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Molecular evidence on potential contribution of marine emissions to aromatic and aliphatic organic sulfur and nitrogen aerosols in the South China Sea

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S1. Sample storage

The collected samples were enveloped in aluminum foil which had previously been subjected to a baking process at 400°C for 8 hours. Subsequently, the samples were stored in a refrigerator maintained at a temperature of –30°C. Following their transportation to the university laboratory, the samples were processed and subjected to chemical analysis consistently. In the preceding organosulfate (OS) loss experiment (using OS standards) by our laboratory, it was demonstrated that the OSs spiked onto the filters (stored at −30°C) exhibited negligible loss for a duration exceeding 28 days (Yang et al., 2024). Furthermore, it has been suggested that the synthesized OS standards can be stored in a refrigerator set at approximately 4°C for a period of two years without undergoing hydrolysis (Huang et al., 2018). Many previous studies have similarly indicated that the $PM_{2.5}$ filters utilized in the OS measurement process were stored at a temperature of –30°C for a period of over five years (Hettiyadura et al., 2018; Brüggemann et al., 2019; Wang et al., 2021b; Hettiyadura et al., 2017).

S2. Identification, classification, and quantification of OSs and relevant limitations.

The analysis of the OSs was conducted using an Acquity UPLC (Waters, USA) coupled to a Xevo G2-XS QToF-MS (Waters, USA) with an electrospray ionization (ESI) source (Yang et al., 2023). The subsequent processing of the mass spectrometry data was conducted using the MassLynx v4.1 software, which facilitated the acquisition of information pertaining to m/z, formula, and signal intensity. A molecular formula calculator was employed to obtain the potential formulae of the identified compounds. These possible formulas were expressed as $C_nH_nO_nS_nN_n$, with a mass tolerance of ± 10 ppm. The identification of OSs (m/z 136.9909-691.4396) was initiated through the preliminary determination of their molecular formulas. The following equation was utilized to facilitate this process (Yang et al., 2023; Wang et al., 2021b; Jiang et al., 2022).

$$n_O / (4n_S + 3n_N) \geq 1 \quad \text{(S1)}$$

where the symbols of n_S, n_N, and n_O indicate the number of sulfur, nitrogen, and oxygen atoms in a given molecular formula, respectively.

The detailed workflow for OS classification was provided in our recent publications (Yang et al., 2023; Yang et al., 2024). Specifically, the identification of 33 types of OS compounds has been validated through the confirmation of sulfur-containing fragment ions (e.g., m/z 80, 81, and 96) by MS/MS analysis (Yang et al., 2023; Wang et al., 2021b). The classification of all potential OSs was further refined into categories based on their provenance. These categories include isoprene-derived OSs (OS_i), monoterpene-derived OSs (OS_m), C_2–C_3 OSs, aliphatic OSs, and aromatic OSs (Yang et al., 2023). The following methodology was employed to classify OS_i. Initially, molecules comprising 4 and 5 carbon atoms were selected. Then, compounds with 4 carbon atoms were characterized by a double bond equivalent (DBE) value ranging from 1 to 2, $n_H \geq 6$, and $n_O \leq 6$. Finally, compounds with 5 carbon atoms were characterized by a DBE value of 0 to 2, $n_H \geq 8$, and $n_O \leq 7$. Notably, $C_7H_9O_7S^-$ was also classified as OS_i (Nozière et al., 2010), which can be further confirmed by a significant correlation (P < 0.01) between $C_7H_9O_7S^-$ and typical OS_i.

The DBE value of each identified molecular formula was calculated according to the following methodology (Lechtenfeld et al., 2014; Xu et al., 2023).

$$DBE = (2n_C + 2 - n_H + n_N) / 2 \quad (S2)$$

where the n_C, n_H, and n_N represent the number of C, H, and N atoms in a molecule, respectively.

The categorization of OS_m was conducted in accordance with the following methodology. The compounds under consideration showed 10 carbon atoms and effective oxygen atoms ($n_{Oeff} = n_O - 2n_N$) that exceed 4. In addition, their DBE values ranged from 2 to 4 (Guo et al., 2022b; Ehn et al., 2012; Yan et al., 2016; Jokinen et al., 2014; Berndt et al., 2016; Berndt et al., 2018). According to the reports of previous studies, $C_9H_{14}NO_8S^-$, $C_9H_{15}O_6S^-$, $C_8H_{13}O_7S^-$, $C_7H_{11}O_6S^-$, and $C_7H_{11}O_7S^-$ were classified into the OS_m category (Yassine et al., 2012; Nozière et al., 2010; Wang et al., 2017; Surratt et al., 2008). Furthermore, a correlation analysis between the selected OSs and the typical OS_m (e.g., $C_{10}H_{17}O_5S^-$) was conducted to validate (r > 0.8, P < 0.01) the identified OS_m species.

OSs characterized by a DBE value of ≥ 2, along with an aromaticity equivalent (X_C) value of ≥ 2.5, were categorized as aromatic OSs (Jiang et al., 2022; Xie et al., 2021; Ma et al., 2022). The X_C value of OSs was calculated according to the following equation, which has been refined to enhance its reliability for chemical classes including sulfoxides, sulfones, sulfinic and sulfonic acids (Yassine et al., 2014;

Ye et al., 2021).

$$X_C = [3(DBE - 0.5(n_O - 4)) - 2]/[DBE - 0.5(n_O - 4)]) \qquad (S3)$$

where the symbol of n_O represent the number of oxygen atoms in a molecule, respectively.

It is important to note that the oxidation of monoterpenes by ·OH or NO_3· can result in the generation of products that possess a DBE value of 2 (Yan et al., 2016; Ehn et al., 2014; Tröstl et al., 2016). Thus, a certain degree of overlap was probable between the identified OS_m and aromatic OS species. In order to resolve the aforementioned issue, a further identification of aromatic OSs with a DBE value of 2 was made through a correlation analysis between unknown aromatic OSs and known aromatic OSs and OS_m (Yang et al., 2024; Yang et al., 2023). The acceptance of compounds was contingent upon the r value to be greater than 0.6 (or the greater one), with a statistical significance level of $P < 0.01$.

OSs exhibiting a DBE value below 2 (e.g., alkanes and certain unsaturated compounds) were classified as aliphatic OSs (Xie et al., 2021; Tao et al., 2014). A previous study has suggested the presence of aliphatic oxygenated organic molecules with a DBE value of 2 (Wang et al., 2021d). Consequently, additional identification of OSs with a DBE value of 2 was undertaken via correlation analysis between unidentified aliphatic OSs and known aliphatic species, as previously referenced. The selected compounds were accepted if their r values exceeded 0.6 ($P < 0.01$). Additionally, the term "OS_a" was used to denote aliphatic and aromatic OSs (Yang et al., 2025; Yang et al., 2023). Several OS_a compounds were identified as either non-aromatic or non-aliphatic categories, which were classified as other OS_a compounds (i.e.,OS_a-other) (Huang et al., 2018; Kundu et al., 2013; Wang et al., 2021b; Yang et al., 2024). In this study, all aliphatic and aromatic OSs and OS_a-other were collectively referred to as OS_a.

Due to the absence of authentic standards, the majority of the identified OSs were quantified using surrogate standards (Hettiyadura et al., 2019; Bryant et al., 2021; Wang et al., 2018; Kanellopoulos et al., 2022; Yang et al., 2023). In view of the fact that OSs with analogous carbon backbone structures tend to demonstrate comparable MS responses, surrogate standards for a given OS compound were predominantly selected on the basis of similarities in the carbon chain structures of the targeted OS species and standard (Hettiyadura et al., 2015; Wang et al., 2021b; Huang et al., 2018). For the OSs reported in previous studies, MS/MS analysis has been conduted to offer futher support in terms of their structural identification (Yang et al., 2023; Wang et al., 2021b). The selection of most OSs lacking structural identification was conducted in accordance with the aforementioned classification rules. The surrogate standards utilized in this study included glycolic acid sulfate (synthesized in the laboratory), α-pinene sulfate (synthesized in the laboratory), limonaketone sulfate (synthesized in the laboratory), lactic acid sulfate (synthesized in the laboratory), sodium octyl sulfate (95%, Sigma-Aldrich), potassium phenyl sulfate (98%, Tokyo Chemical Industry), and methyl sulfate (99%, Macklin) (Huang et al., 2018; Olson et al., 2011; Wang et al., 2018; Wang et al., 2021b). The validation of these standards has been previously documented in our studies (Yang et al., 2023; Wang et al., 2021b). The recoveries of the aforementioned surrogate standards were 88%, 89%, 94%, 84%, 84%, 87%, and 88% respectively. The present study identified a total of up to 155 OSs, of which 92 OS compounds were quantified using the aforementioned surrogate standards. Further details regarding the identification of OS species and data quality control can be found in our recent work (Yang et al., 2024; Yang et al., 2023).

It is imperative to acknowledge the limitations of the OS species quantified in this study. While the quantified OS concentration value should not be regarded as an accurate measurement of OS compounds, it is a best solution in the absence of authentic OS standards. Furthermore, earlier research suggested that the quantification of OSs might be affected by the sampling procedure in the absence of SO_2 denudation (Kristensen et al., 2016; Brüggemann et al., 2021). It is reasonable to assume that if SO_2 can react heterogeneously with components on filters to produce OSs, these processes are also likely to occur on ambient particles prior to being sampled. Consequently, the potential effect of sampling without SO_2 removal on OS quantifications was not considered (Yang et al., 2024). Nevertheless, we also acknowledge that there exists a possibility of an overestimation of OSs in fine aerosols, due to the potential reactivity of SO_2 and NO_x on the filters during sample collection (as indicated by Hartmut Hermman's lab) (Brüggemann et al., 2021).

S3. Analysis of nitrogen-containing organic compounds (NOCs) and identification of NOC precursors

NOCs were analyzed using the same UPLC-MS system (Waters, USA) as for OS measurement. The mass analyzer possesses a mass resolving power of ≥ 40000 at full width at half maximum (FWHM) (m/z 956) (Ma et al., 2024; Wang et al., 2021b). Compounds with identical molecular formulas were summed without making distinctions between isomers since the differentiation of isomers is beyond the scope of the present research. This approach was similar to that employed in previous studies (Sun et al., 2024; Ma et al., 2024; Jiang et al., 2023). The mass range of detected compounds (m/z 50–700) included a variety of compounds, ranging from small organic acids to larger secondary organic aerosol components (Ma et al., 2024).

