



Supplement of

**Molecular characteristics and formation pathways of
organosulfur compounds: a comparative field study across
contrasting atmospheric environments**

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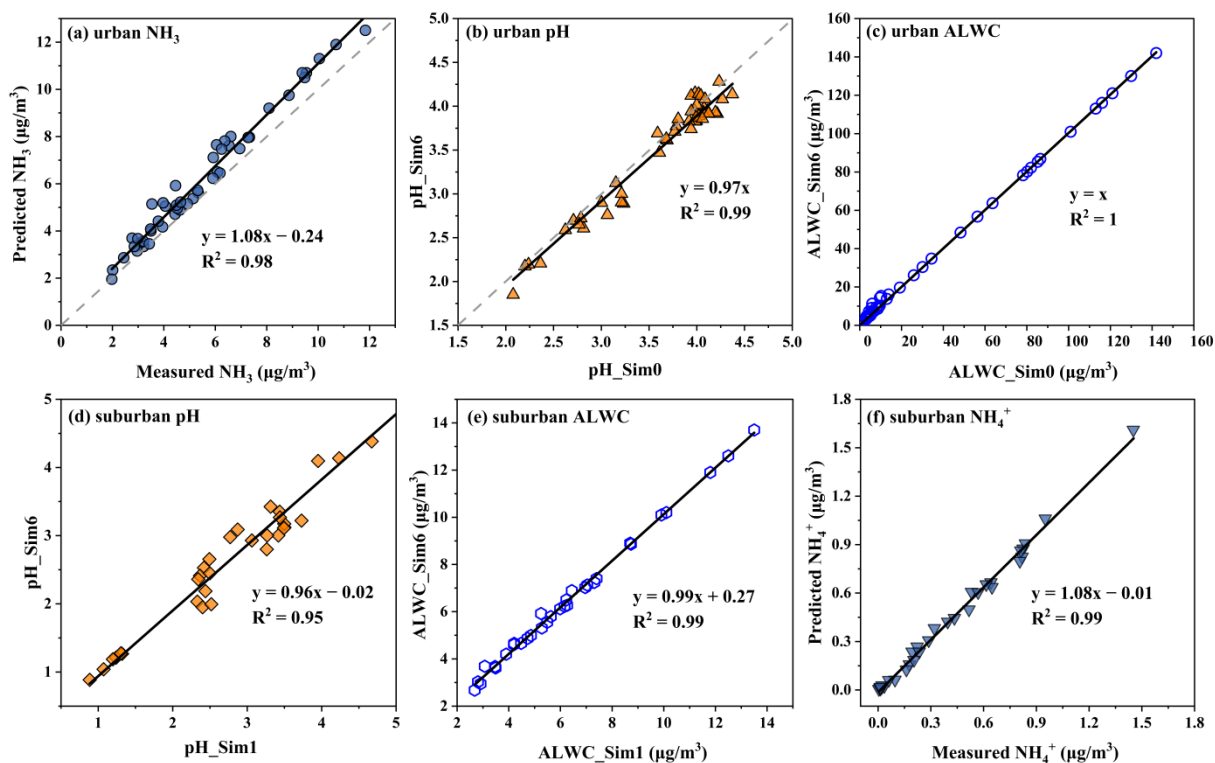


Figure S1. (a) Comparison between observed and ISORROPIA-II-simulated gaseous NH_3 concentrations at the urban site. (b, c) Comparisons of predicted aerosol pH and ALWC, respectively, between simulations constrained by measured gaseous NH_3 (Sim0) and simulations in which gaseous NH_3 was estimated through six iterative runs (Sim6) at the urban site. (d–f) Comparisons of predicted aerosol pH, ALWC, and particulate NH_4^+ , respectively, between the first (Sim1) and sixth (Sim6) iterative runs at the suburban site.

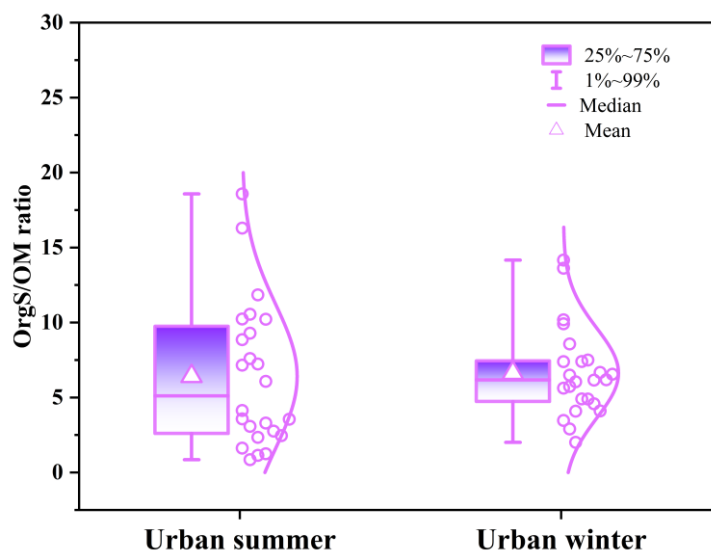


Figure S2. Comparison of OrgS-to-OM ratios between the summer and winter campaigns at the urban site.

