Full length article

Non-targeted analysis of unknown volatile chemicals in medical masks

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ABSTRACT

This paper reports the non-targeted analysis of unknown volatile chemicals in medical masks through headspace gas chromatography-Orbitrap high-resolution mass spectrometry. In view of the difficulties that may be encountered in the qualitative analysis of unknown substances, several typical cases and the corresponding reliable solutions are given from the perspective of comprehensive score and retention index, chemical ionization identification molecular formula, fragment ion detail comparison for distinguishing isomers, and identification of alkanes. With this method, 69 volatile substances were identified in 60 masks. The identified substances were divided into nine categories. Alkanes, esters, benzenes, and alcohols were the top four groups of substances identified in masks and accounted for 34.8%, 15.9%, 10.1%, and 7.2% of the total substances, respectively. In addition, ketones, ethers, phenolics, amides, and other substances were identified. Ethanol, 1,4-dichlorobenzene, toluene, *m*-xylene, dimethyl glutarate, and N,N-dimethylacetamide had high detection rates. The identified substances were further filtered and screened according to their detection rate, toxicity, and response intensity. Finally, 12 high-risk volatile chemicals in medical masks were listed. This study could serve as a reference for identifying unknown substances and a guide for monitoring volatile chemicals in masks and promoting chemical safety improvements in products.

1. Introduction

The Coronavirus Disease 2019 (COVID-19) is rampant worldwide and is intensely contagious among humans. Respiratory droplets and aerosols are the main routes of transmission (Jayaweera et al., 2020; Tang et al., 2020; Yang et al., 2020). As a simple but important personal protective equipment, medical masks are widely used to protect people from viral infections (Jayaweera et al., 2020; Tabatabaeizadeh, 2021). Medical masks can be divided into disposable medical masks, medical surgical masks, and medical protective masks (i.e., N95 masks), whose protection capacity gradually increases (Ma et al., 2020; Zuo et al., 2020). Medical masks are composed of a face mask and a tension band. The former is composed of three layers: an inner layer made of a skin-friendly material (ordinary sanitary gauze or non-woven fabric), a middle layer made of an isolation filter (ultra-fine polypropylene fiber melt-blown material), and an outer layer made of an antibacterial material (ultra-fine polypropylene fiber melt-blown material). The main regulations concerning medical masks include American Standard ASTM F2100 and Guidance for Industry and FDA Staff Surgical Masks-

Premarket Notification [510(K)] Submissions, European Standard EN14683-2019, Chinese YY 0469–2011 (medical surgical masks), and GB 19083–2010 (medical protective masks). However, a mandatory standard or regulatory document to limit the volatile chemicals (except for the disinfectant ethylene oxide) in masks is lacking. The European Safety Union issued a document on its official website that personal protective equipment such as protective masks must comply with the requirements of Registration, Evaluation, Authorization, and Restriction of Chemicals (REACH), which provides some guidelines for the chemical safety of masks.

Studies on masks mainly focused on their physical and biological indicators, including bacterial filtration efficiency, particle filtration efficiency, synthetic blood penetration resistance, and pressure difference (Ramirez et al., 2017, Zuo et al., 2020). Previous works tended to be on the use and protection of masks (Chen et al., 2012). Then, some researchers had paid attention to the application of new materials and new functions in masks (Catel-Ferreira et al., 2015). After the outbreak of COVID-19, researchers began to study the elimination, substitution, extended use, reuse, and disinfection of masks (Maal-Bared et al., 2020;
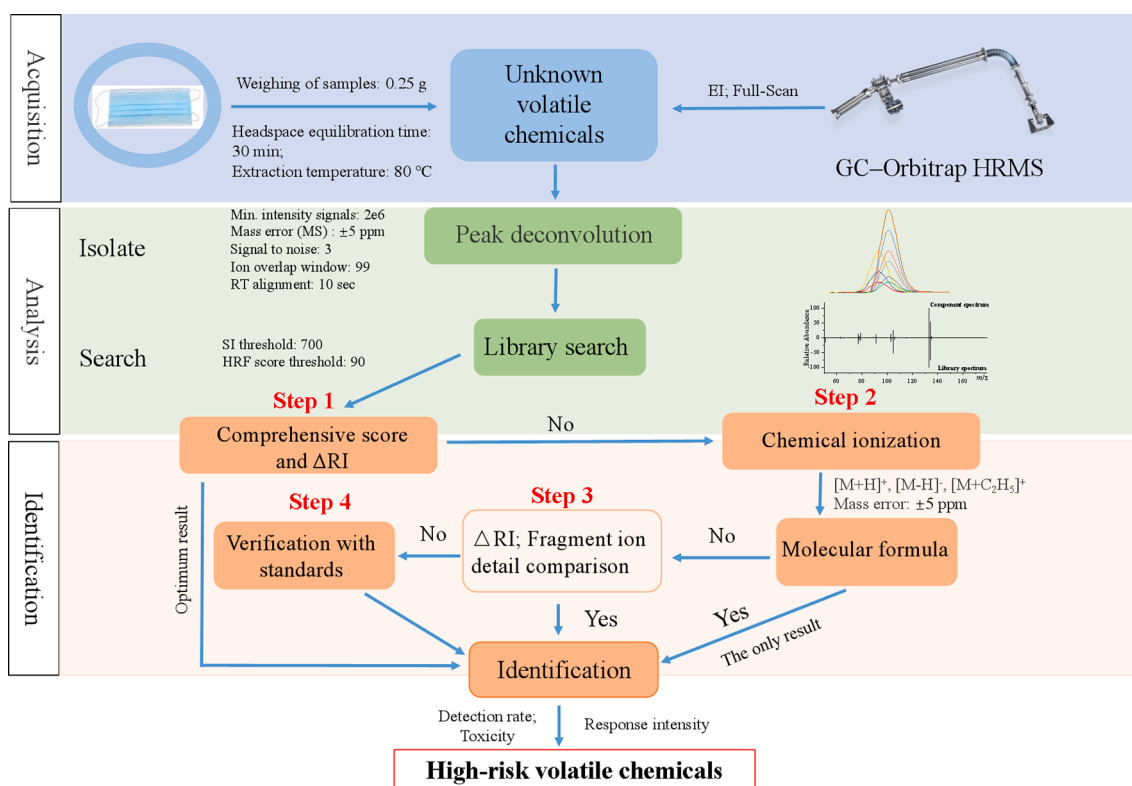
Fig. 1. Workflow of non-targeted analysis for volatile unknown substances in masks.

Zorko et al., 2020), as well as the microplastic inhalation risk posed by wearing masks (Li et al., 2021). Few studies analyzed the chemical risk of masks, and they had a limited list of target chemicals (e.g., ethylene oxide, dimethyldioxirane, hydrogen peroxide, ozone, formaldehyde, isopropanol) used in the disinfection and sterilization of masks (Garcia-Haro et al., 2021; Gnatta et al., 2021; Kumkrong et al., 2021; O'Hearn et al., 2020; Purschke et al., 2020; Yin et al., 2020). If these chemicals and by-products produced in disinfection remain in masks, they might be potentially harmful to the health of users (Gnatta et al., 2021; Paul et al., 2020; Purschke et al., 2020; Viscusi et al., 2009). For example, Salter detected two suspicious toxins, 4-hydroxy-4-methyl-2-pentanone and 2-hydroxy-4-methyl-2-pentanone, in the tension band of N95 masks after they were disinfected with ethylene oxide (Salter et al., 2010). A recent study has shown that masks was a new source of human and environmental exposure to organophosphate esters (Fernández-Arribas et al., 2021). In addition, the potential chemical risks are unknown in the raw materials used in masks and in the production, processing, packaging, and transportation processes, where some chemicals might be introduced. In view of the close contact and frequent use of masks with the human body, the unknown chemicals present in masks must be identified and their chemical risk must be evaluated.