The identification of the precursors of aerosol NOCs presents a significant challenge, owing to the complexity of their sources and the variability of the atmospheric processes. According to previous studies (Nie et al., 2022; Guo et al., 2022b), the potential precursors of organic compounds in aerosols have been classified based on well-established atmospheric reactions. Subsequent refinements to this classification were made by Jiang et al. (2023) for CHON− compounds in ambient aerosols. Additionally, we have refined the identification process to facilitate the classification of Re-NOC (CHN+ and CHON+) precursors. In this study, the CHON− and CHON+ compounds were classified into the following categories, including isoprene-, monoterpene-, aliphatic-, and aromatic-derived Ox-NOCs and aliphatic-, heterocyclic-, and aromatic-derived Re-NOCs. The specific classification procedure was illustrated in Figure S2. The isoprene-CHON and monoterpene-CHON lists mentioned in Figure S2 were derived from previous field observation and laboratory experiments (details in Tables S5 and S6) (Ng et al., 2008; Xu et al., 2021b;

Zhao et al., 2021; Tian et al., 2023; Wu et al., 2021; Shen et al., 2022; Pullinen et al., 2020; Devault and Ziemann, 2021). In particular, an additional identification of isoprene- and monoterpenes-derived NOCs was conducted via a correlation analysis between known and unknown isoprene- and monoterpenes-derived NOCs. The acceptance of compounds was based on the *r* value to be greater than 0.6 (P <0.01). It is important to note that the classification of CHN+ compounds was limited to aliphatic, monoaromatic, and polyaromatic categories (Wang et al., 2021a; Yassine et al., 2014).

S4. Prediction of pH

ISORROPIA-II has been demonstrated to function across a broader range of relative humidity (RH) and air temperature (T), facilitating the prediction of aerosol pH (Guo et al., 2015; Song et al., 2018; Liu et al., 2017; Yang et al., 2024; Nguyen et al., 2016). The model was operated using the particle-phase concentrations of inorganic ions, along with the T and RH as inputs. In addition, the forward mode with the thermodynamically metastable state was selected. This selection is supported by our previous studies (Yang et al., 2024; Ma et al., 2024; Gui et al., 2024; Xu et al., 2023; Xu et al., 2024). The model was run in forward mode for metastable aerosols, yielding more accurate aerosol pH predictions than reverse-mode calculations using only aerosol data input (Wang et al., 2021b; Guo et al., 2015; Hennigan et al., 2015). Previous studies have suggested that gas-phase component input (e.g., NH_3) may influence the accuracy of pH predictions (Guo et al., 2022b). For instance, the pH values reported in the study by Wang et al. (2021c) were increased by one unit to reduce the prediction error when no NH_3 input was incorporated into ISORROPIA-II. In this study, even when a recalibration of the pH scale by one unit was taken into account, the predicted aerosol pH still indicated an acidic nature. Consequently, the pH values documented in this study merely functioned as an important indicator of aerosol acidity.

Table S1. Mean values (± SD) of the major parameters observed during different periods.

Parameter	Aug – Nov (Autumn) (ng m^{-3})	Dec – Feb (Winter) (ng m^{-3})	Mar – May (Spring) (ng m^{-3})	Jun – Aug (Summer) (ng m^{-3})	One-year period
T (°C)	28.6 ± 0.7	27.08 ± 1.2	26.26 ± 2.71	27.98 ± 0.72	27.4 ± 1.79
RH (%)	84.92 ± 1.91	81.6 ± 14.56	85.52 ± 7.43	86.44 ± 2.85	84.29 ± 9.22
NO_2 (μg m^{-3})	4.76 ± 6.62	9.04 ± 5.81	0.52 ± 0.08	4.94 ± 5.36	5.09 ± 5.98
O_3 (μg m^{-3})	55.52 ± 14.25	73.15 ± 25.63	57.87 ± 19.6	48.85 ± 7.85	60.55 ± 20.94
O_x (μg m^{-3})	60.35±13.23	82.18 ± 26.07	58.39 ± 19.63	53.48 ± 15.81	65.66 ± 22.28
pH	3.44 ± 3.73	3.51 ± 2.77	2.2 ± 1	3.2 ± 1.73	3.1 ± 2.56
NO_3^- (μg m^{-3})	0.16 ± 0.1	0.18 ± 0.08	0.14 ± 0.04	0.53 ± 0.27	0.23 ± 0.2
SO_4^{2-} (μg m^{-3})	3.24 ± 1.86	3.88 ± 1.66	5.31 ± 1.22	1.63 ± 0.69	3.67 ± 1.9
Ca^{2+} (μg m^{-3})	0.21 ± 0.15	0.14 ± 0.11	0.21 ± 0.07	0.17 ± 0.08	0.18 ± 0.11
Mg^{2+} (μg m^{-3})	0.09 ± 0.03	0.12 ± 0.06	0.09 ± 0.05	0.2 ± 0.14	0.12 ± 0.08
K^+ (μg m^{-3})	0.08 ± 0.07	0.13 ± 0.09	0.14 ± 0.08	1.32 ± 1.24	0.34 ± 0.7
Na^+ (μg m^{-3})	0.71 ± 0.46	1.36 ± 0.65	0.98 ± 0.39	0.24 ± 0.43	0.9 ± 0.64
NH_4^+ (μg m^{-3})	0.38 ± 0.59	0.67 ± 0.62	1.35 ± 0.46	0.06 ± 0.08	0.66 ± 0.68
Cl^- (μg m^{-3})	0.53 ± 0.41	1.2 ± 0.62	0.78 ± 0.48	2.46 ± 1.85	1.17 ± 1.12
SST (°C)	28.38 ± 0.84	24.94 ± 0.86	26.9 ± 1.98	29.27 ± 0.58	27.4 ± 2.01
Chl *a* (mg m^{-3})	0.12 ± 0.05	0.16 ± 0.05	0.13 ± 0.07	0.12 ± 0.09	0.13 ± 0.07

Table S2. Mean mass concentrations (± SD) of quantified OS_i, OS_m, and C_2–C_3 OSs in $PM_{2.5}$ collected in the Sansha area in different periods.

Formula	MW	Aug – Nov (ng m^{-3})	Dec – Feb (ng m^{-3})	Mar – May (ng m^{-3})	Jun – Aug (ng m^{-3})	Mean (ng m^{-3})
OS_i						
$C_4H_7O_5S^-$	167.0014	0.8 ± 0.07	1.09 ± 0.32	0.81 ± 0.09	0.73 ± 0.06	0.88 ± 0.24
$C_5H_9O_6S^-$	197.0120	0.91 ± 0.15	1.74 ± 1.08	0.97 ± 0.25	0.85 ± 0.12	1.18 ± 0.73
$C_4H_7O_7S^-$	198.9912	0.87 ± 0.14	1.32 ± 0.6	0.97 ± 0.29	0.87 ± 0.13	1.04 ± 0.42
$C_5H_{11}O_6S^-$	199.0276	0.74 ± 0.02	0.82 ± 0.11	0.75 ± 0.04	0.74 ± 0.05	0.77 ± 0.08
$C_5H_7O_7S^-$	210.9912	1.4 ± 0.62	2.03 ± 1.12	1.47 ± 0.54	1.27 ± 0.46	1.6 ± 0.82
$C_5H_9O_7S^-$	213.0069	0.96 ± 0.14	1.29 ± 0.5	0.94 ± 0.18	1.32 ± 0.36	1.13 ± 0.38
$C_5H_{11}O_7S^-$	215.0225	0.82 ± 0.12	0.87 ± 0.15	0.79 ± 0.1	1.02 ± 0.16	0.86 ± 0.15
$C_7H_9O_7S^-$	237.0069	0.78 ± 0.04	1.18 ± 0.57	0.84 ± 0.17	0.77 ± 0.07	0.92 ± 0.38
$C_5H_7O_8S^-$	226.9862	1.15 ± 0.51	1.95 ± 1.18	1.42 ± 0.55	0.99 ± 0.24	1.45 ± 0.85
$C_4H_8NO_7S^-$	243.9763	0.73 ± 0.01	0.78 ± 0.09	0.71 ± 0.02	0.7 ± 0.04	0.73 ± 0.06
$C_4H_7O_8S^-$	214.9862	0.72 ± 0.01	0.75 ± 0.04	0.72 ± 0.03	0.69 ± 0.04	0.72 ± 0.04
$C_4H_5O_7S^-$	196.9756	0.87 ± 0.08	1.12 ± 0.28	0.93 ± 0.12	0.83 ± 0.09	0.96 ± 0.21
$C_4H_6NO_9S^-$	243.9763	0.74 ± 0.02	0.74 ± 0.03	0.71 ± 0.01	0.68 ± 0.04	0.72 ± 0.03
$C_5H_9O_8S^-$	229.0018	0.85 ± 0.14	1.1 ± 0.6	0.85 ± 0.12	0.97 ± 0.14	0.95 ± 0.37
$C_4H_7O_6S^-$	182.9963	1.08 ± 0.21	1.63 ± 0.72	1.08 ± 0.26	0.98 ± 0.12	1.24 ± 0.51
$C_5H_8NO_7S^-$	226.0021	0.75 ± 0.03	0.94 ± 0.25	0.74 ± 0.04	0.72 ± 0.05	0.8 ± 0.17
Total OS_i		10.75 ± 0.81	14.04 ± 4.45	10.82 ± 1.25	11 ± 1.09	11.88 ± 3.03
OS_m						
$C_7H_{11}O_6S^-$	223.0276	1.49 ± 0.45	2.08 ± 1.13	1.14 ± 0.19	1.92 ± 1.63	1.92 ± 1.63
$C_7H_{11}O_7S^-$	239.0225	1.22 ± 0.29	2.28 ± 1.66	1.15 ± 0.2	1.82 ± 1.45	1.82 ± 1.45
$C_{10}H_{15}O_7S^-$	279.0538	1.03 ± 0.1	1.67 ± 0.8	1.01 ± 0.08	1.32 ± 0.67	1.32 ± 0.67
$C_{10}H_{17}O_5S^-$	249.0797	0.02 ± 0	0.03 ± 0.02	0.02 ± 0.01	0.02 ± 0.01	0.02 ± 0.01
$C_9H_{14}NO_8S^-$	296.0440	0.21 ± 0.01	0.25 ± 0.07	0.21 ± 0.02	0.22 ± 0.04	0.22 ± 0.04
$C_{10}H_{16}NO_{10}S^-$	342.0495	0.21 ± 0.01	0.23 ± 0.05	0.2 ± 0	0.21 ± 0.03	0.21 ± 0.03
$C_9H_{15}O_6S^-$	251.0589	0.24 ± 0.02	0.36 ± 0.17	0.23 ± 0.01	0.29 ± 0.12	0.29 ± 0.12
$C_8H_{13}O_7S^-$	253.0382	1.17 ± 0.15	1.44 ± 0.52	1.09 ± 0.11	1.29 ± 0.39	1.29 ± 0.39
Total OS_m		5.59 ± 0.87	8.35 ± 4.05	5.06 ± 0.52	6.26 ± 2.75	7.11 ± 4.02
C_2–C_3 OSs						
$C_3H_5O_4S^-$	136.9909	1.22 ± 0.19	1.4 ± 0.29	1.22 ± 0.13	1.25 ± 0.15	1.28 ± 0.22
$C_2H_3O_5S^-$	138.9701	1.25 ± 0.19	1.45 ± 0.28	1.35 ± 0.17	1.21 ± 0.14	1.33 ± 0.23
$C_3H_5O_5S^-$	152.9858	2.14 ± 0.87	2.78 ± 1.19	1.93 ± 0.45	2.24 ± 0.67	2.31 ± 0.92
$C_2H_3O_6S^-$	154.9650	2.98 ± 2.21	4.66 ± 2.42	4.38 ± 2.02	3.08 ± 0.87	3.9 ± 2.15
$C_3H_7O_5S^-$	155.0014	1.04 ± 0.07	1.56 ± 0.6	1.07 ± 0.16	0.97 ± 0.06	1.2 ± 0.43
$C_3H_5O_6S^-$	168.9807	1.27 ± 0.38	2.03 ± 1.01	1.48 ± 0.51	0.99 ± 0.2	1.52 ± 0.76
Total $C_{2\text{-}3}$ OSs		9.9 ± 3.75	13.87 ± 5.53	11.43 ± 3.21	9.75 ± 2	11.54 ± 4.35

Table S3. Mean mass concentrations (± SD) of quantified anthropogenic OSs in $PM_{2.5}$ collected in the Sansha area in different periods.

