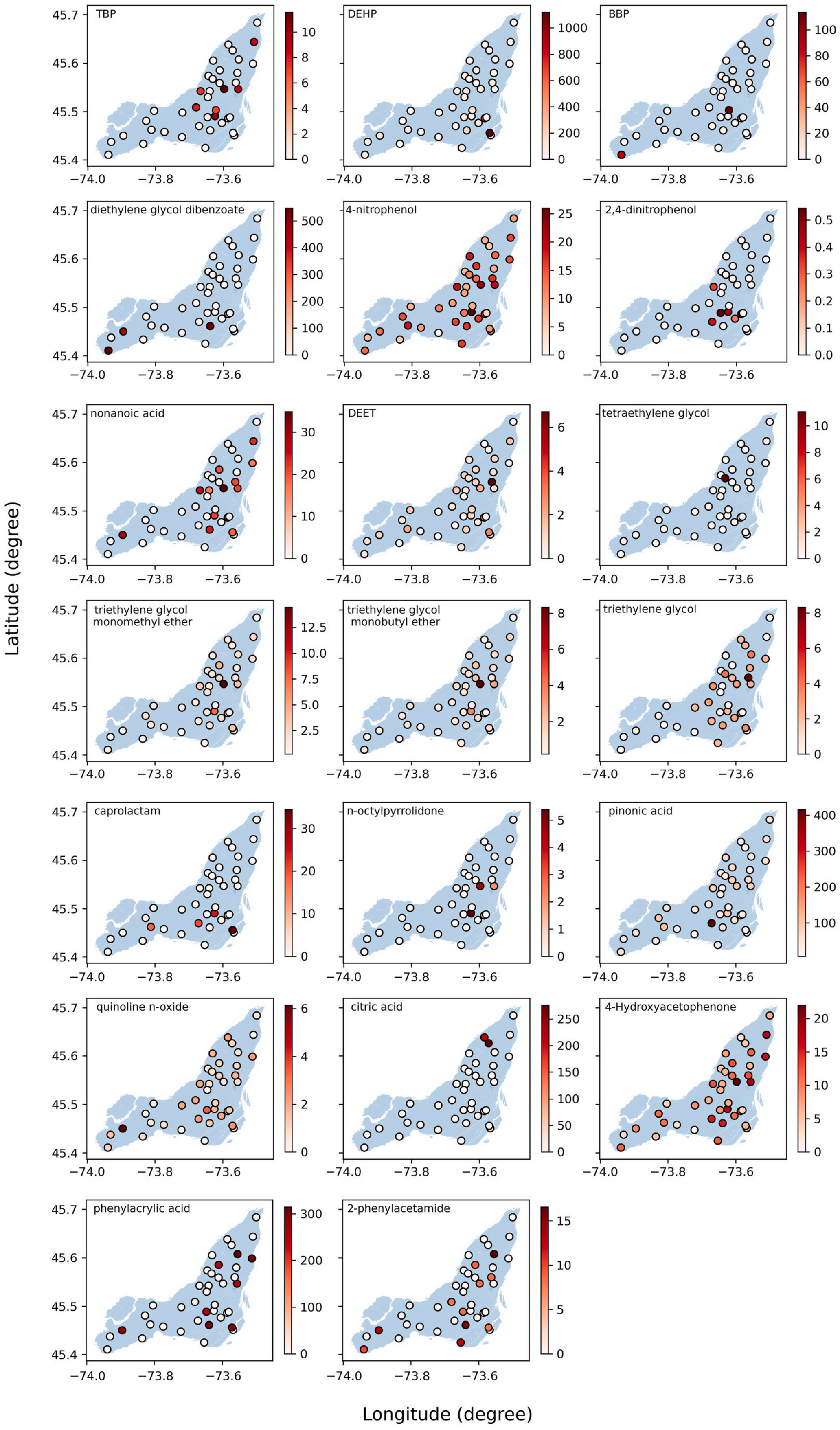

Fig. 3. Spatial variability of the atmospheric gas phase concentrations of 20 compounds confirmed by LC-MS across the Island of Montreal. In each subplot, color bar indicated concentration (ng/m^3) across the 40 sites (LC-MS).