The identification of unknown substances is usually complicated and time consuming, and the reliability of the result is critical. Gas chromatography–mass spectrometry (GC–MS) is commonly used for volatile substances, whereas liquid chromatography–mass spectrometry (LC–MS) is used for thermally unstable and non-volatile substances (Martínez-Bueno et al., 2017; Martínez-Bueno et al., 2019; Onghena et al., 2015; Pleil et al., 2019). The identification of non-targeted substances is based on the use of commercial or in-house standardized spectral libraries. The qualitative analysis of unknown substances depends on the matching of ion mass and abundance ratio between the measured and standard spectra. However, the reliability of unit mass resolution MS identification results is limited if the spectra of homologous compounds are similar or if the differences of isomer fragment ions are negligible (Onghena et al., 2014; Onghena et al., 2015; Pleil et al.,

2019). Orbitrap-based high-resolution mass spectrometry (HRMS) is a powerful tool for such studies, offering resolution, mass accuracy, sensitivity, and selectivity superior to those of traditional mass spectrometry (Eiler et al., 2017; Gómez-Ramos et al., 2019; Pan et al., 2019; Yang et al., 2019). Moreover, HRMS is suited for use in developing non-targeted screening methods and performing retrospective analysis for any suspected or new compounds (Domínguez et al, 2020; Huysman et al., 2019). In addition to the above advantages, GC–Orbitrap MS has enormous potential in the non-targeted high-throughput analysis of unknown volatile substances based on commercial standardized spectral libraries (NIST, Wiley), high-resolution filter (HRF), retention index, and multiple ionization modes (EI, PCI, NCI). (Belmonte-Sánchez et al., 2018; Kwiecien et al., 2015; Yang et al., 2019). As far as we know, this technique has not been applied to the non-targeted screening of volatile substances in masks.

The first objective of this study is to develop a reliable non-targeted analysis method for the rapid and efficient identification of unknown volatile chemicals in medical masks based on headspace GC–Orbitrap MS. The second objective of this study is to unveil high-risk volatile chemicals in medical masks according to the detection rate, toxicity, and response intensity of the identified substances. This study may be the first to identify unknown volatile chemicals in masks by using non-targeted HRMS. Hopefully, this research will capture the current status of volatile chemicals in medical masks and provide technical support for promoting the chemical safety improvement of masks.

2. Materials and methods

2.1. Chemicals and materials

C_{10}-C_{25} saturated alkanes standard mix (1000 µg/mL in n-hexane), C_6-C_9 saturated alkanes standard mix (1000 µg/mL in methanol), 3,4-dimethylbenzaldehyde (CAS 5973-71-7) and 3,5-dimethylbenzaldehyde (CAS 5779-95-3) were all supplied by ANPEL Laboratory Technologies (Shanghai, China). 3,4-Dichlorotoluene (CAS 95-75-0) was purchased
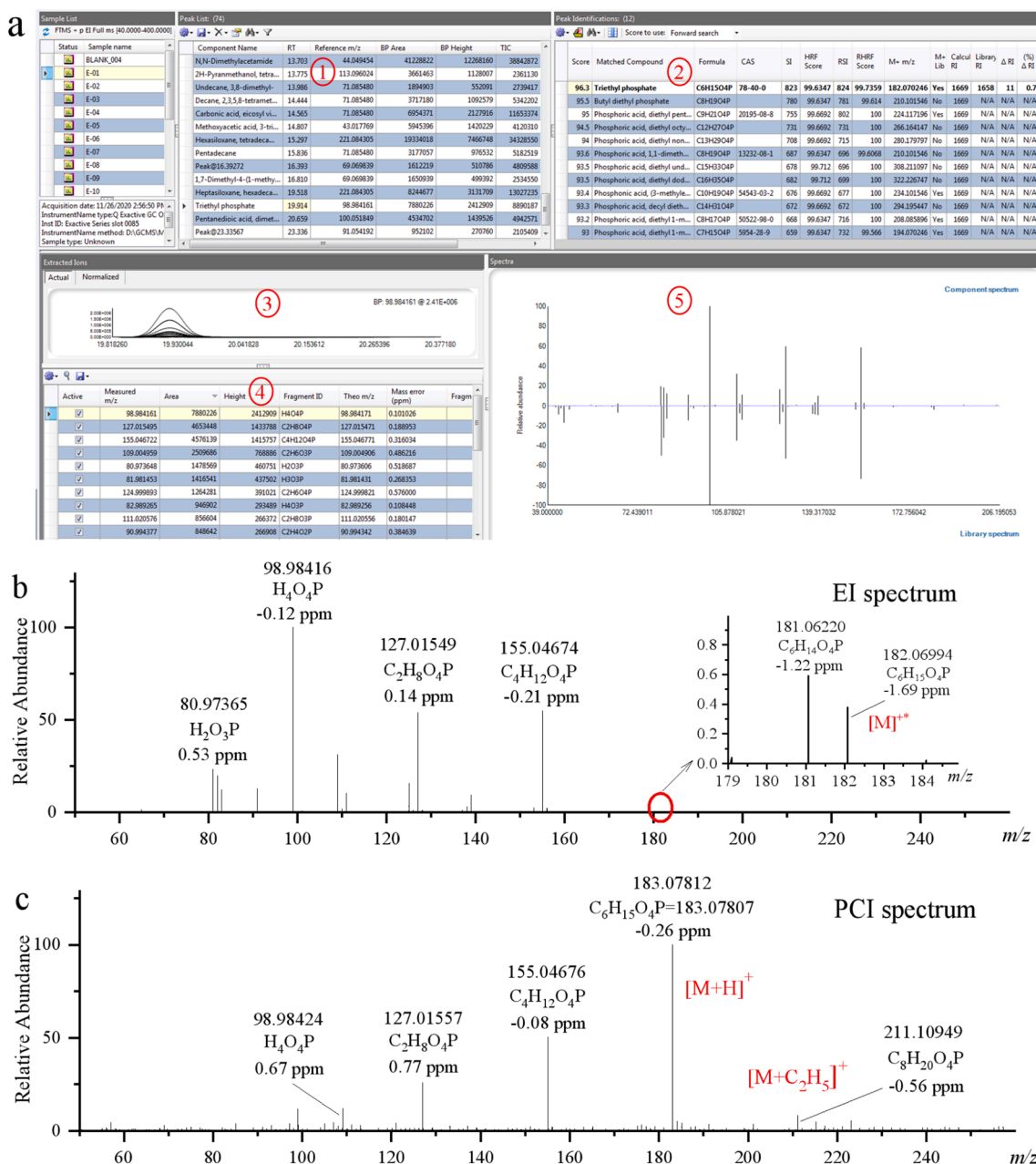
Fig. 2. Identification of triethyl phosphate. (a) ① list of chromatographic peaks in the sample; ② list of substances sorted according to comprehensive scores after retrieval from the NIST library; ③ ion overlay map for substances at the retention time of 19.914 min; ④ abundance of each fragment ion and deviation between the measured mass and the theoretical mass; ⑤ comparison of measured and theoretical mass spectra in the NIST library. (b) EI mass spectra of triethyl phosphate. (c) PCI mass spectra of triethyl phosphate. Notes include measured mass, element composition, theoretical mass, and mass deviation (ppm).

from Tokyo Chemical Industry (Tokyo, Japan). 1,4-Dichlorobenzene (CAS 106-46-7) was obtained from Aladdin (Shanghai China). Other standards were obtained from Dr. Ehrenstorfer GmbH (Augsburg, Germany) and Alfa Aesar (Lancaster, UK). n-Hexane and ethyl acetate were of chromatographic grade and obtained from Fisher Scientific (Waltham, MA, USA).