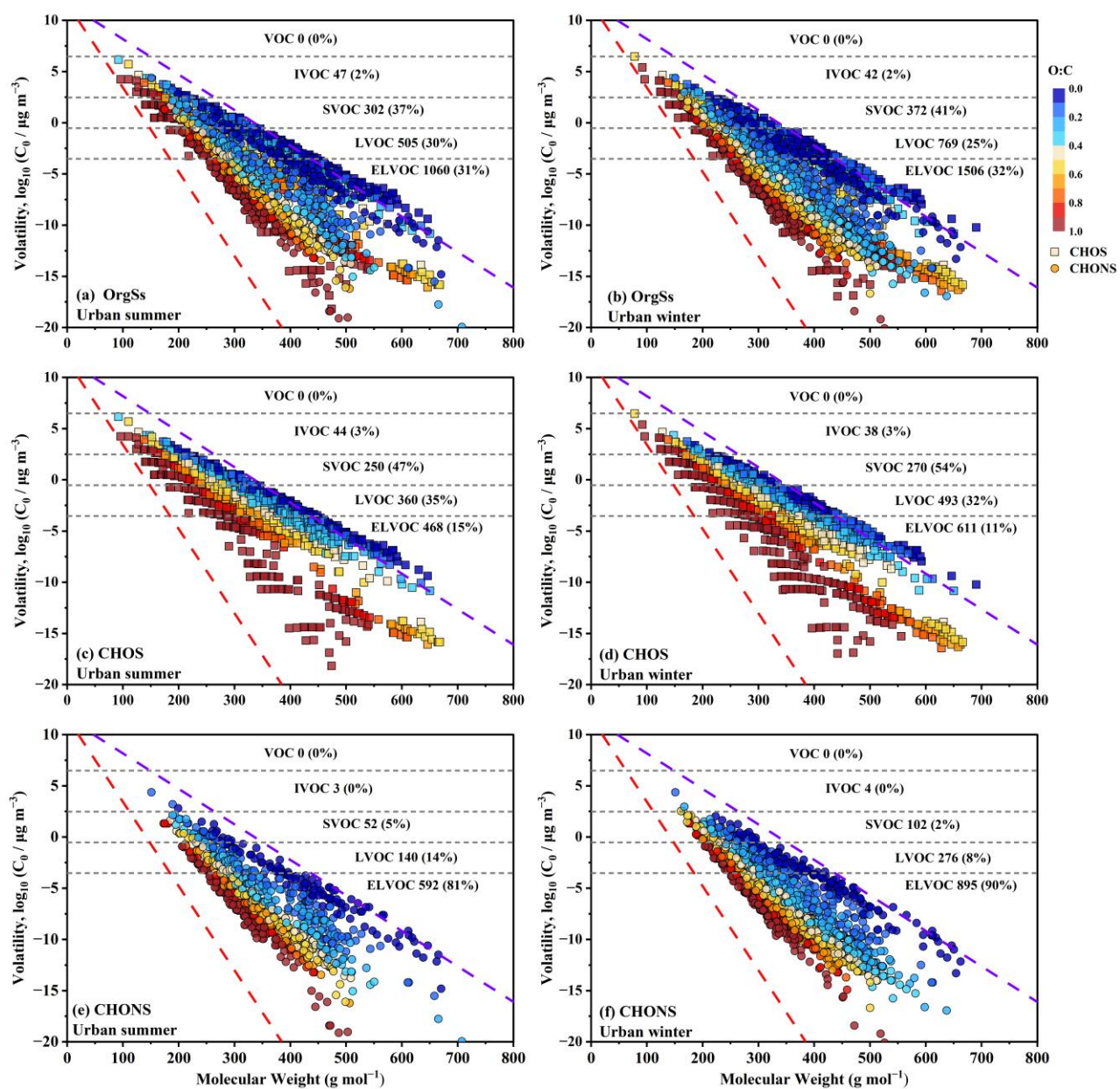


Figure S3. Molecular corridors of molecular weight versus saturation mass concentration (C_0) for total OrgSs, CHOS, and CHONS detected in urban summer (a, c, e) and winter (b, d, f) samples. The two edge dashed lines represent linear n-alkanes $\text{C}_n\text{H}_{2n+2}$ (purple with an O/C ratio = 0) and sugar alcohols $\text{C}_n\text{H}_{2n+2}\text{O}_n$ (red with an O/C ratio = 1). The small markers represent individual compounds identified in each data set color-coded by atomic O/C ratio. The numbers and percentages shown to the left of each volatility-class label denote the total number of each volatility subgroup and their relative peak area-weighted fractions, respectively.