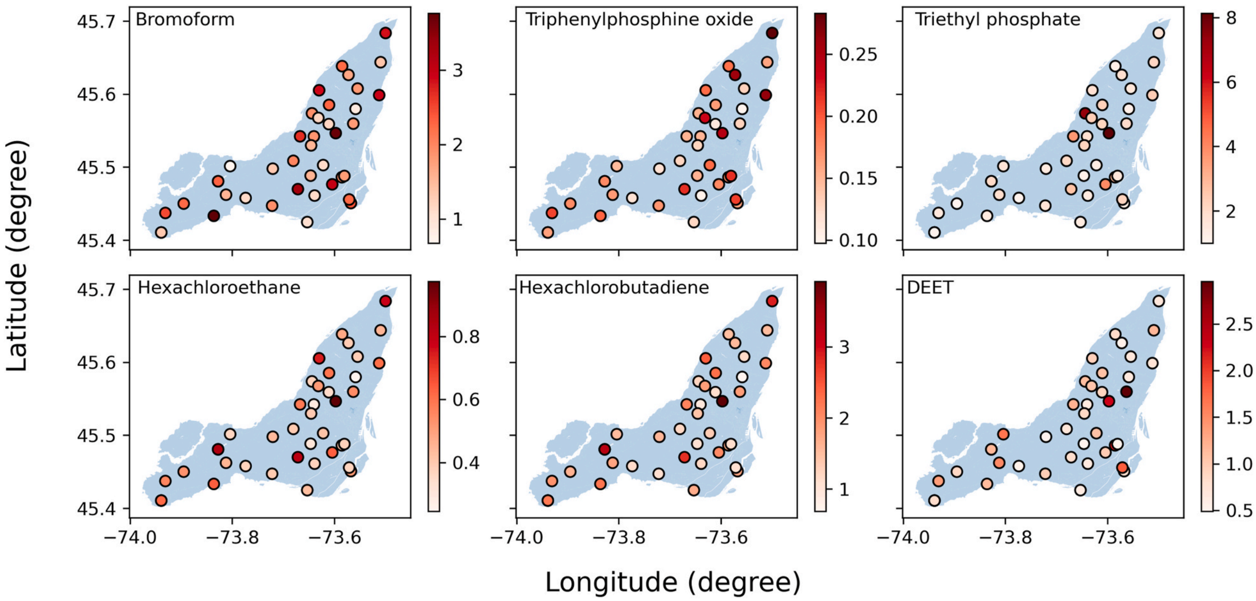

Fig. 4. Spatial variability of the atmospheric gas phase concentrations of 6 compounds confirmed by GC-MS across the Island of Montreal. In each subplot, color bar indicated concentration (ng/m^3) across 38 sites (GC-MS).

DEET levels ranged from 2.8 to 19 ng/m^3 in ambient fine particles collected in North China (Wang et al., 2022), Zaller et al. detected DEET at 4 of 15 sampling sites in eastern Austria (Zaller et al., 2023). DEET has also been detected in indoor air collected using polydimethylsiloxane foam disks (Papazian et al., 2023).

Plasticizers. The presence of three plasticizers was confirmed in the air samples via LC-MS, including the two phthalate esters (PAEs) di(2-ethylhexyl)phthalate (DEHP) and benzyl butyl phthalate (BBP), and the carboxylic ester (CAE) diethylene glycol dibenzoate. DEHP had the highest concentration (range of 29–1100 ng/m^3) and highest detection frequency (22/40 sites). The two sites (47 and 13) with highest DEHP abundance were both in the southeast of Montreal Island (Fig. 3). BBP (88–114 ng/m^3) and diethylene glycol dibenzoate (450–550 ng/m^3) were detected only at 2 (both in public parks) and 3 (two in public park and one in residential area) sampling sites, respectively; and these sites were located in similar regions in the southeast and west of Montreal Island (Fig. 3). PAEs, widely used as plasticizers, are ubiquitous in various environmental media (water, soil, organisms, indoor and outdoor air). One study reported concentration of DEHP in residential outdoor air during winter in Ottawa, Canada, ranging between 20 and 61 ng/m^3 (Feng et al., 2023). DEHP has been recently recognized as one of the dominant PAE in both outdoor particle and gas phase in multiple cities in China, with possible major source including industrial emission, building construction, tire-road wear microplastics emission etc. (Gao et al., 2024; Lu et al., 2023; Liu et al., 2023; Ma et al., 2014) Lu et al. also detected BBP in outdoor air in Hangzhou, China (Lu et al., 2023). Diethylene glycol dibenzoate has been recently detected in ambient PM$_{2.5}$ (Gao et al., 2024), while no study has reported its detection in the gas phase. PAEs and other plasticizers are classified as environmental endocrine disrupting chemicals, with some (e.g. DEHP) also being classified as possible human carcinogens (National Toxicology Program, 2021), suggesting that they have the potential to disrupt the endocrine system and elevate the carcinogenic risk of exposed organisms (Gao et al., 2024; Liu et al., 2023; Zhu et al., 2023).