60 mask samples of different brands (including 18 adult medical surgical masks, 17 adult disposable medical masks, 7 children medical surgical masks, 13 children disposable medical masks, and 5 medical protective masks) were obtained from online shopping and offline pharmacy in Beijing, China.

2.2. Sample preparation

For sampling, the central part of the mask that can contact the nose and mouth was cut into pieces less than 1 cm × 1 cm in size and weighing 250 mg and then quickly placed in a 20 mL headspace vial. The vial was immediately sealed by a metal screw cap with PTFE/silicone septum and then placed in the headspace autosampler. Scissors used for cutting mask samples should be cleaned with absolute ethanol after each sample is processed to avoid cross contamination.

Blank analysis was undertaken in line with the sample to identify any possible systematic or non-systematic contamination that might come from experimental vessels, spacers, column losses, and so on. For each sample and blank, the parallel injection analysis was operated at least three times in random order.

a

	Score	Matched Compound	Formula	CAS	SI	HRF Score	RSI	RHRF Score	M+ m/z	M+ Lib	Calcu RI	Library RI	Δ RI	(%) Δ RI	
No.1	97.2	Benzaldehyde, 2,4-di...	C9H10O	15764-16-6	889	98.62...	894	99.12...	134.072616	Yes	1808	1726	82	4.5	✗
No.2	96.9	Benzaldehyde, 3,4-di...	C9H10O	5973-71-7	872	98.6277	875	99.1329	134.072616	Yes	1808	1790	18	1	√
No.3	96.8	Benzaldehyde, 2,5-di...	C9H10O	5779-94-2	866	98.6277	871	99.1282	134.072616	Yes	1808	1683	125	6.9	✗
No.4	96.3	Benzaldehyde, 2-ethyl-	C9H10O	22927-13-5	843	98.6277	852	99.1181	134.072616	Yes	1808	N/A	N/A	N/A	?
No.5	96.1	Benzaldehyde, 3,5-di...	C9H10O	5779-95-3	833	98.6277	838	99.1294	134.072616	Yes	1808	1837	29	1.6	?
No.6	96.1	Benzaldehyde, 4-ethyl-	C9H10O	4748-78-1	833	98.6277	836	99.1329	134.072616	Yes	1808	1721	87	4.8	✗
No.7	95.5	1H-Inden-5-ol, 2,3-di...	C9H10O	1470-94-6	804	98.6277	806	99.1329	134.072616	Yes	1808	N/A	N/A	N/A	?
No.8	95.4	1-Propanone, 1-(2,4-...	C12H16O	23351-72-6	784	99.1373	788	99.1294	176.119566	Yes	1808	N/A	N/A	N/A	✗✗
No.9	95.4	2,6-Dimethylbenzalde...	C9H10O	1123-56-4	796	98.6277	815	99.0979	134.072616	Yes	1808	1640	168	9.3	✗
No.10	95.2	Furazan-3-carboxylic ...	C13H13N3O4	296244-74-1	759	100	765	100	275.090057	Yes	1808	N/A	N/A	N/A	✗✗
No.11	94.9	4-Ethylbenzoic acid, p...	C15H14O2	118388-89-9	760	99.1373	767	99.1236	226.098831	Yes	1808	N/A	N/A	N/A	✗✗
No.12	94.9	Butanoic acid, 4-(3-et...	C12H14O3	17503-46-7	759	99.1373	763	99.1373	206.093745	Yes	1808	N/A	N/A	N/A	✗✗
No.13	94.8	Benzenebutanoic acid...	C12H14O3	51036-98-7	754	99.1373	758	99.1294	206.093745	Yes	1808	N/A	N/A	N/A	✗✗
No.14	94.8	3,5-Dimethylbenzoic ...	C9H12N2O	42596-61-2	741	100	748	100	164.094414	Yes	1808	N/A	N/A	N/A	✗✗
No.15	94.7	Oxirane, 2-methyl-2-...	C9H10O	2085-88-3	763	98.6277	767	99.1294	134.072616	Yes	1808	1666	142	7.9	✗
No.16	94.6	Benzaldehyde, 3-ethyl-	C9H10O	34246-54-3	757	98.6277	778	99.0941	134.072616	Yes	1808	N/A	N/A	N/A	?

b

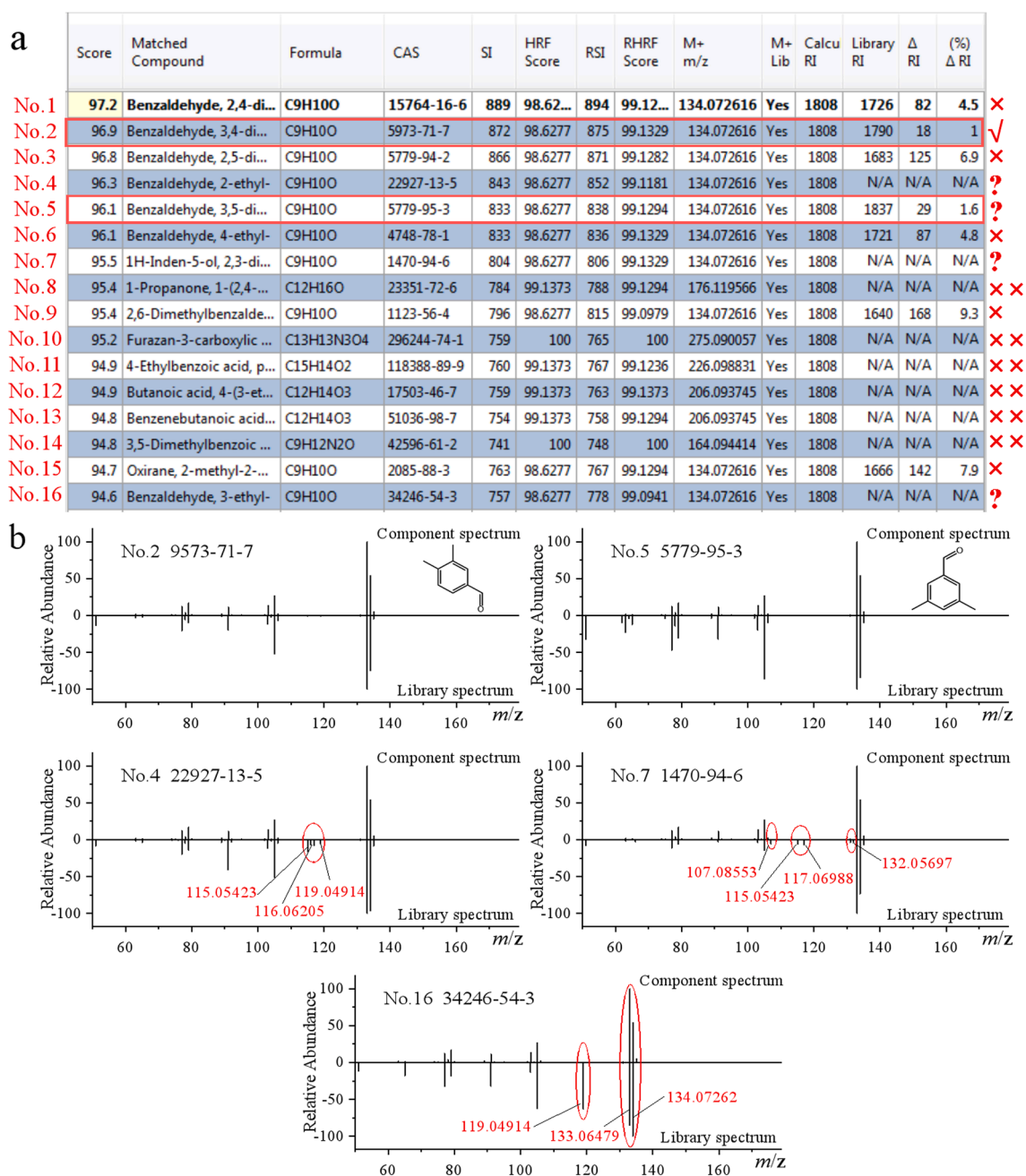**Fig. 3.** Identification of 3,4-dimethylbenzaldehyde. (a) List of candidate substances sorted according to comprehensive scores after retrieval from the spectral library. Compounds marked as "✗✗," "✗," and "?" are excluded according to PCI mass spectra, ΔRI, comparison of the actual spectra with the theoretical spectra, and chemical standard validation. Compounds marked with "√" are the final selected result. (b) Comparison of the actual and theoretical spectra of each candidate.