Formula	MW	Aug – Nov (ng m^{-3})	Dec – Feb (ng m^{-3})	Mar – May (ng m^{-3})	Jun – Aug (ng m^{-3})	Mean (ng m^{-3})
Aliphatic OSs						
$C_{12}H_{21}O_7S^-$	309.1008	0.03 ± 0.01	0.04 ± 0.02	0.03 ± 0.01	0.03 ± 0.01	0.03 ± 0.01
$C_8H_{17}O_4S^-$	210.0926	0.02 ± 0	0.03 ± 0.02	0.02 ± 0	0.02 ± 0.01	0.02 ± 0.01
$C_7H_{15}O_4S^-$	195.0691	0.02 ± 0.01	0.03 ± 0.01	0.03 ± 0	0.03 ± 0.01	0.03 ± 0.01
$C_7H_{15}O_5S^-$	211.064	0.02 ± 0	0.02 ± 0	0.02 ± 0	0.02 ± 0.01	0.02 ± 0
$C_9H_{19}O_4S^-$	223.1004	0.03 ± 0.01	0.05 ± 0.02	0.03 ± 0	0.04 ± 0.01	0.04 ± 0.01
$C_{10}H_{21}O_4S^-$	237.1161	0.06 ± 0.01	0.08 ± 0.02	0.07 ± 0.01	0.07 ± 0.02	0.07 ± 0.02
$C_7H_{13}O_5S^-$	209.0484	0.02 ± 0	0.11 ± 0.17	0.02 ± 0	0.05 ± 0.1	0.05 ± 0.1
$C_9H_{17}O_5S^-$	237.0797	0.02 ± 0	0.02 ± 0.01	0.02 ± 0	0.02 ± 0	0.02 ± 0
$C_{10}H_{19}O_5S^-$	251.0953	0.02 ± 0	0.03 ± 0.01	0.02 ± 0	0.03 ± 0.01	0.03 ± 0.01
$C_9H_{17}O_7S^-$	269.0695	0.03 ± 0	0.03 ± 0.01	0.03 ± 0	0.03 ± 0.01	0.03 ± 0.01
$C_9H_{17}O_6S^-$	253.0746	0.02 ± 0	0.03 ± 0.02	0.02 ± 0	0.03 ± 0.01	0.03 ± 0.01
$C_{13}H_{25}O_6S^-$	293.1423	0.02 ± 0.01	0.03 ± 0.01	0.03 ± 0	0.03 ± 0.01	0.03 ± 0.01
$C_{14}H_{27}O_6S^-$	323.1528	0.02 ± 0	0.03 ± 0.01	0.03 ± 0	0.03 ± 0.01	0.03 ± 0.01
$C_{16}H_{31}O_5S^-$	335.1892	0.02 ± 0	0.03 ± 0.02	0.02 ± 0	0.02 ± 0.02	0.02 ± 0.01
$C_{18}H_{35}O_5S^-$	363.2205	0.03 ± 0.01	0.02 ± 0.01	0.02 ± 0	0.03 ± 0	0.03 ± 0.01
$C_{17}H_{33}O_5S^-$	363.2205	0.02 ± 0	0.06 ± 0.04	0.04 ± 0.01	0.02 ± 0.01	0.02 ± 0.01
$C_{16}H_{31}O_6S^-$	351.1841	0.03 ± 0	0.03 ± 0.01	0.03 ± 0	0.05 ± 0.02	0.04 ± 0.03
$C_8H_{15}O_5S^-$	223.0640	0.02±0	0.03 ± 0.01	0.02 ± 0	0.03 ± 0.01	0.02 ± 0.01
$C_7H_{13}O_6S^-$	225.0433	0.02 ± 0.01	0.04 ± 0.03	0.02 ± 0	0.03 ± 0.02	0.03 ± 0.02
$C_8H_{15}O_6S^-$	239.0589	0.03 ± 0.01	0.06 ± 0.03	0.03 ± 0.01	0.04 ± 0.03	0.04 ± 0.02
$C_{11}H_{21}O_5S^-$	265.1110	0.02 ± 0	0.03 ± 0.01	0.03 ± 0.01	0.03 ± 0.01	0.03 ± 0.01
$C_{10}H_{19}O_6S^-$	267.0902	0.02 ± 0	0.03 ± 0.01	0.02 ± 0	0.02 ± 0.01	0.02 ± 0.01
$C_7H_{13}O_9S^-$	273.0280	0.02 ± 0	0.02 ± 0	0.02 ± 0	0.02 ± 0	0.02 ± 0
$C_{10}H_{17}O_5S^-$	249.0797	0.03 ± 0	0.02 ± 0.01	0.02 ± 0	0.03 ± 0.01	0.03 ± 0.01
$C_9H_{15}O_6S^-$	251.0589	0.02 ± 0	0.04 ± 0.01	0.03 ± 0	0.03 ± 0.02	0.02 ± 0
$C_9H_{15}O_5S^-$	235.0640	0.02 ± 0	0.04 ± 0.02	0.02 ± 0	0.02 ± 0	0.02 ± 0.02
$C_8H_{13}O_6S^-$	237.0433	0.04 ± 0.02	0.07 ± 0.05	0.03 ± 0.02	0.05 ± 0.04	0.04 ± 0.04
$C_9H_{15}O_7S^-$	267.0538	0.02 ± 0.01	0.03 ± 0.02	0.02 ± 0	0.02 ± 0.02	0.02 ± 0.01
Total ali. OSs		0.68 ± 0.06	1.07 ± 0.5	0.72 ± 0.07	0.69 ± 0.07	0.82 ± 0.34
Aromatic OSs						
$C_{11}H_{19}O_{11}S^-$	359.0648	0.13 ± 0.01	0.19 ± 0.07	0.14 ± 0.01	0.13 ± 0.01	0.15 ± 0.05
$C_{10}H_{17}O_{12}S^-$	361.0441	0.11 ± 0	0.11 ± 0.01	0.11 ± 0	0.11 ± 0.01	0.11 ± 0.01
$C_7H_{11}O_{10}S^-$	287.0073	0.11 ± 0	0.14 ± 0.03	0.12 ± 0.01	0.11 ± 0.01	0.12 ± 0.02
$C_8H_{13}O_9S^-$	285.0280	0.11 ± 0	0.14 ± 0.03	0.12 ± 0.01	0.11 ± 0.01	0.12 ± 0.02
$C_8H_{13}O_{10}S^-$	301.0229	0.12 ± 0	0.15 ± 0.04	0.13 ± 0.02	0.12 ± 0.01	0.13 ± 0.03
$C_{11}H_{17}O_{11}S^-$	357.0492	0.13 ± 0.03	0.12 ± 0.01	0.11 ± 0	0.11 ± 0.01	0.12 ± 0.02
$C_9H_{11}O_{13}S^-$	358.9920	0.12 ± 0	0.14 ± 0.02	0.13 ± 0.01	0.12 ± 0.01	0.13 ± 0.01
$C_8H_{12}NO_{11}S^-$	330.0131	0.12 ± 0.01	0.15 ± 0.06	0.11 ± 0.01	0.11 ± 0.01	0.13 ± 0.04