Organohalogen Compounds. Bromoform was detected at 32/38 sites by GC-MS (0.68–3.9 ng/m^3). As a naturally occurring organohalogen compound in the atmosphere (Mehlmann et al., 2020), primarily produced by marine algae, it is also a major by-product of the chlorination of cooling water in coastal power plants (Kuyper et al., 2012; Maas et al., 2021). The main route of human exposure to bromoform is from drinking water that has been disinfected with chlorine, bromine or bromine compounds (Agency for Toxic Substances and Disease Registry (ATSDR), 1990). EPA considers it to be a probable human carcinogen (EPA's Group B2), and estimated an inhalation unit risk (1.1 × 10^{-6} per μg/m^3) for the probability of a person developing cancer from breathing air containing bromoform (U.S. Environmental Protection Agency, 1999).

Hexachloroethane (detected at 37/38 sites by GC-MS, Table 1) was reported to be used in Canada as a chemical intermediate, as a flux agent for grain refining and degassing of aluminum alloys, and as a flame retardant in industrial laminating resins (Environment and Climate Change Canada and Health Canada, 2016). Hexachloroethane may be a constituent of lubricating greases and oils, non-structural caulking compounds and sealants, automotive chemicals, laundry and ironing aids and dry cleaning agents, and could also be produced during the chlorination of water and sewage, all of which could be a pathway to atmosphere (Environment and Climate Change Canada and Health Canada, 2016). No previous study has reported the detection of hexachloroethane in ambient air.

Hexachlorobutadiene (HCBD) has no natural source and is mainly generated as a by-product in the manufacturing of chlorinated hydrocarbons. The Global Atmospheric Passive Sampling network reported steadily and rapidly increasing concentrations of HCBD globally between 2009 and 2016 (Shunthirasingham et al., 2024). HCBD has been listed in the Stockholm Convention since 2015 due to its persistence, toxicity, and potential for bioaccumulation and long-range transport (The Persistent Organic Pollutants Review Committee, 2011). It is no longer commercially produced and imported into Canada. Zhan et al. recently reported uniform concentrations of HCBD in the Canadian atmosphere (Zhan et al., 2024). In the current study, the almost ubiquitous detection of HCBD in the PASs (detected in 37/38 sites by GC-MS, Table 1) at concentrations (0.25–1.0 ng/m^3, mean of 1.9 ng/m^3) comparable to those reported by Zhan et al. (2024) suggest long range transport as a source, although we cannot exclude the possibility of unintentional release from chemical production processes using chlorine (Yang et al., 2023).

Organophosphorus Compounds. Triphenylphosphine oxide (TPPO) was detected in 36 out 38 PAS sites in the GC-MS extracts with concentration ranging from 0.1 to 0.3 ng/m^3 (Table 1). TPPO has been recently reported as one of the dominant organophosphorus compounds in $PM_{2.5}$ from Thessaloniki, Greece, with concentrations ranging from 0.09 to 1.9 ng/m^3 (Pantelaki and Voutsa, 2024). TPPO was also present in road dust from Dalian, China with mean concentration of 435 ± 106 ng/g (Zhang et al., 2020b). TPPO is extensively used as an intermediate when producing pharmaceuticals, and as ligand for transition metals (Zhang et al., 2020b). TPPO could possibly also originate from the oxidation of triphenylphosphine, which is used as heat stabilizer, light stabilizer, antioxidant, flame retardant and rubber antiozonant. Numerous such uses can be found in urban area and become a source of triphenylphosphine.