2.3. Instrument parameters

The analysis was performed using a Trace 1310 GC coupled to a quadrupole–Orbitrap MS (Thermo Fisher Scientific, Bremen, Germany) with a TriPlus RSH automatic sampler (including headspace injection function). The injection port temperature was 250 °C. In electron ionization (EI) mode, split injection was adopted, with split ratio of 20:1 and injection volume of 1 mL. In positive chemical ionization (PCI) mode, splitless injection was used, with injection volume of 1.5 mL. Helium (99.999% purity) was used as the carrier gas at a constant flow of 1 mL/min. Separations were performed on a DB-WAX column (30 m × 0.25 mm × 0.25 μm) using the following temperature program: 40 °C (held for 1 min) and 5 °C /min to 230 °C (held for 5 min).

Full scan MS acquisition was conducted at an *m/z* range of 40 to 500.

Each sample was analyzed in EI and PCI mode respectively. The electron energy of EI was 70 eV. Methane was used as a reaction gas in PCI mode, and the flow rate was 1.5 mL/min. The MS transfer line was 250 °C. The ion source temperature of EI and PCI were 280 °C and 230 °C, respectively. Nitrogen gas (99.999% purity) was used for the C-trap and HCD cell. The solvent delay time was 0 min. The mass resolution was set at 60,000 FWHM at *m/z* 200 and the TIC intensity threshold at $2e^6$. The maximum injection time was set to 200 ms and the mass tolerance window was set to ± 5 ppm.

The headspace equilibration temperature was operated at 80 °C with 30 min equilibration time, while the syringe temperature was 100 °C. The volatile components were released from the samples to the headspace under the conditions settings. Then 1 mL (or 1.5 mL) of the headspace gas was injected and analyzed by GC-Orbitrap MS.
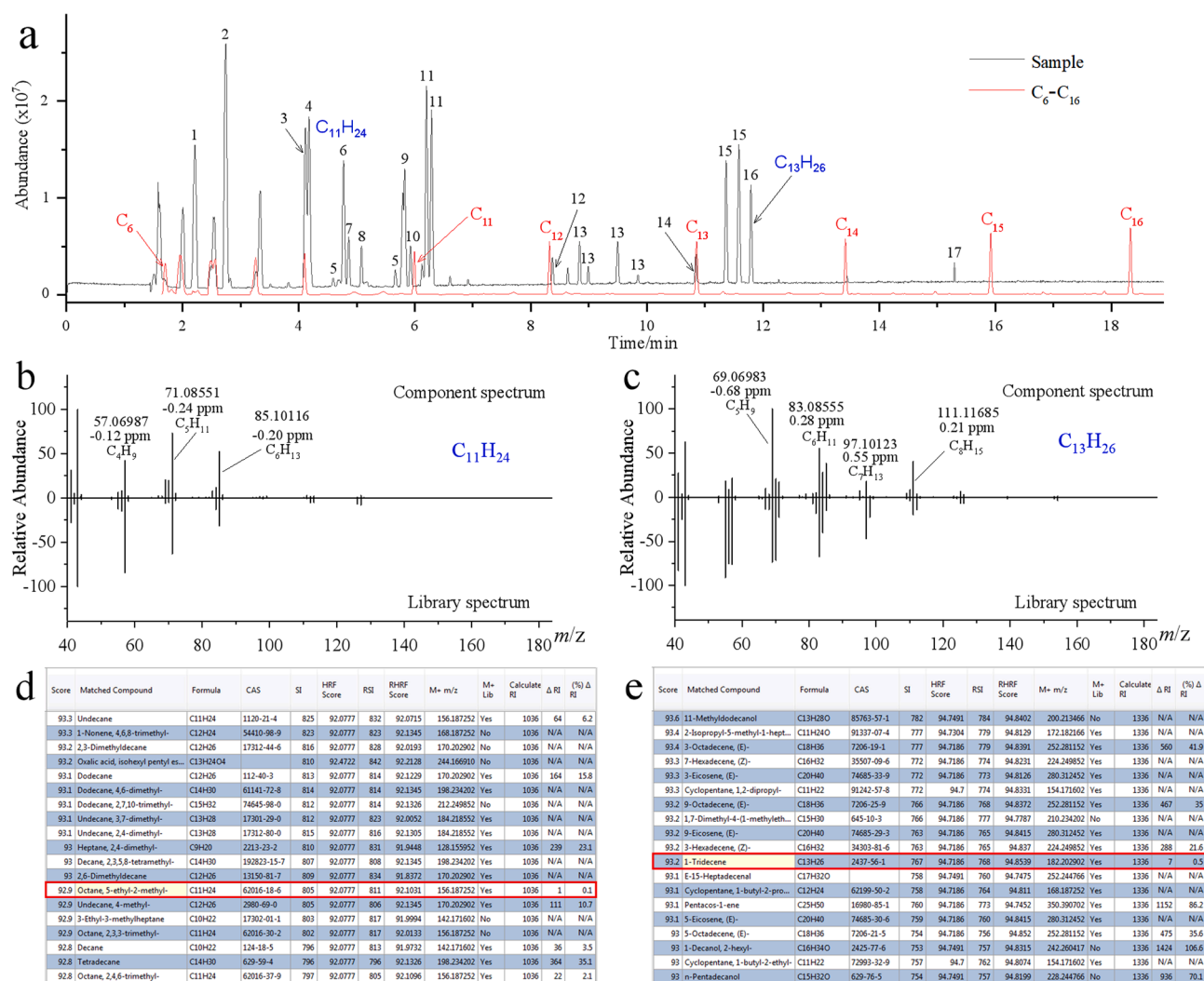
a