$C_8H_7O_5S^-$	215.0014	0.12 ± 0.01	0.14 ± 0.03	0.12 ± 0.01	0.11 ± 0.01	0.13 ± 0.02
$C_8H_7NO_5S^-$	229.0045	0.15 ± 0.04	0.23 ± 0.18	0.15 ± 0.03	0.19 ± 0.04	0.18 ± 0.11
$C_9H_9O_6S^-$	245.0120	0.11 ± 0	0.12 ± 0.01	0.11 ± 0	0.11 ± 0.01	0.11 ± 0.01
$C_8H_7O_4S^-$	199.0065	0.17 ± 0.01	0.17 ± 0.02	0.17 ± 0.01	0.15 ± 0.01	0.17 ± 0.01
$C_9H_7O_7S^-$	258.9912	0.11 ± 0	0.14 ± 0.05	0.11 ± 0	0.11 ± 0.01	0.12 ± 0.03
$C_8H_5O_6S^-$	228.9807	0.12 ± 0.01	0.14 ± 0.03	0.12 ± 0.01	0.11 ± 0.01	0.12 ± 0.02
$C_9H_7O_6S^-$	242.9963	0.12 ± 0	0.14 ± 0.04	0.11 ± 0	0.11 ± 0.01	0.12 ± 0.03
$C_9H_3O_{11}S^-$	318.9396	0.11 ± 0	0.12 ± 0.01	0.11 ± 0	0.11 ± 0.01	0.11±0.01
$C_{10}H_5O_{12}S^-$	348.9502	0.11 ± 0	0.11 ± 0	0.11 ± 0	0.11 ± 0.01	0.11 ± 0
$C_{43}H_{63}O_5S^-$	691.4396	0.13 ± 0.02	0.12 ± 0.02	0.11 ± 0.01	0.2 ± 0.16	0.14 ± 0.08
$C_7H_{11}O_9S^-$	271.0124	0.12 ± 0.01	0.15 ± 0.04	0.12 ± 0.01	0.12 ± 0.01	0.13 ± 0.03
$C_{10}H_7O_{11}S^-$	334.9709	0.11 ± 0	0.11 ± 0	0.11 ± 0.01	0.11 ± 0.01	0.11 ± 0.01
$C_{10}H_5O_{11}S^-$	332.9553	0.11 ± 0	0.11 ± 0.01	0.11 ± 0	0.11 ± 0.01	0.11 ± 0.01
$C_{12}H_7O_{13}S^-$	390.9607	0.12 ± 0	0.12 ± 0	0.12 ± 0	0.11 ± 0.01	0.12±0.01
$C_7H_5O_5S^-$	200.9858	0.12 ± 0	0.17 ± 0.07	0.12 ± 0.01	0.11 ± 0.01	0.13 ± 0.05
$C_9H_9O_4S^-$	213.0222	0.15 ± 0.03	0.2 ± 0.09	0.17 ± 0.05	0.14 ± 0.03	0.17 ± 0.06
$C_{23}H_{19}O_7S^-$	439.0851	0.2 ± 0.17	0.12 ± 0.01	0.13 ± 0.01	0.15 ± 0.04	0.15 ± 0.09
$C_{25}H_{21}O_7S^-$	465.1008	0.12 ± 0.01	0.12 ± 0.01	0.11 ± 0	0.11 ± 0.01	0.12 ± 0.01
$C_{24}H_{17}O_4S^-$	401.0848	0.14 ± 0.01	0.32 ± 0.39	0.14 ± 0.01	0.13 ± 0.01	0.2 ± 0.23
$C_{27}H_{21}O_7S^-$	489.1008	0.11 ± 0	0.11 ± 0	0.11 ± 0	0.1 ± 0.01	0.11 ± 0
$C_6H_5O_4S^-$	172.9909	0.11 ± 0.01	0.13 ± 0.01	0.11 ± 0	0.11 ± 0.01	0.12 ± 0.01
$C_7H_7O_4S^-$	187.0065	0.11 ± 0.01	0.13 ± 0.02	0.11 ± 0	0.11 ± 0.01	0.12 ± 0.01
$C_{12}H_{21}N_2O_{11}S^-$	401.0866	0.14 ± 0.01	0.32 ± 0.39	0.14 ± 0.01	0.13 ± 0.01	0.2 ± 0.23
Total aro. OSs		3.91 ± 0.23	4.67 ± 1.42	3.79 ± 0.17	3.79 ± 0.29	4.1 ± 0.9
OS_a-other[a]						
$C_4H_7O_4S^-$	151.0065	0.15 ± 0.02	0.16 ± 0.02	0.14 ± 0.02	0.14 ± 0.01	0.15 ± 0.02
$C_5H_7O_6S^-$	194.9963	1.21 ± 0.17	1.54 ± 0.4	1.21 ± 0.15	1.14 ± 0.13	1.3 ± 0.31
$C_6H_9O_6S^-$	209.0120	1.48 ± 0.35	4.45 ± 3.82	2 ± 1.2	1.69 ± 0.42	2.61 ± 2.57

[a]The term "OS_a" was used to denote aliphatic and aromatic OSs (Yang et al., 2024). However, several OS species were identified as either non-aromatic or non-aliphatic categories. Thus, these componuds were classified as other OS_a compounds (i.e.,OS_a-other) (Huang et al., 2018; Kundu et al., 2013; Wang et al., 2021b; Yang et al., 2024). All aliphatic and aromatic OSs and OS_a-other were collectively referred to as OS_a.

Table S4. Mean mass concentrations of various OSs in $PM_{2.5}$ at different locations worldwide.

Sampling site	Period		OS_i (ng m^{-3})	OS_m (ng m^{-3})	OS_a (ng m^{-3})	C_2-C_3 OSs (ng m^{-3})	Total (ng m^{-3})	Reference
Urban site								
Shanghai, China	**2021**	**Summer**	**85.38**	**30.61**	**19.31**	**23.38**	**158.68**	**(Yang et al., 2023)**
Pearl River Delta, China	2012	Summer	0.68	-	-	-	0.68	(He et al., 2014)
Guangzhou, China	2019	Summer	181.8	10.8	-	-	192.6	(Bryant et al., 2021)
Shanghai, China	2012	Spring	0.017	0.20	0.219	-	0.44	(Ma et al., 2014)
		Summer	23.1	26.7	0.77	-	50.57	
		Autumn	0.063	0.77	0.79	-	1.62	
		Winter	0.82	0.90	0.72	-	2.44	
Xi'an, China	2014	Winter	-	-	0.14	77.3	77.44	(Huang et al., 2018)
Beijing, China	2016	Summer	12.3	15.1	-	-	27.4	(Wang et al., 2020)
		Winter	2.0	6.0	-	-	8.0	
Tianjing, China	2019	Winter	600	-	-	-	600	(Ding et al., 2022)
		Summer	400	-	-	-	400	
Beijing, China	**2016**	**Spring**	**16.2**	**13.0**	**-**	**19.5**	**48.7**	(Wang et al., 2018)
Xi'an, China	**2018**	**Winter**	**260.32**	**40.09**	**74.91**	**25.81**	**401.13**	(Yang et al., 2025)
Guangzhou, China	**2018**	**Winter**	**86.65**	**57.81**	**37.60**	**25.22**	**207.28**	(Yang et al., 2025)
Hong Kong, China	2016	Summer	163.19	2.95	-	-	166.14	(Wang et al., 2022)
	2017	Winter	97.96	17.26	-	-	115.22	
Guangzhou, China	2016	Summer	460.2	26.22	-	-	486.42	
	2017	Winter	88.03	20.96	-	-	108.99	
Beijing, China	2016	Summer	236.64	21.7	-	-	258.34	
	2017	Winter	176.32	36.01	-	-	212.33	

Shanghai, China	2016	Summer	326.4	34.9	-	-	361.3	
	2017	Winter	70.31	32.32	-	-	102.63	
Patra, Greece	2018	Winter	31.5	20.7	3.1	-	55.3	(Kanellopoulos et al., 2022)
		Spring	75.7	32.4	1.3	-	109.4	
		Summer	658	37.7	1.6	-	697.3	
		Autumn	53.2	25.4	1.1	-	79.7	
		Mean	204.6	29.05	1.78	-	235.43	
Pasadena, USA	2010	Summer	-	-	1.03	-	1.03	(Riva et al., 2015)
Copenhagen, Denmark	2011	Summer	11.31	0.87	-	-	18.18	(Nguyen et al., 2014)
Atlanta, GA, USA	**2014**	**Summer**	**1122.98**	**67.9**	**-**	**58.5**	**1249.38**	(Hettiyadura et al., 2019)
Manaus, Brazil	2016	Summer	1200.90	116.30	-	194.20	1511.40	(Riva et al., 2019)
Rotterdam, Netherlands	2013	Winter	3.32	22.91	9.07	-	35.30	(Glasius et al., 2018)
Bakersfield, CA, USA	2010	Summer	0.6	-	-	-	0.6	(Olson et al., 2011)
Riverside, CA, USA	2005	Summer	0.8	-	-	-	0.8	
Cleveland, OH, USA	2007	Summer	0.4	-	-	-	0.4	
Lahore, Pakistan		Winter	3.8	-	2.02	-	5.82	(Kundu et al., 2013)
Fresno, CA, USA	2016	Winter	74.00	-	-	-	74.00	(Chen et al., 2021)
		Summer	44.00	-	-	-	44.00	
Suburban and rural sites								
Zion, Illinois, USA	**2013**	**Spring**	**121.1**	**8.7**	**-**	**-**	**129.8**	(Hughes et al., 2021)
Towson, MD, USA	**2012**	Spring	3.75	2.62	1.6	0.7	8.67	(Meade et al., 2016)
		Summer	19.96	0.8	1.4	0.24	22.4	
		Autumn	2.22	2.9	1.4	0.35	6.87	
		Winter	0.5	2.41	0.9	0.3	4.11	
		Mean	**6.60**	**2.18**	**1.32**	**0.40**	**10.51**	

Birkenes, Norway	**2013**	Winter	0.96	1.53	0.65	-	3.14	(Glasius et al., 2018)
Risoe, Denmark		**Winter**	**2.28**	**6.39**	**2.16**	**-**	**10.83**	
Centreville, AL, USA	**2013**	**Summer**	**15.40**	**-**	**1.16**	**20.83**	**37.39**	(Hettiyadura et al., 2017)
Cabauw, Netherlands	**2013**	**Winter**	**1.98**	**16.10**	**6.67**	**-**	**24.75**	(Glasius et al., 2018)
Melpitz, Germany		Winter	11.12	49.33	32.83	-	93.28	
Vavihill, Sweden		Winter	2.75	6.39	4.15	-	13.29	
Lille Valby, Denmark	2009	Summer	0.27	2.4	-	-	2.67	(Yttri et al., 2011)
Yorkville, GA, USA	2010	Summer	115.11	-	-	-	115.11	(Lin et al., 2013)
Wangdu, China		Summer	-	36.7	-	-	36.7	(Brüggemann et al., 2019)
Forest site								
The Amazon forest	**2014**	**Spring**	**1733.1**	**116.3**	**-**	**268.4**	**2117.8**	(Riva et al., 2019)
Look Rock, TN, USA	2013	Summer	1256.75	-	-	-	1256.75	(Budisulistiorini et al., 2015)
Brasschaat, Belgium	2007	Summer	12.07	1.51	-	-	13.58	(Gómez-González et al., 2012)
Fichtelgebirge, Germany	2002	Summer	-	5.00	-	-	5.00	(Iinuma et al., 2010)
Hyytiälä, Finland	2009	Summer	-	4.91	1.47	-	6.38	(Yttri et al., 2011)
Silkeborg, Denmark	2008	Spring	0.03	0.52	-	-	0.55	(Kristensen and Glasius, 2011)
Polar and marine sites								
Station Nord, Greenland	**2010**	**Winter**	**5.03**	**0.43**	**-**	**-**	**5.46**	(Hansen et al., 2014)
Zeppelin Mountain, Svalbard	2010	Winter	1.34	0.14	-	-	1.48	(Hansen et al., 2014)
The Yellow Sea	**2019**	Spring	5.04	8.28	-	8.23	21.55	(Wang et al., 2023)
		Summer	22.98	7.53	-	12.7	43.21	
		Autumn	8.50	3.02	-	11.36	22.88	
		Winter	4.77	36.87	-	8.61	50.25	
		Mean	**10.32**	**13.93**	-	**10.22**	**34.47**	
Sansha, China	**2017-**	Autumn	10.75	5.59	7.43	9.9	33.67	This study

	2018	Winter	14.04	8.35	11.89	13.87	48.15	
		Spring	10.82	5.06	7.87	11.43	35.18	
		Summer	11.00	6.26	7.45	9.75	34.46	
		Mean	**11.88**	**7.11**	**8.66**	**11.54**	**39.19**	

The bold data were shown in Figure 1.

Table S5. The molecular formula list of potential isoprene-derived CHON compounds.