Tributyl phosphate (TBP) was detected at 8 out of 40 sites (7.0–12 ng/m^3) in LC-MS extracts, while triethyl phosphate (TEP) was detected at 31 out 38 sites (1.0–8.3 ng/m^3) in GC-MS extracts. Organophosphorus ester, used as plasticizer for resins, plastics, and as flame retardant, are commonly detected in urban air (Rodgers et al., 2023). TBP has been previously detected in the outdoor gas phase globally, including several locations in Canada (urban Greater Toronto Area, Montreal landfill area, St. Lawrence estuary, and Southern Salish Sea region) (Saini et al., 2019; Kerric et al., 2021; Li et al., 2025a, 2025b). In contrast to Li et al., who observed elevated levels in the proximity of airports (Li et al., 2025a), TBP was not detected in PAS deployed at sites close to Montreal Pierre Elliott Trudeau Airport (site 109 and 110, Fig. 3). Pantelaki et al. detected TEP in $PM_{2.5}$ from Thessaloniki, Greece with concentration ranging from 4.6 to 280 ng/m^3 (Pantelaki and Voutsa, 2024). TEP has also been reported in PASs in Toronto, Canada, with concentration between 11 and 1020 pg/m^3 (Saini et al., 2019).

Other Industrial Chemicals. Other identified industrial chemicals include four synthetic ethylene glycol oligomers (EGs) and their ethers (EGEs). Triethylene glycol monomethyl ether (0.2–14.4 ng/m^3) and triethylene glycol monobutyl ether (0.2–8.3 ng/m^3) were detected at all 40 deployment sites, both with the highest abundance at site 44 (Fig. 3, Table 1). The concentration of these two EGEs showed a strong correlation (correlation coefficient 0.9621) across the 40 sites, indicating that they originate from the same source. Triethylene glycol (2.1–8.3 ng/m^3) was detected at 20 out of 40 sites, with highest abundance at site 112. Tetraethylene glycol (11 ng/m^3) was only detected at site 113. Notably, the highest concentrations of the four ethylene glycols were recorded at three sites in close proximity (44, 112, 113). EGs and EGEs are commonly used as plasticizers for the manufacturing of polymer fibers, as antifreeze agent in the coolant of automobile and air-conditioning systems, and as additives in hydraulic fluids, brake fluids, cleaning and sanitizer products, personal care products, inks, paints, *etc.* (Fruijtier-Polloth, 2005) Although they are widely present in daily life, few studies investigated human exposure to EGs and EGEs. Papazian et al. tentatively (level 2) identified triethylene glycol in indoor PAS extracts (Papazian et al., 2023). Alves et al. reported detection of triethylene glycol and tetraethylene glycol in $PM_{2.5}$ and indicated both industry and traffic as possible sources (Alves et al., 2023). Recent detection of larger polyethylene glycols and their ethers (number of carbon $\geq$18, low volatility) in children's urine indicates the potential for absorption and accumulation of this type of compound by human (Tkalec et al., 2022).

Two cyclic nitrogen-containing organics, caprolactam and n-octylpyrrolidone, were detected at 3–4 sites in central Montreal, with concentration in the range of 18–35 ng/m^3 and 2.1–5.4 ng/m^3, respectively. Caprolactam is mainly used in the production of synthetic fibers (e.g. Nylon 6). Other applications include its use in brush bristles, textile stiffeners, film coatings, synthetic leather, plasticizers, plastics, paint vehicles, cross-linkers for polyurethanes and in the synthesis of lysine (U.S. Department of Health and Human Services, 1993; U.S. Environmental Protection Agency, 1988). Caprolactam has been detected in $PM_{2.5}$ (0.13–70 ng/m^3) in the Lower Fraser Valley, Canada (Cheng et al., 2006), and as one of the two most abundant cyclic nitrogen-containing organics in $PM_{2.5}$ on the North China Plain (23–212 ng/m^3) (Wang et al., 2022). Exposure to caprolactam has been reported to cause both acute and chronic effects on the respiratory system, as well as eye and skin irritation in both animals and humans (U.S. Environmental Protection Agency, 1988; International Agency for Research on Cancer (IARC), 1979). N-octylpyrrolidone is used as a solvent or an intermediate in the manufacturing of agrochemicals, ink, and coating formulations as well as a coating stripper in the electronics industry. Its presence in the atmosphere has not previously been reported.