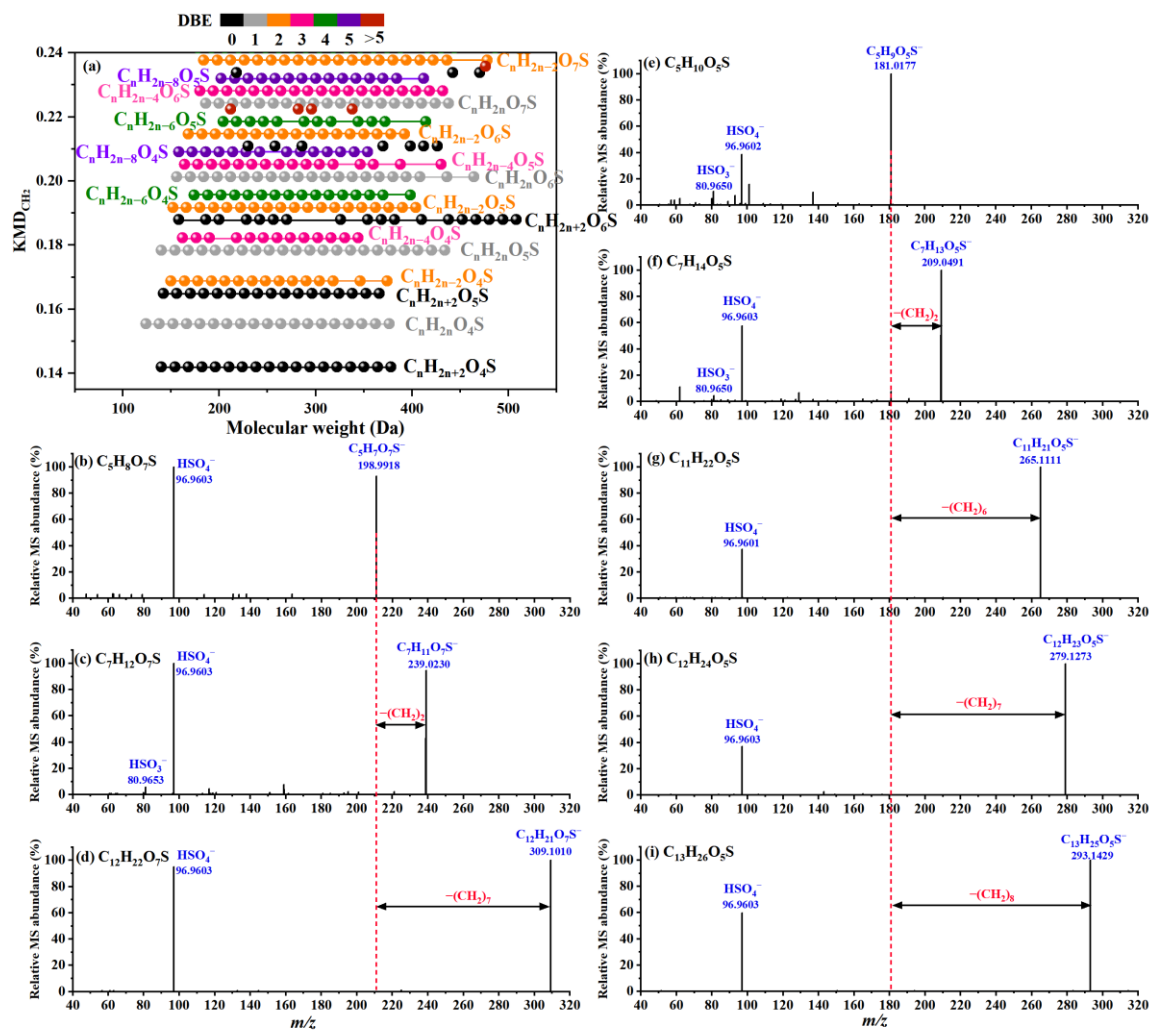


Figure S4. (a) CH₂-based Kendrick mass defect (KMD) diagram of potential OSs. (b–i) MS/MS fragmentation spectra of eight representative sulfur-containing ions. The parent ions chosen for fragmentation were (b–d) C_nH_{2n-2}O₇S (n = 5, 7, and 12) and (e–i) C_nH_{2n}O₅S (n = 5, 7, 11, 12, and 13).