Formula[a]		
$C_4H_7N_1O_5$	$C_5H_8N_1O_9$	$C_5H_9N_3O_{13}$
$C_4H_7N_1O_6$	$C_5H_9N_1O_9$	$C_5H_{11}N_3O_{13}$
$C_4H_7N_1O_7$	$C_5H_{11}N_1O_9$	$C_5H_9N_4O_{12}$
$C_4H_9N_1O_7$	$C_5H_{13}N_1O_9$	$C_5H_{10}N_4O_{12}$
$C_4H_7N_1O_8$	$C_5H_8N_1O_{10}$	$C_5H_{10}N_4O_{13}$
$C_4H_7N_1O_9$	$C_5H_9N_1O_{10}$	$C_{10}H_{15}N_1O_{10}$
$C_4H_6N_2O_6$	$C_5H_{11}N_1O_{10}$	$C_{10}H_{16}N_2O_8$
$C_4H_6N_2O_7$	$C_5H_{10}N_1O_{11}$	$C_{10}H_{16}N_2O_9$
$C_4H_8N_2O_7$	$C_5H_{10}N_2O_6$	$C_{10}H_{16}N_2O_{10}$
$C_4H_6N_2O_8$	$C_5H_8N_2O_7$	$C_{10}H_{16}N_2O_{11}$
$C_4H_8N_2O_8$	$C_5H_{10}N_2O_7$	$C_{10}H_{18}N_2O_{11}$
$C_4H_7N_2O_9$	$C_5H_6N_2O_8$	$C_{10}H_{16}N_2O_{12}$
$C_4H_8N_2O_9$	$C_5H_8N_2O_8$	$C_{10}H_{16}N_2O_{13}$
$C_4H_8N_2O_{10}$	$C_5H_{10}N_2O_8$	$C_{10}H_{16}N_2O_{14}$
$C_4H_7N_3O_9$	$C_5H_8N_2O_9$	$C_{10}H_{16}N_2O_{15}$
$C_4H_7N_3O_{10}$	$C_5H_9N_2O_9$	$C_{10}H_{16}N_2O_{17}$
$C_4H_7N_3O_{11}$	$C_5H_{10}N_2O_9$	$C_{10}H_{17}N_3O_{12}$
$C_5H_7N_1O_4$	$C_5H_{12}N_2O_9$	$C_{10}H_{13}N_3O_{13}$
$C_5H_9N_1O_4$	$C_5H_8N_2O_{10}$	$C_{10}H_{17}N_3O_{13}$
$C_5H_7N_1O_5$	$C_5H_9N_2O_{10}$	$C_{10}H_{15}N_3O_{14}$
$C_5H_9N_1O_5$	$C_5H_{10}N_2O_{10}$	$C_{10}H_{17}N_3O_{14}$
$C_5H_7N_1O_6$	$C_5H_{12}N_2O_{10}$	$C_{10}H_{17}N_3O_{15}$
$C_5H_9N_1O_6$	$C_5H_8N_2O_{11}$	$C_{10}H_{17}N_3O_{16}$
$C_5H_{11}N_1O_6$	$C_5H_{10}N_2O_{11}$	$C_{10}H_{17}N_3O_{17}$
$C_5H_7N_1O_7$	$C_5H_{12}N_2O_{11}$	$C_{10}H_{17}N_3O_{18}$
$C_5H_9N_1O_7$	$C_5H_9N_3O_9$	$C_{10}H_{18}N_4O_{16}$
$C_5H_{11}N_1O_7$	$C_5H_{11}N_3O_9$	$C_{10}H_{18}N_4O_{17}$
$C_5H_7N_1O_8$	$C_5H_9N_3O_{10}$	$C_{10}H_{17}N_5O_{18}$
$C_5H_8N_1O_8$	$C_5H_{11}N_3O_{10}$	$C_{15}H_{24}N_4O_{18}$
$C_5H_9N_1O_8$	$C_5H_9N_3O_{11}$	$C_{15}H_{24}N_4O_{21}$
$C_5H_{11}N_1O_8$	$C_5H_{11}N_3O_{11}$	$C_{15}H_{24}N_4O_{22}$
$C_5H_7N_1O_9$	$C_5H_9N_3O_{12}$	$C_{15}H_{25}N_5O_{21}$

[a]The molecular formulas were derived from previous studies (Guo et al., 2022b; Xu et al., 2021b; Zhao et al., 2021; Tian et al., 2023; Wu et al., 2021; Ng et al., 2008).

Table S6. The molecular formula list of potential monoterpene-derived CHON compounds.

Formula[a]				
$C_6H_7N_1O_6$	$C_8H_{17}N_1O_5$	$C_9H_{13}N_1O_9$	$C_{10}H_{15}N_1O_6$	$C_{10}H_{12}N_2O_9$
$C_6H_7N_1O_7$	$C_8H_{11}N_1O_6$	$C_9H_{14}N_1O_9$	$C_{10}H_{16}N_1O_6$	$C_{10}H_{14}N_2O_9$
$C_6H_7N_1O_8$	$C_8H_{11}N_1O_7$	$C_9H_{15}N_1O_9$	$C_{10}H_{17}N_1O_6$	$C_{10}H_{15}N_2O_9$
$C_6H_9N_1O_9$	$C_8H_{12}N_1O_7$	$C_9H_{13}N_1O_{10}$	$C_{10}H_{13}N_1O_7$	$C_{10}H_{16}N_2O_9$
$C_6H_7N_1O_{10}$	$C_8H_{11}N_1O_8$	$C_9H_{14}N_1O_{10}$	$C_{10}H_{15}N_1O_7$	$C_{10}H_{18}N_2O_9$
$C_6H_7N_1O_{11}$	$C_8H_{12}N_1O_8$	$C_9H_{15}N_1O_{10}$	$C_{10}H_{16}N_1O_7$	$C_{10}H_{12}N_2O_{10}$
$C_6H_6N_2O_9$	$C_8H_{13}N_1O_8$	$C_9H_{13}N_1O_{11}$	$C_{10}H_{17}N_1O_7$	$C_{10}H_{14}N_2O_{10}$
$C_6H_{10}N_2O_{10}$	$C_8H_{15}N_1O_8$	$C_9H_{14}N_1O_{11}$	$C_{10}H_{13}N_1O_8$	$C_{10}H_{15}N_2O_{10}$
$C_7H_9N_1O_5$	$C_8H_{11}N_1O_9$	$C_9H_{15}N_1O_{11}$	$C_{10}H_{15}N_1O_8$	$C_{10}H_{16}N_2O_{10}$
$C_7H_{11}N_1O_5$	$C_8H_{12}N_1O_9$	$C_9H_{13}N_1O_{12}$	$C_{10}H_{16}N_1O_8$	$C_{10}H_{14}N_2O_{11}$
$C_7H_9N_1O_6$	$C_8H_{13}N_1O_9$	$C_9H_{14}N_1O_{12}$	$C_{10}H_{17}N_1O_8$	$C_{10}H_{15}N_2O_{11}$
$C_7H_{11}N_1O_6$	$C_8H_{11}N_1O_{10}$	$C_9H_{15}N_1O_{12}$	$C_{10}H_{13}N_1O_9$	$C_{10}H_{16}N_2O_{11}$
$C_7H_7N_1O_7$	$C_8H_{12}N_1O_{10}$	$C_9H_{13}N_1O_{13}$	$C_{10}H_{15}N_1O_9$	$C_{10}H_{14}N_2O_{12}$
$C_7H_9N_1O_7$	$C_8H_{13}N_1O_{10}$	$C_9H_{14}N_1O_{13}$	$C_{10}H_{16}N_1O_9$	$C_{10}H_{15}N_2O_{12}$
$C_7H_{11}N_1O_7$	$C_8H_{11}N_1O_{11}$	$C_9H_{15}N_1O_{13}$	$C_{10}H_{17}N_1O_9$	$C_{10}H_{16}N_2O_{12}$
$C_7H_7N_1O_8$	$C_8H_{12}N_1O_{11}$	$C_9H_{13}N_1O_{14}$	$C_{10}H_{15}N_1O_{10}$	$C_{10}H_{17}N_2O_{12}$
$C_7H_8N_1O_8$	$C_8H_{13}N_1O_{11}$	$C_9H_{14}N_1O_{14}$	$C_{10}H_{16}N_1O_{10}$	$C_{10}H_{14}N_2O_{13}$
$C_7H_9N_1O_8$	$C_8H_{11}N_1O_{12}$	$C_9H_{15}N_1O_{14}$	$C_{10}H_{17}N_1O_{10}$	$C_{10}H_{15}N_2O_{13}$
$C_7H_{10}N_1O_8$	$C_8H_{12}N_1O_{12}$	$C_9H_{13}N_2O_7$	$C_{10}H_{15}N_1O_{11}$	$C_{10}H_{16}N_2O_{13}$
$C_7H_{11}N_1O_8$	$C_8H_{13}N_1O_{12}$	$C_9H_{14}N_2O_8$	$C_{10}H_{16}N_1O_{11}$	$C_{10}H_{18}N_2O_{13}$
$C_7H_9N_1O_9$	$C_8H_{11}N_1O_{13}$	$C_9H_{10}N_2O_9$	$C_{10}H_{17}N_1O_{11}$	$C_{10}H_{14}N_2O_{14}$
$C_7H_{10}N_1O_9$	$C_8H_{10}N_2O_8$	$C_9H_{11}N_2O_9$	$C_{10}H_{18}N_1O_{11}$	$C_{10}H_{15}N_2O_{14}$
$C_7H_{11}N_1O_9$	$C_8H_{10}N_2O_{14}$	$C_9H_{12}N_2O_9$	$C_{10}H_{15}N_1O_{12}$	$C_{10}H_{16}N_2O_{14}$
$C_7H_9N_1O_{10}$	$C_9H_{11}N_1O_2$	$C_9H_{10}N_2O_{10}$	$C_{10}H_{16}N_1O_{12}$	$C_{10}H_{18}N_2O_{14}$
$C_7H_{10}N_1O_{10}$	$C_9H_{13}N_1O_2$	$C_9H_{11}N_2O_{10}$	$C_{10}H_{17}N_1O_{12}$	$C_{10}H_{14}N_2O_{15}$
$C_7H_{11}N_1O_{10}$	$C_9H_{17}N_1O_3$	$C_9H_{12}N_2O_{10}$	$C_{10}H_{15}N_1O_{13}$	$C_{10}H_{15}N_2O_{15}$
$C_7H_9N_1O_{11}$	$C_9H_{13}N_1O_4$	$C_9H_{10}N_2O_{11}$	$C_{10}H_{16}N_1O_{13}$	$C_{10}H_{16}N_2O_{15}$
$C_7H_{10}N_1O_{11}$	$C_9H_{14}N_1O_4$	$C_9H_{11}N_2O_{11}$	$C_{10}H_{17}N_1O_{13}$	$C_{10}H_{14}N_2O_{16}$
$C_7H_{11}N_1O_{11}$	$C_9H_{15}N_1O_4$	$C_9H_{12}N_2O_{11}$	$C_{10}H_{15}N_1O_{14}$	$C_{10}H_{15}N_2O_{16}$
$C_7H_9N_1O_{12}$	$C_9H_{11}N_1O_5$	$C_9H_{10}N_2O_{12}$	$C_{10}H_{16}N_1O_{14}$	$C_{10}H_{16}N_2O_{16}$
$C_7H_{10}N_1O_{12}$	$C_9H_{13}N_1O_5$	$C_9H_{11}N_2O_{12}$	$C_{10}H_{17}N_1O_{14}$	$C_{10}H_{15}N_3O_{11}$
$C_7H_{11}N_1O_{12}$	$C_9H_{12}N_1O_6$	$C_9H_{12}N_2O_{12}$	$C_{10}H_{15}N_1O_{15}$	$C_{10}H_{17}N_3O_{12}$
$C_7H_{11}N_1O_{15}$	$C_9H_{13}N_1O_6$	$C_9H_{14}N_2O_{12}$	$C_{10}H_{16}N_1O_{15}$	$C_{10}H_{15}N_3O_{13}$
$C_7H_8N_2O_8$	$C_9H_{16}N_1O_6$	$C_{10}H_{15}N_1O_3$	$C_{10}H_{17}N_1O_{15}$	$C_{10}H_{17}N_3O_{13}$
$C_7H_8N_2O_{10}$	$C_9H_{13}N_1O_7$	$C_{10}H_{17}N_1O_3$	$C_{10}H_{12}N_2O_5$	$C_{10}H_{15}N_3O_{14}$
$C_7H_8N_2O_{11}$	$C_9H_{14}N_1O_7$	$C_{10}H_{15}N_1O_4$	$C_{10}H_{20}N_2O_6$	$C_{10}H_{17}N_3O_{14}$
$C_7H_8N_2O_{12}$	$C_9H_{15}N_1O_7$	$C_{10}H_{17}N_1O_4$	$C_{10}H_{12}N_2O_8$	$C_{10}H_{15}N_3O_{15}$
$C_7H_8N_2O_{13}$	$C_9H_{13}N_1O_8$	$C_{10}H_{19}N_1O_4$	$C_{10}H_{14}N_2O_8$	$C_{10}H_{17}N_3O_{15}$
$C_7H_8N_2O_{14}$	$C_9H_{14}N_1O_8$	$C_{10}H_{15}N_1O_5$	$C_{10}H_{15}N_2O_8$	$C_{10}H_{17}N_3O_{16}$
$C_7H_{10}N_2O_{14}$	$C_9H_{15}N_1O_8$	$C_{10}H_{17}N_1O_5$	$C_{10}H_{16}N_2O_8$	$C_{11}H_{23}N_1O_3$
$C_8H_{13}N_1O_5$	$C_9H_{16}N_1O_8$	$C_{10}H_{13}N_1O_6$	$C_{10}H_{18}N_2O_8$	$C_{11}H_{17}N_1O_5$