b Component spectrum

71.08551 -0.24 ppm C_5H_{11}

57.06987 -0.12 ppm C_4H_9

85.10116 -0.20 ppm C_6H_{13}

$C_{11}H_{24}$

Library spectrum

c Component spectrum

69.06983 -0.68 ppm C_5H_9

83.08555 0.28 ppm C_6H_{11}

111.11685 0.21 ppm C_8H_{15}

97.10123 0.55 ppm C_7H_{13}

$C_{13}H_{26}$

Library spectrum

d

Score	Matched Compound	Formula	CAS	SI	HRF Score	RSI	RHRF Score	M+ m/z	M+ Lib	Calculate RI	ΔRI	(%) Δ RI
93.3	Undecane	C11H24	1120-21-4	825	92.0777	832	92.0715	156.187252	Yes	1036	64	6.2
93.3	1-Nonene, 4,6,8-trimethyl-	C12H24	54410-98-9	823	92.0777	823	92.1345	168.187252	No	1036	N/A	N/A
93.2	2,3-Dimethyldecane	C12H26	17312-44-6	816	92.0777	828	92.0193	170.202902	No	1036	N/A	N/A
93.2	Oxalic acid, isohexyl pentyl es...	C13H24O4		810	92.4722	842	92.2128	244.166910	No	1036	N/A	N/A
93.1	Dodecane	C12H26	112-40-3	813	92.0777	814	92.1229	170.202902	Yes	1036	164	15.8
93.1	Dodecane, 4,6-dimethyl-	C14H30	61141-72-8	814	92.0777	814	92.1345	198.234202	No	1036	N/A	N/A
93.1	Dodecane, 2,7,10-trimethyl-	C15H32	74645-98-0	812	92.0777	814	92.1326	212.249852	No	1036	N/A	N/A
93.1	Undecane, 3,7-dimethyl-	C13H28	17301-29-0	812	92.0777	823	92.0052	184.218552	Yes	1036	N/A	N/A
93.1	Undecane, 2,4-dimethyl-	C13H28	17312-80-0	815	92.0777	816	92.1305	184.218552	Yes	1036	N/A	N/A
93	Heptane, 2,4-dimethyl-	C9H20	2213-23-2	810	92.0777	831	91.9448	128.155952	Yes	1036	239	23.1
93	Decane, 2,3,5,8-tetramethyl-	C14H30	192823-15-7	807	92.0777	808	92.1345	198.234202	Yes	1036	N/A	N/A
93	2,6-Dimethyldecane	C12H26	13150-81-7	809	92.0777	834	91.8372	170.202902	No	1036	N/A	N/A
92.9	Octane, 5-ethyl-2-methyl-	C11H24	62016-18-6	805	92.0777	811	92.1031	156.187252	Yes	1036	1	0.1
92.9	Undecane, 4-methyl-	C12H26	2980-69-0	805	92.0777	806	92.1345	170.202902	No	1036	111	10.7
92.9	3-Ethyl-3-methylheptane	C10H22	17302-01-1	803	92.0777	817	91.9994	142.171602	No	1036	N/A	N/A
92.9	Octane, 2,3,3-trimethyl-	C11H24	62016-30-2	802	92.0777	817	92.0133	156.187252	No	1036	N/A	N/A
92.8	Decane	C10H22	124-18-5	796	92.0777	813	91.9732	142.171602	Yes	1036	36	3.5
92.8	Tetradecane	C14H30	629-59-4	796	92.0777	796	92.1326	198.234202	Yes	1036	364	35.1
92.8	Octane, 2,4,6-trimethyl-	C11H24	62016-37-9	797	92.0777	805	92.1096	156.187252	Yes	1036	22	2.1

e

Score	Matched Compound	Formula	CAS	SI	HRF Score	RSI	RHRF Score	M+ m/z	M+ Lib	Calculate RI	ΔRI	(%) Δ RI
93.6	11-Methyldodecanol	C13H28O	85763-57-1	782	94.7491	784	94.8402	200.213466	No	1336	N/A	N/A
93.4	2-Isopropyl-5-methyl-1-hept...	C11H24O	91337-07-4	777	94.7304	779	94.8129	172.182166	Yes	1336	N/A	N/A
93.4	3-Octadecene, (E)-	C18H36	7206-19-1	777	94.7186	779	94.8391	252.281152	Yes	1336	560	41.9
93.3	7-Hexadecene, (Z)-	C16H32	35507-09-6	772	94.7186	774	94.8231	224.249852	Yes	1336	N/A	N/A
93.3	3-Eicosene, (E)-	C20H40	74685-33-9	772	94.7186	773	94.8126	280.312452	Yes	1336	N/A	N/A
93.3	Cyclopentane, 1,2-dipropyl-	C11H22	91242-57-8	772	94.7	774	94.8331	154.171602	Yes	1336	N/A	N/A
93.2	9-Octadecene, (E)-	C18H36	7206-25-9	766	94.7186	768	94.8372	252.281152	Yes	1336	467	35
93.2	1,7-Dimethyl-4-(1-methyleth...	C15H30	645-10-3	766	94.7186	777	94.7787	210.234202	No	1336	N/A	N/A
93.2	9-Eicosene, (E)-	C20H40	74685-29-3	763	94.7186	765	94.8415	280.312452	Yes	1336	N/A	N/A
93.2	3-Hexadecene, (Z)-	C16H32	34303-81-6	763	94.7186	765	94.837	224.249852	Yes	1336	288	21.6
93.2	1-Tridecene	C13H26	2437-56-1	767	94.7186	768	94.8539	182.202902	Yes	1336	7	0.5
93.1	E-15-Heptadecenal	C17H32O		758	94.7491	760	94.7475	252.244766	Yes	1336	N/A	N/A
93.1	Cyclopentane, 1-butyl-2-pro...	C12H24	62199-50-2	758	94.7186	764	94.811	168.187252	Yes	1336	N/A	N/A
93.1	Pentacos-1-ene	C25H50	16980-85-1	760	94.7452	773	94.7452	350.390702	Yes	1336	1152	86.2
93.1	5-Eicosene, (E)-	C20H40	74685-30-6	759	94.7186	760	94.8415	280.312452	Yes	1336	N/A	N/A
93	5-Octadecene, (E)-	C18H36	7206-21-5	754	94.7186	756	94.852	252.281152	Yes	1336	475	35.6
93	1-Decanol, 2-hexyl-	C16H34O	2425-77-6	753	94.7491	757	94.8315	242.260417	No	1336	1424	106.6
93	Cyclopentane, 1-butyl-2-ethyl-	C11H22	72993-32-9	757	94.7	762	94.8074	154.171602	Yes	1336	N/A	N/A
93	n-Pentadecanol	C15H32O	629-76-5	754	94.7491	757	94.8199	228.244766	No	1336	936	70.1

Fig. 4. Identification of alkanes. (a) Overlap of mask sample with n-alkane chromatogram. (b) Comparison of the actual and theoretical spectra of a candidate of $C_{11}H_{24}$. (c) Comparison of the actual and theoretical spectra of a candidate of $C_{13}H_{26}$. (d) List of candidate substances sorted according to comprehensive scores after retrieval from the spectral library ($C_{11}H_{24}$). (e) List of candidate substances sorted according to comprehensive scores after retrieval from the spectral library ($C_{13}H_{26}$).
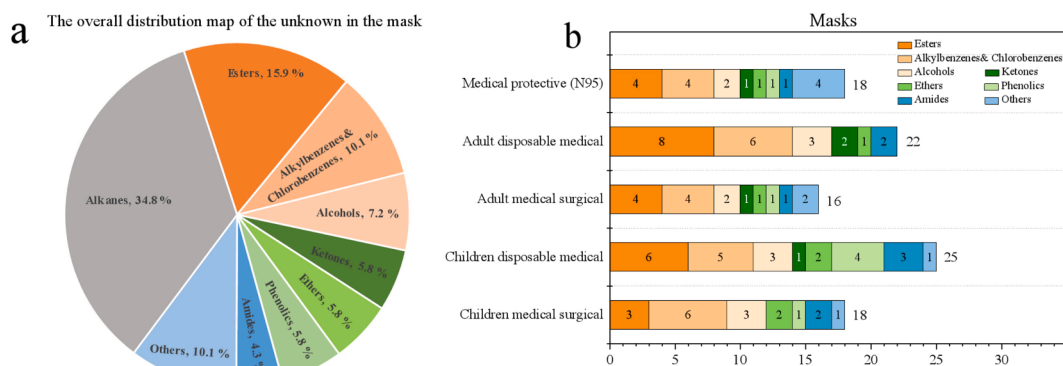
a The overall distribution map of the unknown in the mask