2-phenyl acetamide, which is widely used in the production of agricultural chemicals, dyes, medicines and perfumes, as well as a plasticizers for plastics and resins was detected at 11 out of 40 sites (8.0–17 ng/m^3). Quinoline n-oxide, a metabolite of quinolone in humans (Reign et al., 1996), was detected at 35 out of the 40 sites (0.5–6.1 ng/m^3), with no prior reports of its presence in atmospheric samples.

Natural Products. Beside nonanoic acid, which is both a naturally occurring compound and an herbicide, four other naturally occurring chemicals were identified by LC-MS in negative ion mode. Pinonic acid (6.9–416 ng/m^3) and 4′-hydroxyacetophenone (2.4–22 ng/m^3) were among the most frequently detected (40 and 39 out of 40 sites, respectively) and most abundant (ranked as the top 27 and 28, respectively) of the 780 FMFs in ESI^-. Pinonic acid is the major oxidation product of the biogenic monoterpene α-/β-pinene (Jo et al., 2023) and a marker of biogenically sourced secondary organic aerosol (Pereira et al., 2021; Zhang et al., 2010; Amarandei et al., 2023; Cheng et al., 2004). Possible anthropogenic source of α-/β-pinene include its use as a fragrance component, as well as emissions from building materials, agricultural burning and traffic (Jo et al., 2023). 4′-hydroxy-acetophenone, which is a phenolic antioxidant metabolite common in plants and fungi, has not been reported in the outdoor gas phase before. It was reported at low concentration in secondary aerosol formed from the photo-oxidation of *m*-ethyltoluene, and *p*-ethyltoluene within an outdoor smog chamber (Forstner et al., 1997). Cinnamic acid, also called phenylacrylic acid and naturally occurring in fruits and vegetables, ranked 17th among the most abundant FMF in ESI^-, with an estimated concentration of 250–314 ng/m^3. Similarly to pinonic acid, it is a marker for biomass combustion, and has been reported in $PM_{2.5}$ at concentration up to 30 ng/m^3 near a large industrial complex in Portugal (Alves et al., 2023). Citric acid (both a naturally occurring compound and an industrial chemical) was detected in two neighboring parks in northern Montreal (225 ng/m^3 at site 102; 276 ng/m^3 at site 105).

4. Conclusions

In contrast to earlier studies on the outdoor atmosphere which mainly focused on particles, the current study used an NTA approach combining LC-MS and GC-MS for the first comprehensive characterization of the varied organic chemical mixture in the urban outdoor gas phase. The confirmation of multiple compounds, including previously unreported ones, adds to the understanding of the complex composition of the atmosphere, and highlights the need for further monitoring of potentially hazardous contaminants in urban air. Statistical analyses separated samples deployed in residential areas and in parks, indicating the impact of anthropogenic activities on spatial distribution. Notably, a small group of sampling sites showed a high detection frequency of the molecular features with the highest abundance. Because these sites were different between LC-MS and GC-MS, non-polar vapors, preferentially detected by GC-MS, may display a different spatial pattern in the urban atmosphere, and therefore have different sources, from the more polar vapors that are more likely to be detected by LC-MS. Further spatial analysis that integrates detailed data on land use is required to fully explore the relationship between chemical distribution pattern and their potential source/origin. Additional PAS sampling during different seasons and over different deployment times may yield information on the temporal pattern of the MFs of interest, as well as on short-lived compounds. Complementary toxicity analyses could aid in evaluating impacts, specifically facilitate an assessment of the risk to human health associated with exposure to airborne chemical mixtures.

CRediT authorship contribution statement

Lan Liu: Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Data curation, Conceptualization. **Antoine P. Gillet:** Writing – review & editing, Methodology, Investigation, Conceptualization. **Caren Akiki:** Methodology, Investigation, Formal analysis, Conceptualization. **Lei Tian:** Writing – review & editing, Methodology, Formal analysis, Conceptualization. **Yue Ma:** Formal analysis, Data curation. **Xianming Zhang:** Writing – review & editing, Supervision, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **David T. Bowman:** Writing – review & editing, Methodology, Formal analysis, Data curation. **Frank Wania:** Writing – review & editing, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Géraldine Delbès:** Writing – review & editing, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Philippe Apparicio:** Writing – review & editing, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Stéphane Bayen:** Writing – review & editing, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Data curation, Conceptualization.

Declaration of competing interest

The authors report no conflict of interest for the following manuscript submitted for your review (Original Article).

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Appendix A. Supplementary data

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Data availability

Data will be made available on request.

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