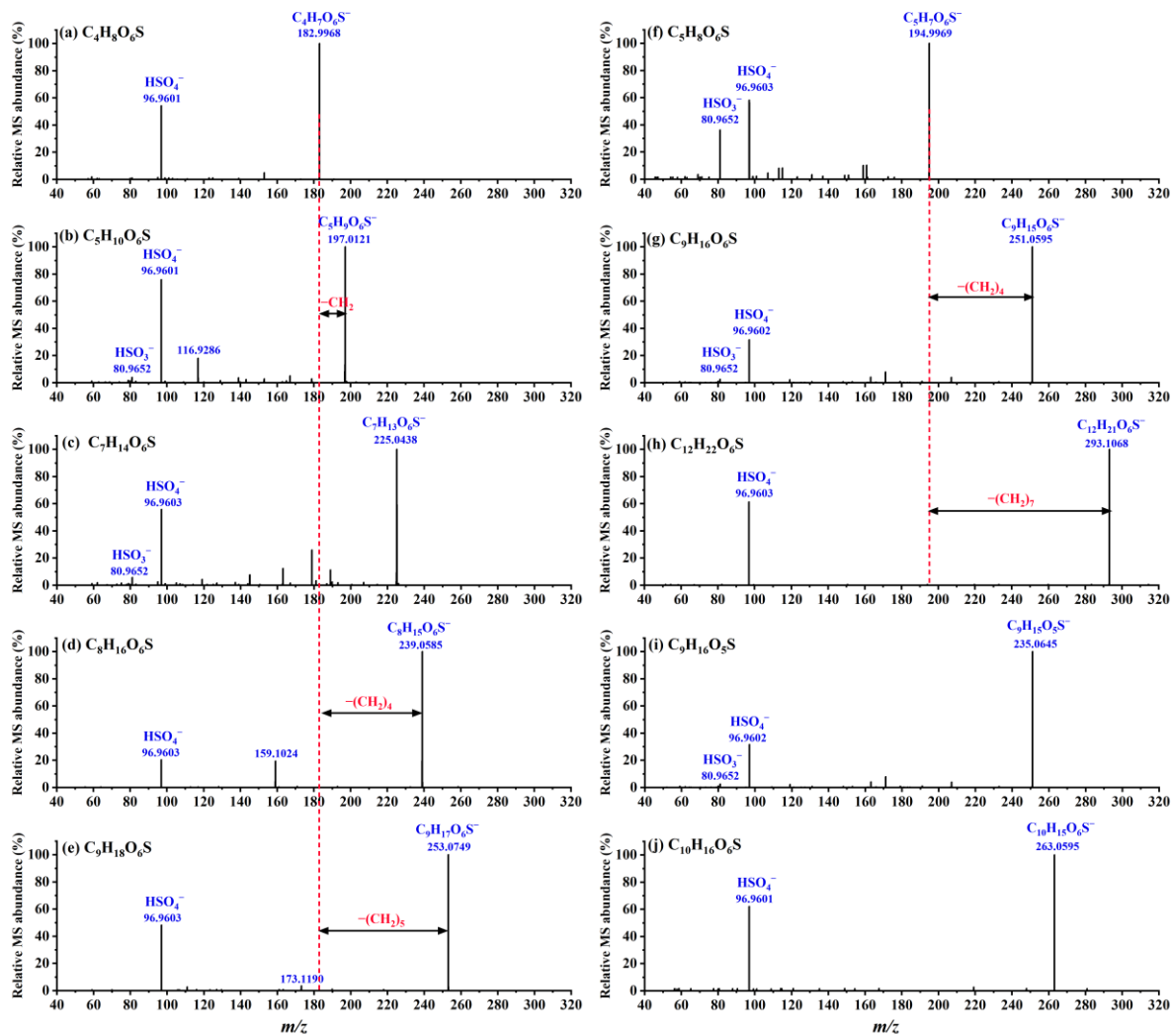
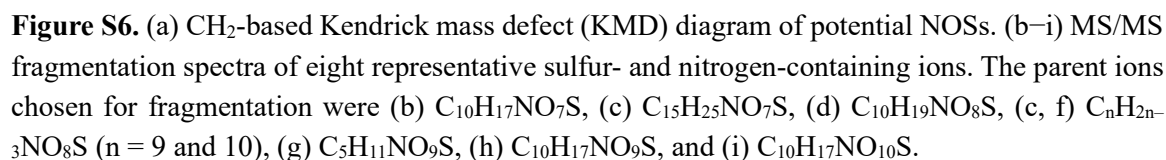


Figure S5. MS/MS fragmentation spectra of ten representative sulfur-containing ions. The parent ions chosen for fragmentation were (a–e) $C_nH_{2n}O_6S$ ($n = 4, 5, 7, 8,$ and 9), (f–h) $C_nH_{2n-2}O_6S$ ($n = 5, 9,$ and 12), (i) $C_9H_{16}O_5S$, and (j) $C_{10}H_{16}O_6S$.