Esters, 15.9 %
Alkylbenzenes & Chlorobenzenes, 10.1 %
Alcohols, 7.2 %
Ketones, 5.8 %
Ethers, 5.8 %
Phenolics, 5.8 %
Amides, 4.3 %
Others, 10.1 %
Alkanes, 34.8 %

b Masks

Legend: Esters, Alkylbenzenes & Chlorobenzenes, Alcohols, Ethers, Amides, Ketones, Phenolics, Others

Mask type	Total
Medical protective (N95)	18
Adult disposable medical	22
Adult medical surgical	16
Children disposable medical	25
Children medical surgical	18

Fig. 5. (a) Overall distribution of the unknown substances in the mask. (b) Number of substances detected in different types of masks.

The quantitative analysis method refered to the method reported earlier by our team (Wang et al., 2018). An automated HS sampler (DANI 86.50, Italy) equipped with GC–MS system (Agilent 6890–5975, USA). The HS operating conditions were as follows: equilibration time = 15 min; equilibration temperature = 160 °C; pressing pressure = 70 kPa; pressing time = 10 s; sample loop fill time = 10 s; and injecting time = 20 s. The GC operating conditions were as follows: carrier gas was helium at a flow rate of 1 mL/min; injection port was held at 230 °C and used in the split mode with a split ratio of 20:1. The samples were cut into pieces smaller than 5 mm. Afterward, 0.2 g of the sample was
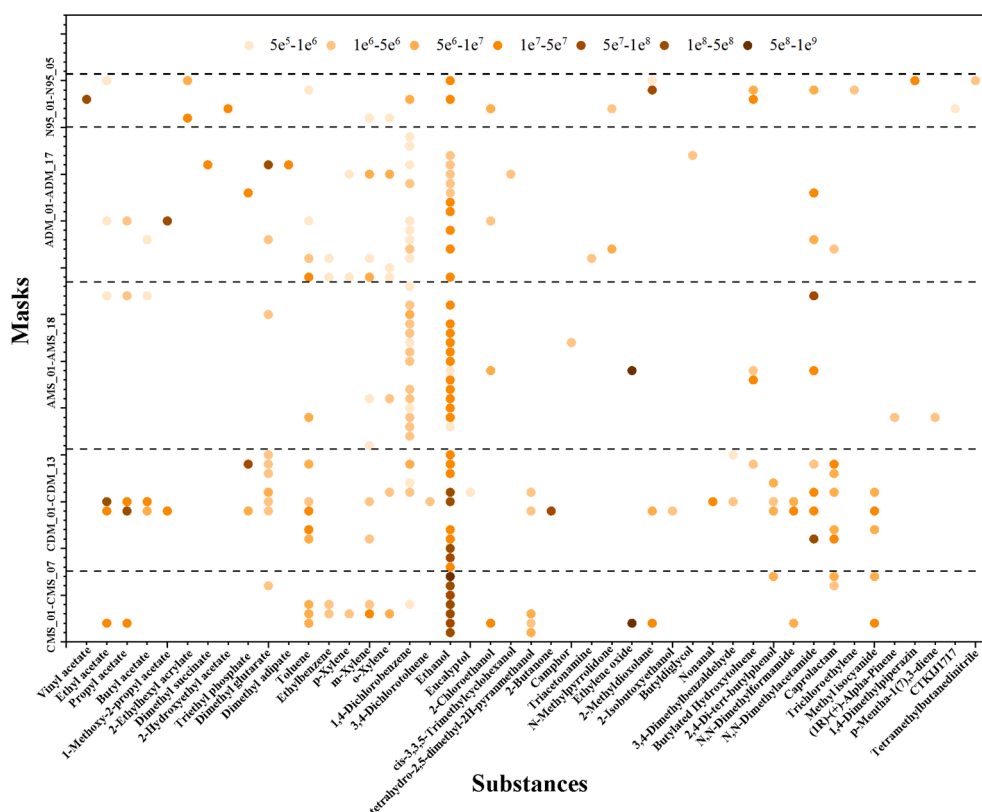
Fig. 6. Summary statistics of non-targeted identified 45 substances in 60 masks. CMS: children medical surgical masks. CDM: children disposable medical masks. AMS: adult medical surgical masks. ADM: adult disposable medical masks. N95: medical protective masks.

transferred into a 20 mL HS vial, and then 20 μL of ethyl acetate was added. The vial was immediately sealed with an aluminum cap and PTFE/silicone septum and then placed in the autosampler.

2.4. Data analysis

Data were collected and processed using Thermo Scientific™ TraceFinder™ 4.1 software. Fig. 1 shows the workflow of the non-targeted analysis method for masks. It is mainly composed of data acquisition, data analysis, and identification of unknown substances. First, the volatile substances released from the samples were analyzed using GC–Orbitrap MS in EI full scan mode. Second, the peaks were resolved into a pure mass spectrum using the Deconvolution Plugin of TraceFinder software. After the blanks were subtracted, the unique peaks in each sample were recognized and then searched in the standard spectrum library NIST 2014 (the positive matching index SI was involved). The matching results were further filtered using the accurate mass information. The HRF value represents the percentage of the accurate mass of the fragment ions in the mass spectrum consistent with the elemental composition of the corresponding fragment ions in the standard spectrum library. Therefore, the higher the HRF and SI values, the higher the reliability of the results. Before sample analysis, the mixed solution of C_6–C_{25} n-alkanes was analyzed using the same separation method to determine the retention time of each n-alkane, which was used to calculate the retention index of unknown substances. The deviation of retention index (ΔRI) was finally calculated by comparing it with the retention index of compounds included in the library. A smaller ΔRI means that the result is more reliable. Third, the qualitative analysis of unknown substances was carried out according to four identification steps. Step 1 is based on the comprehensive score (SI, HRF, etc.) and ΔRI. In theory, the reliability of tentative identification is high when the only substance which meets these conditions that SI ≥ 700, HRF ≥ 90, and ΔRI ≤ 100. In step 2, if multiple results meet the above

requirements, the molecular ion peak and the molecular formula were confirmed by measuring the PCI data to distinguish the interferents with similar scores. In step 3, the most likely substances were verified from various isomers by comparing the tiny differences in the details of characteristic fragment ions, isotope information, and ΔRI. Relatively reliable tentatively qualitative results were obtained in the above three steps. In step 4, individual substances, especially isomers with very similar structures, were finally identified by available chemical standards. Finally, all identified volatiles in the samples were classified and analyzed, and then a list of high-risk volatile substances in medical masks was introduced according to the detection rate, toxicity, and response intensity of these substances.

3. Results and discussion

3.1. Non-targeted analysis of unknown substances

3.1.1. Qualitative analysis based on comprehensive score and PCI

After the deconvolution process and the deduction of blanks, all unknown peaks detected above the threshold $2e^6$ in each sample were considered. The search results were ranked according to the comprehensive score of SI and HRF. ΔRI is also an important parameter for qualitative analysis. However, some compounds do not have retention index data in the NIST library; therefore, their ΔRI cannot be obtained.