$C_{11}H_{20}N_2O_5$	$C_{18}H_{28}N_2O_{12}$	$C_{19}H_{31}N_3O_{16}$	$C_{20}H_{30}N_2O_{12}$	$C_{20}H_{34}N_4O_{15}$
$C_{11}H_{18}N_2O_{10}$	$C_{18}H_{29}N_3O_{13}$	$C_{19}H_{31}N_3O_{17}$	$C_{20}H_{32}N_2O_{12}$	$C_{20}H_{30}N_4O_{16}$
$C_{12}H_{23}N_1O_3$	$C_{18}H_{29}N_3O_{14}$	$C_{19}H_{31}N_3O_{18}$	$C_{20}H_{30}N_2O_{13}$	$C_{20}H_{34}N_4O_{16}$
$C_{13}H_{25}N_1O_2$	$C_{19}H_{41}N_1O_2$	$C_{19}H_{31}N_3O_{19}$	$C_{20}H_{31}N_2O_{13}$	$C_{20}H_{30}N_4O_{17}$
$C_{13}H_{26}N_1O_{12}$	$C_{19}H_{38}N_1O_3$	$C_{19}H_{30}N_4O_{13}$	$C_{20}H_{32}N_2O_{13}$	$C_{20}H_{34}N_4O_{17}$
$C_{14}H_{26}N_1O_{10}$	$C_{19}H_{29}N_1O_4$	$C_{19}H_{30}N_4O_{15}$	$C_{20}H_{30}N_2O_{14}$	$C_{20}H_{30}N_4O_{18}$
$C_{14}H_{24}N_2O_5$	$C_{19}H_{29}N_1O_5$	$C_{19}H_{31}N_5O_{17}$	$C_{20}H_{31}N_2O_{14}$	$C_{20}H_{34}N_4O_{18}$
$C_{15}H_{30}N_1O_{14}$	$C_{19}H_{33}N_1O_5$	$C_{19}H_{31}N_5O_{18}$	$C_{20}H_{32}N_2O_{14}$	$C_{20}H_{30}N_4O_{19}$
$C_{16}H_{35}N_1O_3$	$C_{19}H_{29}N_1O_6$	$C_{19}H_{31}N_5O_{19}$	$C_{20}H_{30}N_2O_{15}$	$C_{20}H_{34}N_4O_{19}$
$C_{16}H_{32}N_1O_{13}$	$C_{19}H_{33}N_1O_6$	$C_{20}H_{31}N_1O_4$	$C_{20}H_{31}N_2O_{15}$	$C_{20}H_{30}N_4O_{20}$
$C_{16}H_{32}N_1O_{14}$	$C_{19}H_{31}N_1O_7$	$C_{20}H_{31}N_1O_5$	$C_{20}H_{32}N_2O_{15}$	$C_{20}H_{34}N_4O_{20}$
$C_{16}H_{32}N_1O_{15}$	$C_{19}H_{33}N_1O_7$	$C_{20}H_{35}N_1O_5$	$C_{20}H_{30}N_2O_{16}$	$C_{20}H_{30}N_4O_{21}$
$C_{17}H_{22}N_1O_6$	$C_{19}H_{35}N_1O_7$	$C_{20}H_{31}N_1O_6$	$C_{20}H_{31}N_2O_{16}$	$C_{20}H_{30}N_4O_{22}$
$C_{17}H_{28}N_1O_9$	$C_{19}H_{33}N_1O_8$	$C_{20}H_{33}N_1O_6$	$C_{20}H_{32}N_2O_{16}$	$C_{21}H_{35}N_1O_7$
$C_{17}H_{27}N_1O_{12}$	$C_{19}H_{35}N_1O_8$	$C_{20}H_{35}N_1O_6$	$C_{20}H_{30}N_2O_{17}$	$C_{21}H_{35}N_1O_8$
$C_{17}H_{32}N_1O_{13}$	$C_{19}H_{29}N_1O_{10}$	$C_{20}H_{31}N_1O_7$	$C_{20}H_{32}N_2O_{17}$	$C_{21}H_{23}N_1O_{10}$
$C_{17}H_{34}N_1O_{13}$	$C_{19}H_{31}N_1O_{10}$	$C_{20}H_{33}N_1O_7$	$C_{20}H_{32}N_2O_{18}$	$C_{21}H_{40}N_1O_{14}$
$C_{17}H_{34}N_1O_{14}$	$C_{19}H_{29}N_1O_{11}$	$C_{20}H_{35}N_1O_7$	$C_{20}H_{32}N_2O_{19}$	$C_{21}H_{40}N_1O_{15}$
$C_{17}H_{27}N_1O_{15}$	$C_{19}H_{31}N_1O_{11}$	$C_{20}H_{37}N_1O_7$	$C_{20}H_{32}N_2O_{20}$	$C_{21}H_{42}N_1O_{15}$
$C_{17}H_{34}N_1O_{15}$	$C_{19}H_{29}N_1O_{12}$	$C_{20}H_{31}N_1O_8$	$C_{20}H_{31}N_3O_{12}$	$C_{22}H_{44}N_1O_{14}$
$C_{17}H_{28}N_2O_9$	$C_{19}H_{31}N_1O_{12}$	$C_{20}H_{33}N_1O_8$	$C_{20}H_{33}N_3O_{12}$	$C_{22}H_{30}N_1O_{15}$
$C_{17}H_{26}N_2O_{12}$	$C_{19}H_{29}N_1O_{13}$	$C_{20}H_{31}N_1O_9$	$C_{20}H_{31}N_3O_{13}$	$C_{24}H_{36}N_1O_9$
$C_{17}H_{26}N_2O_{13}$	$C_{19}H_{31}N_1O_{13}$	$C_{20}H_{33}N_1O_9$	$C_{20}H_{33}N_3O_{13}$	$C_{25}H_{32}N_2O_5$
$C_{17}H_{28}N_2O_{13}$	$C_{19}H_{31}N_1O_{14}$	$C_{20}H_{39}N_1O_9$	$C_{20}H_{31}N_3O_{14}$	$C_{25}H_{28}N_2O_{13}$
$C_{17}H_{26}N_2O_{14}$	$C_{19}H_{38}N_1O_{14}$	$C_{20}H_{31}N_1O_{10}$	$C_{20}H_{33}N_3O_{14}$	$C_{26}H_{34}N_2O_4$
$C_{17}H_{26}N_2O_{15}$	$C_{19}H_{31}N_1O_{15}$	$C_{20}H_{31}N_1O_{11}$	$C_{20}H_{31}N_3O_{15}$	$C_{26}H_{34}N_2O_5$
$C_{17}H_{26}N_2O_{16}$	$C_{19}H_{38}N_1O_{15}$	$C_{20}H_{31}N_1O_{12}$	$C_{20}H_{33}N_3O_{15}$	$C_{26}H_{47}N_3O_{20}$
$C_{17}H_{26}N_2O_{17}$	$C_{19}H_{38}N_1O_{16}$	$C_{20}H_{33}N_1O_{12}$	$C_{20}H_{31}N_3O_{16}$	$C_{26}H_{47}N_5O_{25}$
$C_{17}H_{26}N_2O_{18}$	$C_{19}H_{30}N_1O_{17}$	$C_{20}H_{31}N_1O_{13}$	$C_{20}H_{32}N_3O_{16}$	$C_{27}H_{34}N_2O_4$
$C_{18}H_{27}N_1O_5$	$C_{19}H_{36}N_1O_{17}$	$C_{20}H_{40}N_1O_{14}$	$C_{20}H_{33}N_3O_{16}$	$C_{27}H_{36}N_2O_4$
$C_{18}H_{31}N_1O_7$	$C_{19}H_{24}N_2O_2$	$C_{20}H_{31}N_1O_{15}$	$C_{20}H_{31}N_3O_{17}$	$C_{27}H_{36}N_2O_5$
$C_{18}H_{31}N_1O_8$	$C_{19}H_{34}N_2O_8$	$C_{20}H_{33}N_1O_{15}$	$C_{20}H_{32}N_3O_{17}$	$C_{27}H_{24}N_2O_6$
$C_{18}H_{27}N_1O_{10}$	$C_{19}H_{30}N_2O_{10}$	$C_{20}H_{38}N_1O_{15}$	$C_{20}H_{33}N_3O_{17}$	$C_{27}H_{44}N_6O_{16}$
$C_{18}H_{28}N_1O_{13}$	$C_{19}H_{30}N_2O_{11}$	$C_{20}H_{40}N_1O_{15}$	$C_{20}H_{31}N_3O_{18}$	$C_{28}H_{43}N_1O_{18}$
$C_{18}H_{32}N_1O_{14}$	$C_{19}H_{30}N_2O_{12}$	$C_{20}H_{33}N_1O_{16}$	$C_{20}H_{32}N_3O_{18}$	$C_{28}H_{38}N_2O_4$
$C_{18}H_{34}N_1O_{14}$	$C_{19}H_{30}N_2O_{13}$	$C_{20}H_{38}N_1O_{16}$	$C_{20}H_{33}N_3O_{18}$	$C_{28}H_{38}N_2O_5$
$C_{18}H_{36}N_1O_{14}$	$C_{19}H_{30}N_2O_{14}$	$C_{20}H_{40}N_1O_{16}$	$C_{20}H_{31}N_3O_{19}$	$C_{28}H_{44}N_2O_{16}$
$C_{18}H_{29}N_1O_{15}$	$C_{19}H_{32}N_2O_{14}$	$C_{20}H_{32}N_2O_8$	$C_{20}H_{32}N_3O_{19}$	$C_{28}H_{45}N_5O_{16}$
$C_{18}H_{34}N_1O_{15}$	$C_{19}H_{30}N_2O_{15}$	$C_{20}H_{34}N_2O_8$	$C_{20}H_{33}N_3O_{19}$	$C_{28}H_{45}N_5O_{17}$
$C_{18}H_{36}N_1O_{15}$	$C_{19}H_{30}N_2O_{16}$	$C_{20}H_{30}N_2O_9$	$C_{20}H_{31}N_3O_{20}$	$C_{28}H_{43}N_5O_{22}$
$C_{18}H_{35}N_1O$	$C_{19}H_{30}N_2O_{17}$	$C_{20}H_{32}N_2O_9$	$C_{20}H_{33}N_3O_{20}$	$C_{29}H_{44}N_2O_{22}$
$C_{18}H_{34}N_2O_5$	$C_{19}H_{30}N_2O_{18}$	$C_{20}H_{32}N_2O_{10}$	$C_{20}H_{31}N_3O_{21}$	$C_{29}H_{47}N_3O_{19}$
$C_{18}H_{30}N_2O_7$	$C_{19}H_{30}N_2O_{19}$	$C_{20}H_{32}N_2O_{11}$	$C_{20}H_{30}N_4O_{14}$	$C_{29}H_{45}N_3O_{20}$
$C_{18}H_{28}N_2O_{11}$	$C_{19}H_{31}N_3O_{15}$	$C_{20}H_{34}N_2O_{11}$	$C_{20}H_{30}N_4O_{15}$	$C_{29}H_{47}N_3O_{21}$