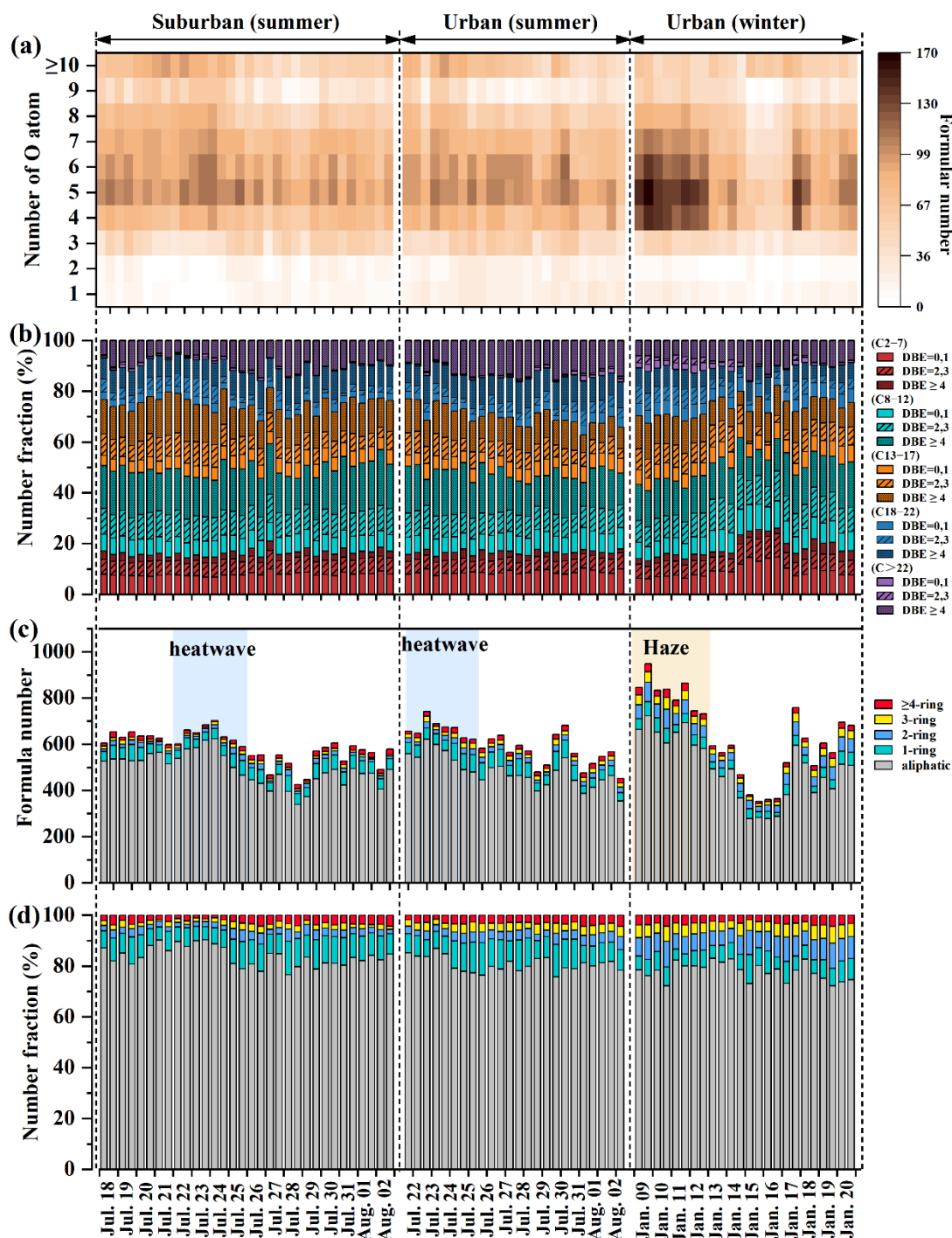


Figure S7. (a) Number distribution of the total CHOS species sorted by the oxygen atom number in the molecular formulas across the three field campaigns. (b) Formular number percentages of each subgroup which were divided based on the DBE value and the length of carbon skeleton in the CHOS formulas; (c) Formular number and (d) number percentages of each subgroup which were divided based on the Xc value of formulas.