Fig. 2a shows the unknown peak at 19.914 min in the E-01 sample. The highest comprehensive score was triethyl phosphate, its SI value was 823, the HRF value was 99.6347, and the ΔRI was 11. The score difference between it and other candidates was not very significant. In addition, other candidates had no ΔRI to refer to. However, the molecular formula of these candidates varied. Thus, the molecular ion peak of the compound can be determined by PCI. As a soft ionization method, the molecular adduct ions ($[M + H]^+$ and $[M + C_2H_5]^+$) can be obtained by PCI when using methane as the reaction gas so that the molecular

Table 1
High-risk volatile chemicals in masks.

No.	Compounds	Retention time (min)	Formula	CAS No.	SI score	HRF score	ΔRI	Base peak ion (m/z) error (ppm)	[M]$^+$ peak ion (m/z) error (ppm)	[M + H]$^+$ peak ion (m/z) error (ppm)	Identification step	Detection rate (%)	Notes
1	1,4-Dichlorobenzene	14.450	$C_6H_4Cl_2$	106–46–7	842	86.00	7	145.96836 (-0.69)	145.96836 (-0.69)	146.97627 (-0.07)	4	46.67	Group 2B carcinogen, Restricted by Oeko-Tex Standard 100
2	Toluene	4.841	C_7H_8	108–88–3	898	100.00	3	91.05428 (0.37)	92.06196 (-0.98)	93.07001 (1.40)	3	21.67	Group 3 carcinogen
3–5	Xylenes (p, m, o)	6.774, 6.918, 7.926	C_8H_{10}	106–42–3, 108–38–3, 95–47–6	924	98.33	4	91.05419 (-0.51)	106.07763 (-0.66)	107.08563 (0.93)	3	5.00, 16.67, 11.67	Group 3 carcinogen
6	Ethylene oxide	1.809	C_2H_4O	75–21–8	925	99.92	57	44.02567 (0.08)	44.02567 (0.40)	45.03336 (-2.89)	3	3.33	Group 1 carcinogen
7	Ethylbenzene	6.607	C_8H_{10}	100–41–4	884	98.36	3	91.05422 (-0.08)	106.07771 (0.08)	107.08558 (0.60)	3	6.67	Group 2B carcinogen
8	Caprolactam	30.511	$C_6H_{11}NO$	105–60–2	719	99.98	/	85.05219 (-0.30)	113.08352 (0.50)	114.09146 (1.05)	2	13.33	Group 4 carcinogen
9	N,N-Dimethylacetamide	13.682	C_4H_9NO	127–19–5	900	99.79	4	87.06785 (-0.29)	87.06782 (-0.57)	88.07577 (0.91)	1	15.00	Restricted by Oeko-Tex Standard 100 and AAFA RSL
10	N,N-Dimethylformamide	11.614	C_3H_7NO	68–12–2	894	99.93	3	73.05222 (0.06)	73.05219 (-0.41)	74.06010 (0.81)	3	5.00	Restricted by Oeko-Tex Standard 100 and AAFA RSL
11	N-Methylpyrrolidone	20.248	C_5H_9NO	872–50–4	704	96.90	12	98.06010 (0.61)	99.06788 (0.10)	100.07569 (-0.01)	2	3.33	Restricted by REACH
12	Dimethyl glutarate	20.656	$C_7H_{12}O_4$	1119–40–0	780	99.79	7	100.05174 (-1.41)	/	161.08090 (0.37)	3	16.67	/

weight and molecular formula of the compound can be clearly identified. The mass spectra of the unknown substance in EI and PCI ionization modes are shown in Fig. 2b and 2c, respectively. The basic peak m/z 183.07812 in Fig. 2c can be inferred as the protonated molecular ion peak ($[M + H]^+$). On the basis of the possible element composition and isotopic information, the molecular formula of the substance was calculated to be $C_6H_{14}O_4P$. In addition, m/z 211.10949 was very significant, that is, the $[M + C_2H_5]^+$ addition peak of the substance. The deviations of the two ions from their theoretical accurate masses were −0.26 and −0.56 ppm, respectively. As shown in Fig. 2b, the deviation of all fragment ions from the theoretical accurate mass was less than ± 1 ppm. In EI mode, a weak molecular ion peak can also be observed. Therefore, the unknown substance can be tentatively identified as triethyl phosphate.

3.1.2. Detailed comparison of fragment ions for distinguishing isomers

Although PCI data can aid in determining the molecular ion of unknown substances, unknown substances are still not easy to identify - when most of the candidates are isomers. For example, in identifying 3,4-dimethylbenzaldehyde, deconvolution results provided 16 candidates, most of which are isomers. The candidate compounds were numbered one by one, as shown in Fig. 3a, to facilitate the description of the results. The scores of these substances were very close. Four of them had ΔRI values less than 100, and nine of them had no library RI to refer to.

First, the molecular mass of 134.07262 was determined by PCI, and the candidates of No. 8 and Nos. 10–14 can be excluded (marked with the symbol XX). Then, the remaining 10 isomers with molecular formula $C_9H_{10}O$ were further identified. The ΔRI values of No. 1, 3, 6, 9, and 15 candidates were greater than 80. Thus, they can be excluded and marked as X. Then, the candidate Nos. 4, 7, and 16 can be excluded by comparing the actual spectrum with the theoretical spectrum, marked as ?. As shown in Fig. 3b, No. 4 could produce the fragment ions m/z 115.05423, 116.06205, and 119.0914, but these ions were not found in the sample spectrum. Similarly, the characteristic ions of Nos. 7 and 16 were slightly different from the unknown substance, which are marked in red in Fig. 3b.

For No. 2 and 5 candidates, the evaluation indexes (SI, HRF, and ΔRI) were in line with the theoretical requirements. Although the score and ΔRI of No. 2 was slightly superior, the structural difference between them was only the position of the methyl group. We used the chemical standard for confirmation to obtain accurate identification results. Results showed that the retention times of 3,4-dimethylbenzaldehyde and 3,5-dimethylbenzaldehyde were 23.00 and 22.70 min, respectively. The retention time of the former is consistent with that of the unknown peak.

3.1.3. Identification of alkanes

On the basis of the preliminary screening results, the components with the highest content and detection rate were different alkanes. As we all know, the mass spectrum information of alkane isomers has a strong similarity, which makes the accurate identification of alkanes very complex. Alkanes can be studied according to the retention behavior, chain length, and molecular weight of alkanes and fragment ions in the database. Alkanes with the same carbon number can be divided into an isomer group (Xu et al., 2020). Some researchers also indicated that most of the studies on alkanes are n-alkanes, and only the number of C needs to be studied for branched alkanes (Zhang et al., 2021). We have carried out some exploration to obtain detailed results.