$C_{29}H_{48}N_4O_{18}$	$C_{30}H_{47}N_1O_{18}$	$C_{30}H_{49}N_3O_{18}$	$C_{30}H_{47}N_3O_{24}$	$C_{30}H_{48}N_4O_{21}$
$C_{29}H_{46}N_4O_{19}$	$C_{30}H_{47}N_1O_{19}$	$C_{30}H_{47}N_3O_{19}$	$C_{30}H_{48}N_4O_{16}$	$C_{30}H_{48}N_4O_{22}$
$C_{29}H_{46}N_4O_{20}$	$C_{30}H_{48}N_2O_{18}$	$C_{30}H_{49}N_3O_{20}$	$C_{30}H_{48}N_4O_{17}$	$C_{30}H_{48}N_4O_{23}$
$C_{29}H_{46}N_4O_{22}$	$C_{30}H_{46}N_2O_{22}$	$C_{30}H_{47}N_3O_{21}$	$C_{30}H_{48}N_4O_{18}$	$C_{30}H_{48}N_4O_{24}$
$C_{29}H_{46}N_4O_{23}$	$C_{30}H_{48}N_2O_{23}$	$C_{30}H_{49}N_3O_{22}$	$C_{30}H_{48}N_4O_{19}$	$C_{30}H_{49}N_5O_{20}$
$C_{29}H_{46}N_4O_{24}$	$C_{30}H_{47}N_3O_{18}$	$C_{30}H_{47}N_3O_{23}$	$C_{30}H_{48}N_4O_{20}$	

[a]The molecular formulas were derived from previous studies (Shen et al., 2022; Guo et al., 2022b; Pullinen et al., 2020; Devault and Ziemann, 2021; Draper et al., 2015; Guo et al., 2022a; Xu et al., 2021a).

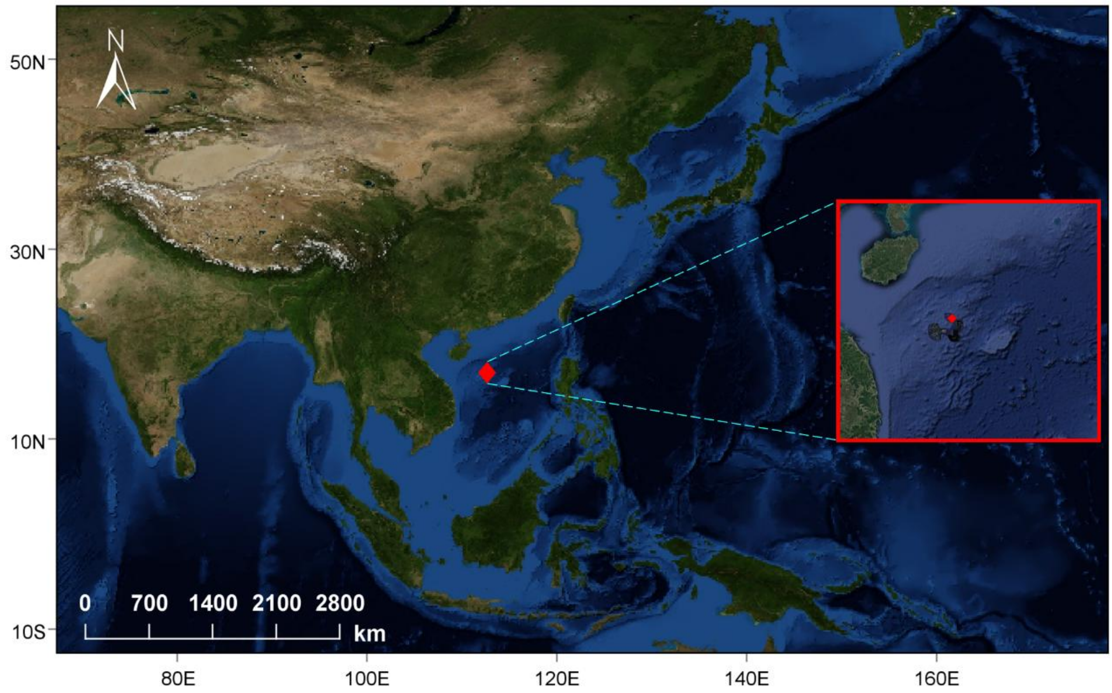

Figure S1. The location of the sampling site (112.33°E, 16.83°N). The map was derived from Baidu Maps (BIDU, China). The figure may contain a territory that is disputed according to the United Nations.

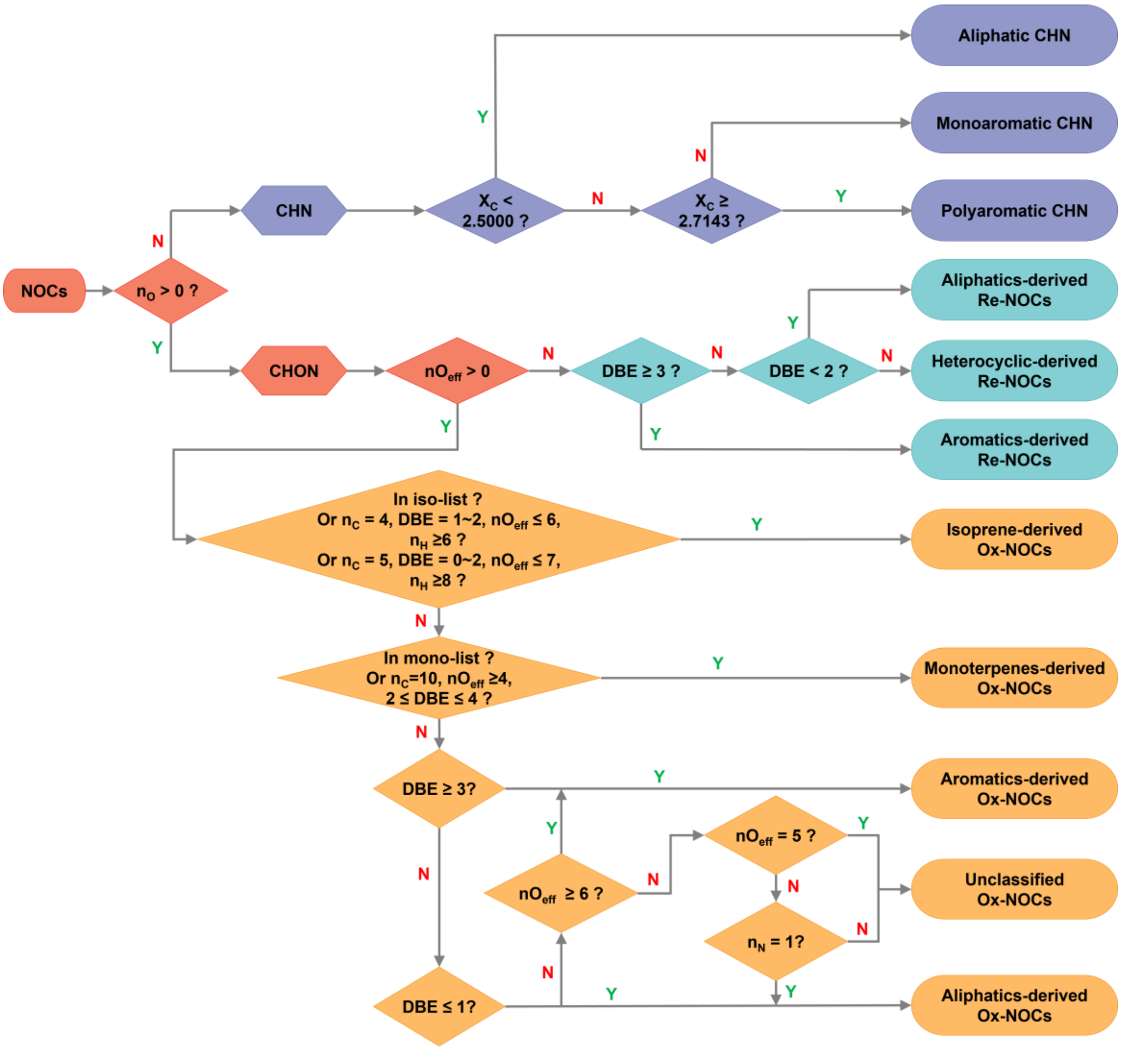

Figure S2. Workflow for the identification of the potential precursors of NOCs. The symbols n_C, n_N, n_H, n_O, and nO_{eff} represent the number of carbon, nitrogen, hydrogen, oxygen, and effective oxygen atoms in each NOC molecule, respectively. The symbols "Y" and "N" denote affirmative and negative responses, respectively.