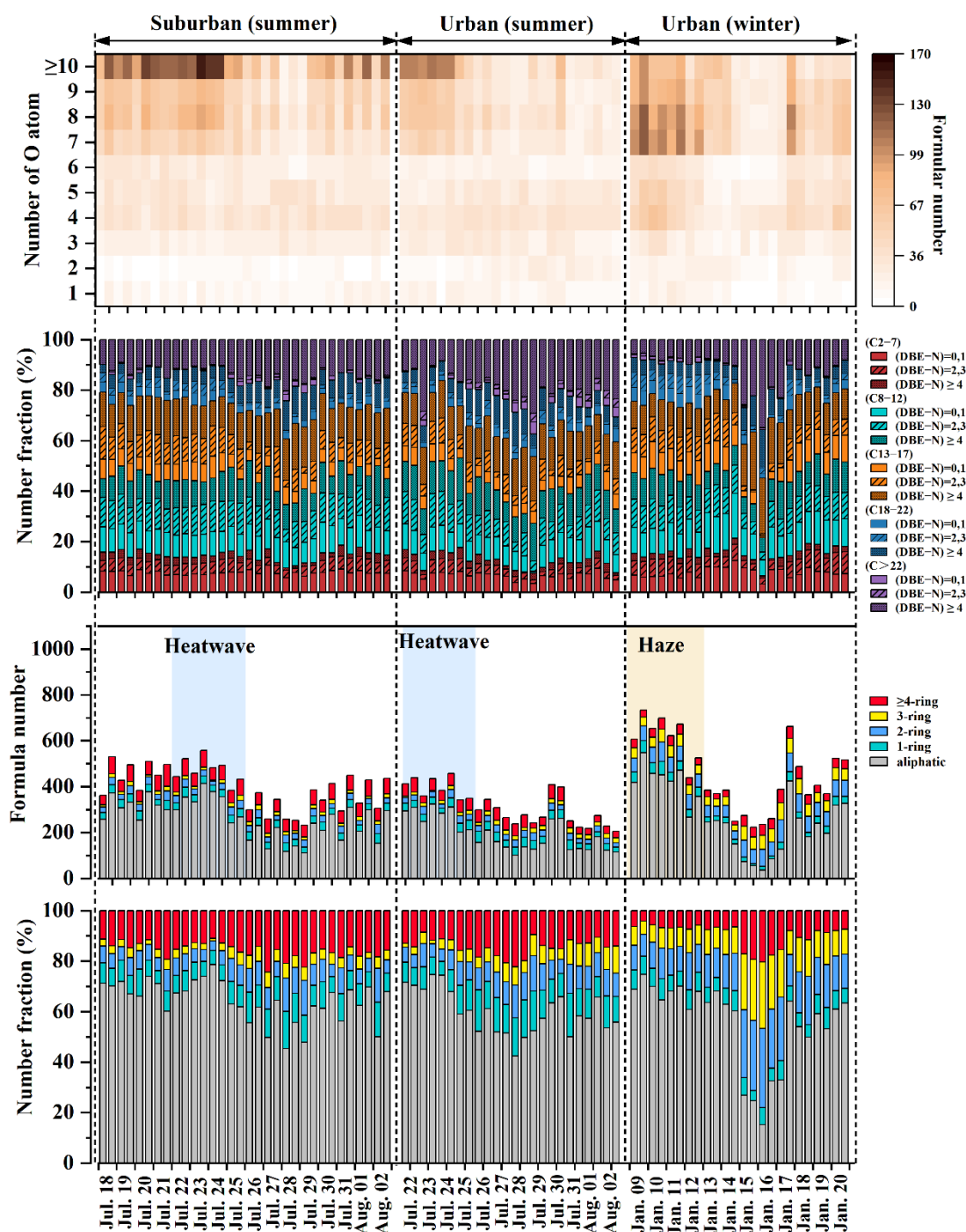


Figure S8. (a) Number distribution of the total CHONS species sorted by the oxygen atom number in the molecular formulas across the three field campaigns. (b) Formular number percentages of each subgroup which were divided based on the (DBE-N) value and the length of carbon skeleton in the CHONS formulas; (c) Formular number and (d) number percentages of each subgroup which were divided based on the Xc value of formulas.