Fig. 4a is the overlap of the chromatograms of a mask sample and a standard solution of C_6-C_{16} n-alkanes under the same separation conditions. Twenty-four peaks were preliminarily identified as alkanes and subjected to further analysis. Fig. 4b and 4c provide the characteristic fragments of saturated and unsaturated alkanes, respectively. We aimed to obtain the molecular ion peaks of these compounds by the soft ionization PCI method. However, the molecular ion peak of most alkanes cannot be obtained even in PCI mode because of the poor stability of the
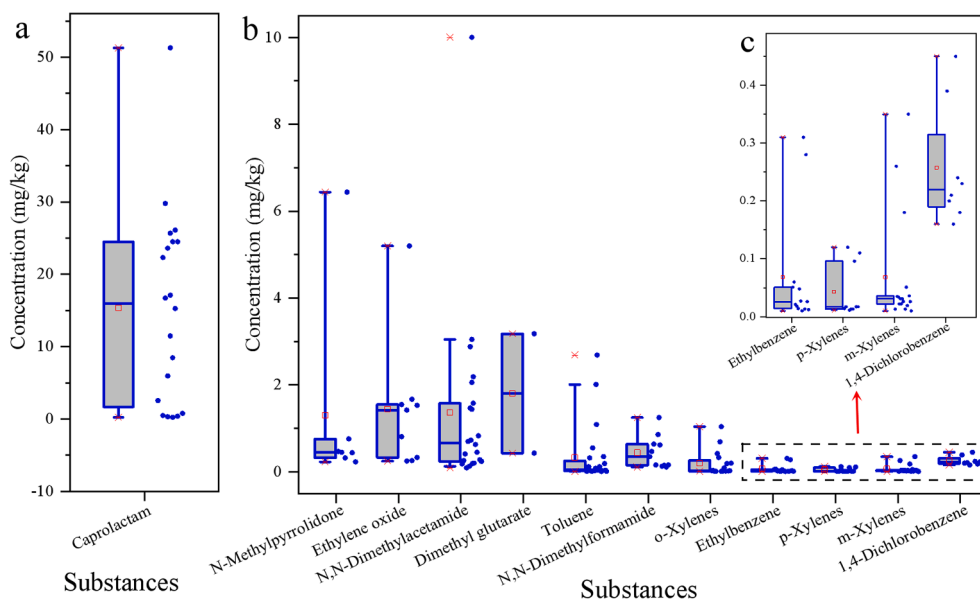
Fig. 7. Residue detection results of 12 high-risk substances in masks. (Boxes represent the 25th to 75th percentiles, solid lines in the boxes are the median values, red squares are the mean values, and error bars represent the 5th and 95th percentiles).

C-C bond of alkanes. Finally, we identified partial alkanes according to the peak time of n-alkanes, positive and negative correlation scores (SI and RSI), HRF, ΔRI, and characteristic fragment ions. Taking 1-tridecene as an example, the unknown compound was determined to be an unsaturated alkane by the characteristic ions 69.06983, 83.08555, and 97.10123 in Fig. 4c. Fig. 4e shows a variety of candidate results of this unknown compound. It was tentatively identified as 1-tridecane according to the comprehensive score and ΔRI. Fig. 4b and 4d show the identification process of saturated alkanes. The identification process of compounds with substance names in Table S1 (Supplementary material) referred to the identification process of 1-tridecene. Compounds without substance names in Table S1 were only identified as the molecular formula.

3.2. Screening of volatile chemicals in masks

On the basis of the above non-targeted qualitative method, 69 substances were found in 60 samples of masks in all. The identified substances were divided into nine categories. Fig. 5a shows the categories and proportions of these substances. Alkanes, esters, benzenes, and alcohols were the top four groups of substances identified in masks and accounted for 34.8%, 15.9%, 10.1%, and 7.2% of the total substances, respectively. In addition, ketones, ethers, phenolics, amides, and other substances were identified. Fig. 5b shows the distribution of identified substances in different types of masks. The test results for different masks were slightly different. Relatively more chemical substances were detected in disposable medical masks for adults and children.

Except for alkanes, the semi-quantitative analysis of 45 other identified substances was carried out. In Fig. 6, the abscissa is the substances, the ordinate is the mask samples, the circle represents the detection of the substance, and the depth of the circle color represents the peak area of the extracted base peak ion of the substance. Ethanol had the highest detection rate in mask samples, reaching 70.0%, and its content in the samples was relatively high, especially in children's medical surgical masks. In addition, the detection rates of 1,4-dichlorobenzene (46.7%), toluene (21.7%), *m*-xylene (16.7%), dimethyl glutarate (16.7%), N,N-dimethylacetamide (15.0%), caprolactam (13.3%), *o*-xylene (11.7%) were relatively high. Although ethylene oxide was only detected in two masks, they all had response values as high as $5e^8$–$1e^9$. According to available data, more substances were detected in children's masks than in adult masks, which may be related to the colored patterns on the

surface of children's masks.

The detailed information of all the non-targeted identified substances is presented in Tables S1 and S2 (Supplementary material). The identified substances were further filtered and screened according to their detection rate, toxicity, and response intensity. Finally, 12 high-risk volatile chemicals in masks were listed. Table 1 lists the name, CAS number, scores, ion mass deviation (ion error), detection rate, hazards of substances, and regulations involved. According to Schymanski's confidence level criteria (Schymanski et al., 2014), the substances in Table 1 belong to level 1 (confirmed structure) after they were verified by standards. In Table S2, the substance marked as 4 in the identification step also belongs to level 1, and other substances belong to level 2 (probable structure).

Some of these substances were considered carcinogenic. For example, ethylene oxide was classified as group 1 carcinogens (carcinogenic to humans) by the International Agency for Research on Cancer (IARC, 2020). 1,4-Dichlorobenzene and ethylbenzene were classified as group 2B carcinogen (possibly carcinogenic to humans). Toluene, and xylene were categorized as group 3 carcinogens (not classifiable as to their carcinogenicity to humans). Some substances were restricted in textile related regulations. For example, 1,4-dichlorobenzene, N,N-dimethylacetamide, and N,N-dimethylformamide were restricted by the International Environmental Textile Association Oeko-Tex Standard 100. The latter two were also listed in the RSL list of the American Apparel and Footwear Association. N-Methylpyrrolidone was restricted by REACH regulations. Other substances, such as dimethyl glutarate, can irritate the human eye, respiratory system, and skin.

A few months later, we supplemented the experiment and quantitatively analyzed the residues of high-risk substances in mask samples. The mask samples were partially inconsistent with the previous non-targeted screening samples, but the test results were basically the same. Caprolactam was detected in 20 samples with a content range of 0.23–51.3 mg/kg, which has not been paid attention to before. It is worth noting that it is not very prominent in Fig. 6, which is related to its high boiling point (272.5 °C). Therefore, the amount of volatilization is not only related to the content, but also related to the boiling point. Ethylene oxide was detected in 9 samples, with the content of 0.25–5.2 mg/kg, which was less than the limit of 10 mg/kg in China's mask standards. N-methylpyrrolidone was detected in 7 samples, and the content was 0.23–6.4 mg/kg, which was far less than the limit of 3000 mg/kg in REACH regulations. See Fig. 7 for detailed detection results of

other substances. The potential risks to people caused by the presence of these substances in masks need to be further studied.

4. Conclusion

A non-targeted headspace GC-Orbitrap MS method was developed for the screening of unknown volatile substances in medical masks. Several typical cases and solutions with different levels of difficulty were provided to solve the problems encountered in the qualitative analysis. As such, the accuracy of identifying unknown substances can be ensured. A total of 69 volatile substances were identified in the masks. These substances were further filtered and screened, and 12 high-risk volatile chemicals in masks were finally listed. This work can provide a new path and certain guidance for screening potential chemical hazards of masks and other products. The next step is to expand the variety of mask products and carry out exposure assessment and risk assessment of identified high-risk substances to provide scientific data for evaluating the impact of masks on human health and promoting product safety.

CRediT authorship contribution statement

Yahui Liu: Writing – original draft, Methodology, Data curation, Formal analysis. **Zhijuan Wang:** Methodology, Data curation, Formal analysis. **Wan Wang:** Formal analysis, Validation. **Jiangtao Xing:** Validation, Software. **Qing Zhang:** Supervision, Conceptualization. **Qiang Ma:** . **Qing Lv:** Writing – review & editing, Methodology, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envint.2022.107122.

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