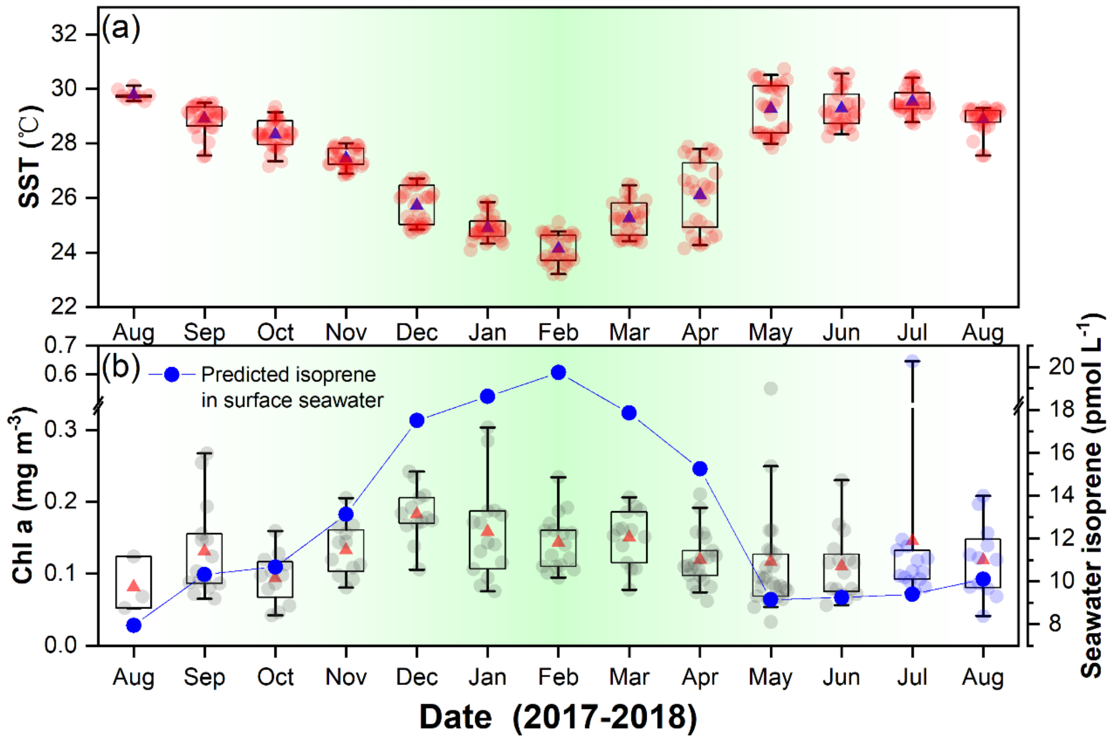

Figure S3. Distributions of (a) sea surface temperature (SST) and (b) the concentrations of chlorophyll *a* (Chl *a*) and predicted surface seawater isoprene over months in the Sansha area. Each box encompasses the 25th–75th percentiles. Whiskers are the 5th and 95th percentiles. The solid triangles inside boxes indicate the mean. SST data (0.25°×0.25°) were derived from NOAA Optimum Interpolation Sea Surface Temperature Version 2 (OISSTv2) dataset (Schneider et al., 2013). Chl *a* data (0.5°×0.5°) were derived from the MODIS Level-3 product. To prevent the extraction of missing values, the nearest available values within the radius of 0.75° and 1° around the sampling location were averaged. Isoprene concentrations in surface seawater were predicted by temperature-dependent empirical formulas (Wang et al., 2023).

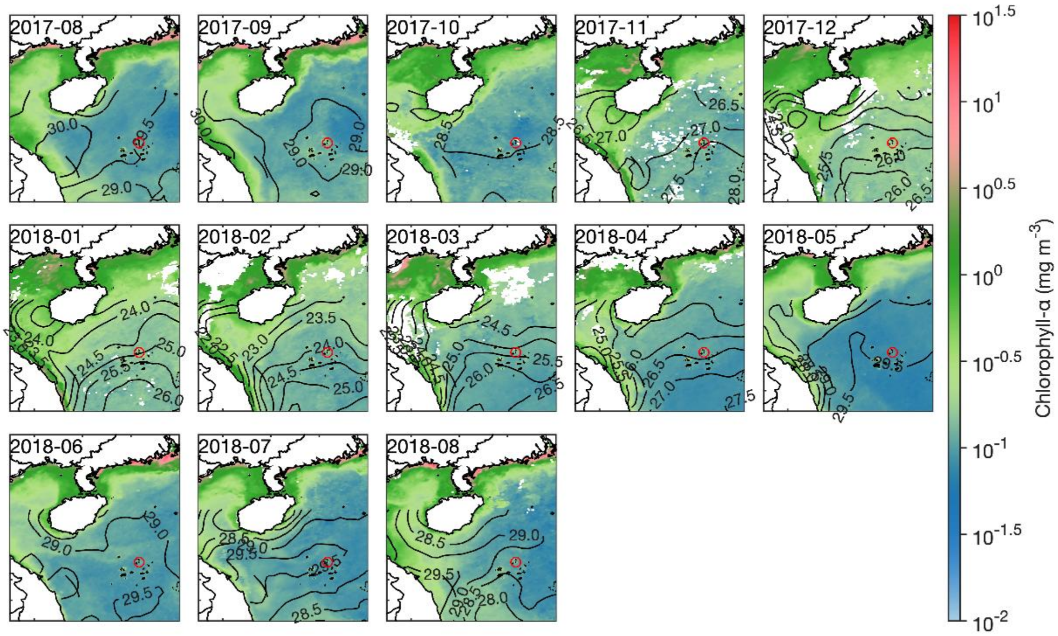

Figure S4. Illustrations showing the variations in sea surface temperature (shown as isothermal line in each panel) and Chl *a* concentrations over months in the Sansha area. The red circle indicates the location of Sansha.

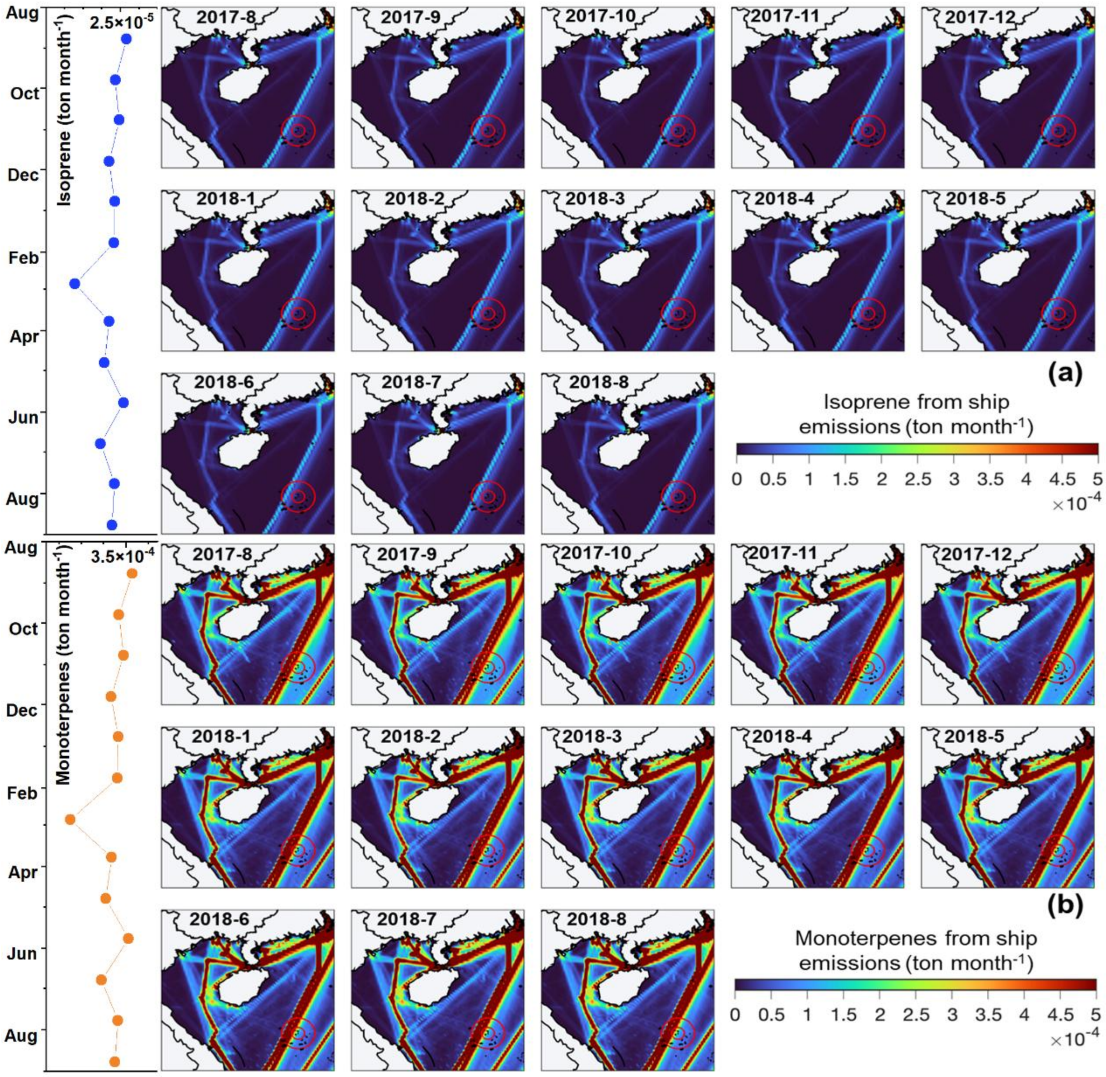

Figure S5. Illustrations presenting the variation in the amount of (a) isoprene and (b) monoterpenes emitted from ships over months in the Sansha area. The data (0.1°×0.1°) were derived from the HTAP_v3 emission mosaic (Crippa et al., 2023; Huang et al., 2017). The small and large red circles in panels (a) and (b) show radii of 0.25° and 0.75°, respectively.

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