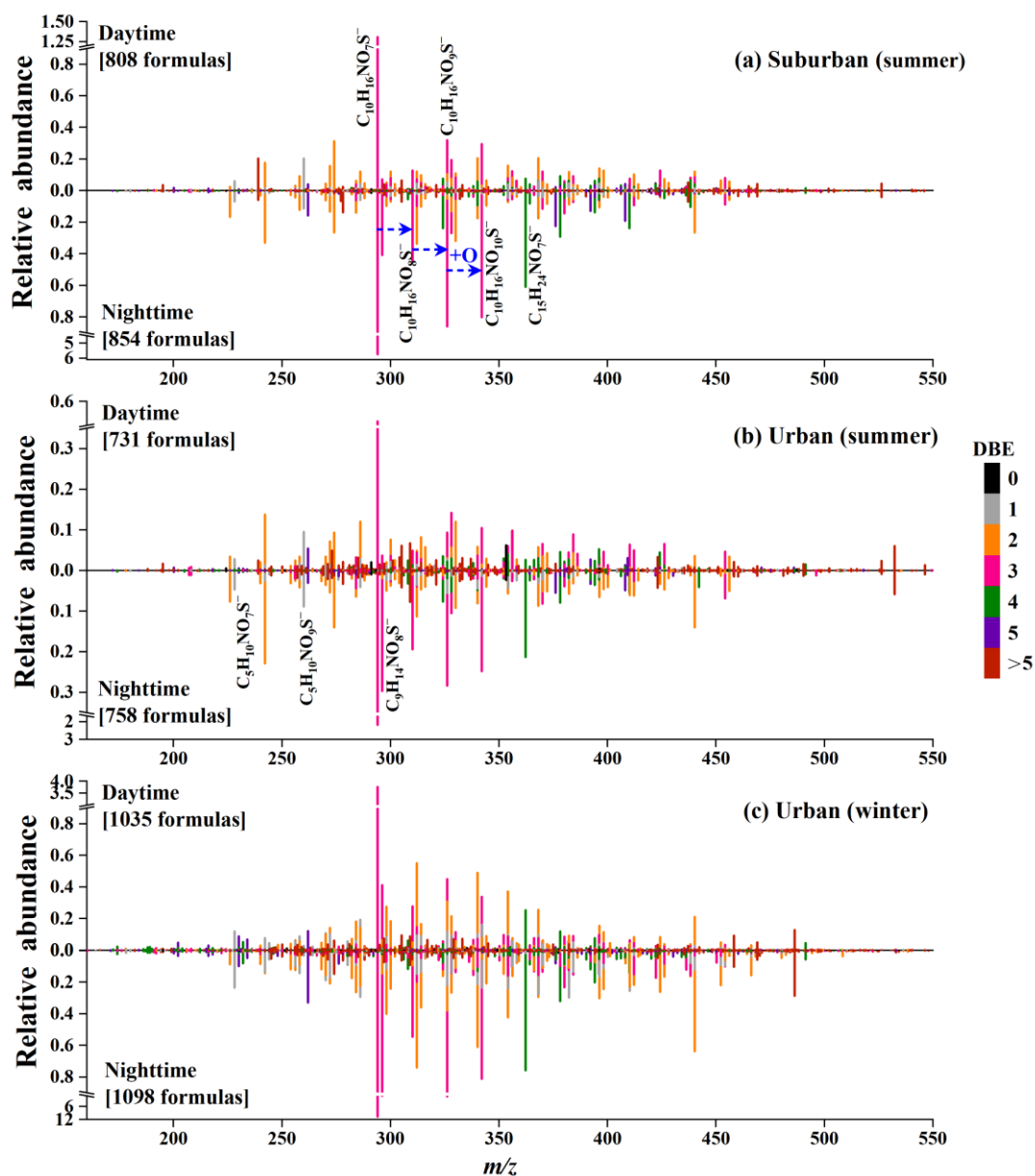


Figure S9. The relative abundance distribution of detected CHONS compounds in the suburban (a, summer) and urban (b, summer; c, winter). The color bar denotes the DBE of CHONS compounds. Note that the abundances of IS in each sample were set arbitrarily to 100%.

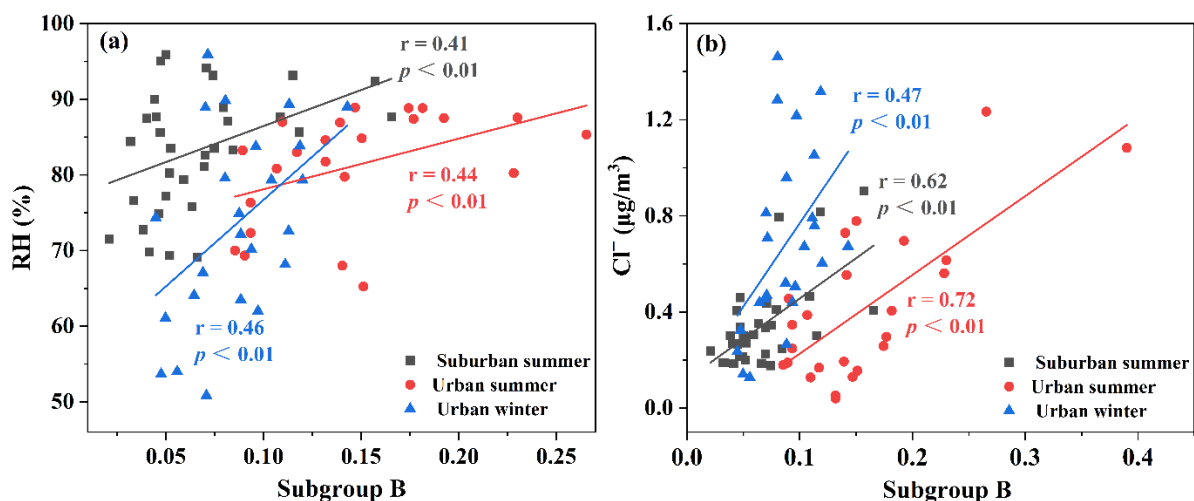


Figure S10. Significant correlations of the sum-normalized peak areas of OSs classified into subgroup B (with $\text{DBE} \leq 2$, $\text{C} > 8$, $3 < \text{O} < 7$ for CHOS) with RH (a) and Cl^- (b).

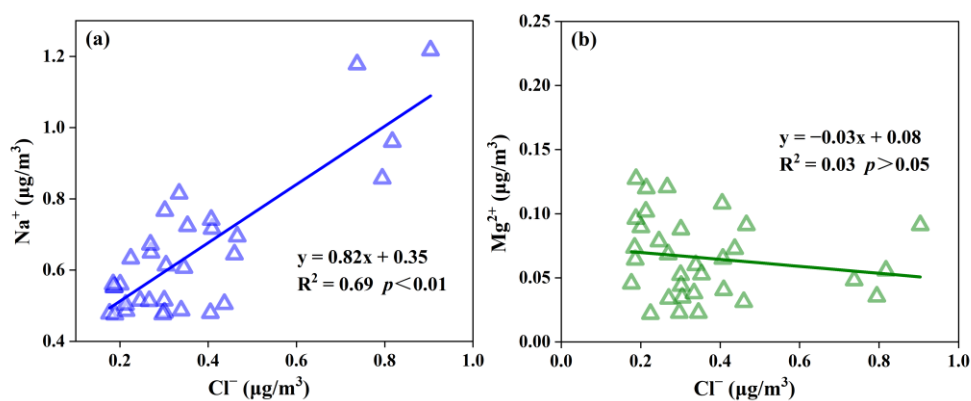


Figure S11. Correlations of Cl^- with (a) Na^+ and (b) Mg^{2+} concentrations in suburban summer.

Table S1. The concentrations of PM_{2.5}, gaseous pollutants, and meteorological parameters in the suburban (summer) and urban (summer, winter) of Shanghai. The involved abbreviations included temperature (T), relative humidity (RH), and wind speed (WS).

	Suburban summer	Daytime	Nighttime	Urban summer	Daytime	Nighttime	Urban winter	Daytime	Nighttime
I. PM _{2.5} and gaseous pollutants ($\mu\text{g m}^{-3}$)									
PM _{2.5}	14.6 ± 7.67	16.7 ± 8.15	12.5 ± 6.50	17.9 ± 9.44	20.5 ± 9.41	15.4 ± 8.76	50.8 ± 34.0	50.1 ± 31.4	51.6 ± 36.4
SO ₂	2.21 ± 0.61	2.05 ± 0.60	2.16 ± 0.60	4.56 ± 1.15	5.05 ± 1.37	4.06 ± 0.90	8.08 ± 2.18	8.34 ± 2.29	7.81 ± 2.03
NO _x	17.7 ± 8.91	13.1 ± 5.80	22.9 ± 9.11	25.7 ± 8.22	23.7 ± 7.35	27.6 ± 9.26	56.5 ± 26.5	53.8 ± 21.8	59.2 ± 30.4
CO	456 ± 88.7	477 ± 70.7	435 ± 99.2	779 ± 80.1	785 ± 76.2	774 ± 83.3	1174 ± 271	1108 ± 266	1239 ± 282
O ₃	78.5 ± 25.2	95.3 ± 33.7	61.7 ± 13.8	61.3 ± 17.3	75.9 ± 24.3	46.7 ± 11.7	42.8 ± 22.5	50.9 ± 21.4	34.6 ± 23.2
OC	2.51 ± 5.59	3.49 ± 2.82	1.52 ± 1.87	3.46 ± 2.55	4.09 ± 3.04	2.87 ± 1.82	6.60 ± 5.47	6.36 ± 4.08	6.84 ± 6.55
EC	0.49 ± 0.48	0.66 ± 0.54	0.31 ± 0.32	1.03 ± 0.90	1.23 ± 1.07	0.83 ± 0.62	2.77 ± 1.77	2.73 ± 1.31	2.80 ± 2.13
II. Meteorological parameters									
T (°C)	28.7 ± 1.70	29.9 ± 1.39	27.4 ± 0.83	30.8 ± 1.54	32.4 ± 1.38	29.1 ± 0.59	7.64 ± 3.28	9.43 ± 3.44	5.84 ± 3.13
RH (%)	83.3 ± 7.78	78.1 ± 6.95	88.6 ± 4.29	80.8 ± 7.60	76.0 ± 7.94	85.5 ± 2.78	75.7 ± 13.9	67.6 ± 14.3	83.7 ± 7.26
WS (m s ⁻¹)	2.45 ± 1.14	2.85 ± 0.98	2.05 ± 1.16	4.70 ± 1.13	5.07 ± 1.21	4.33 ± 0.91	3.39 ± 1.60	3.90 ± 1.16	2.88 ± 1.81

Table S2. Summary of MS/MS analysis for potential OSs and NOSs.

Compound category	Number of compounds showing diagnostic fragment ions	Fraction of total signal intensity (%)	Major diagnostic fragment ions	Representative spectra
Potential OSs	117	52.7	HSO ₄ ⁻ <i>m/z</i> 96.9601, HSO ₃ ⁻ <i>m/z</i> 80.9652	Fig. S4–S5
Potential NOSs	63	64.1	HSO ₄ ⁻ <i>m/z</i> 96.9601, SO ₃ ⁻ <i>m/z</i> 79.9574, NO ₃ ⁻ <i>m/z</i> 61.9884	Figs. S6

Note: The fraction of total signal intensity was calculated as the summed signal intensity of compounds showing diagnostic MS/MS fragment ions divided by the total signal intensity of all potential OSs or NOSs within the corresponding category. Only representative MS/MS spectra are presented in Figs. S4–S6 because of the large number of compounds examined.

Table S3. Summary of molecular characteristics of CHOS and CHONS compounds detected in suburban and urban PM_{2.5} samples from Shanghai.

Sample ID	Group	Subgroup	Number of formulas	% of total OrgS number	% of total OrgS Intensity	% of formulas number with $(4s+3n)/o \leq 1$	% of formulas intensity with $(4s+3n)/o \leq 1$	MW _w	H/C _w	O/C _w	DBE _w	Xc _w
Suburban Summer	CHOS	CHOS ₁	418–688	58.4±3.33	64.8±16.0	88.2±3.80	86.1±13.9	300±16.2	1.87±0.06	0.58±0.15	2.05±0.46	0.37±0.24
		Total	425–703 (1069)	59.8±3.41	65.2±16.1	86.6±3.71	86.2±13.8	300±16.0	1.88±0.06	0.58±0.14	2.06±0.46	0.37±0.24
Urban Summer	CHOS	CHOS ₁	439–677	64.8±3.36	76.7±12.4	84.4±2.38	85.3±11.6	301±16.4	1.82±0.04	0.53±0.11	2.11±0.43	0.42±0.26
		Total	452–689 (1127)	66.4±3.56	77.1±12.6	83.2±2.53	85.2±11.5	302±16.5	1.81±0.04	0.53±0.11	2.18±0.44	0.43±0.27
Urban Winter	CHOS	CHOS ₁	324–846	59.5±4.07	73.8±8.44	89.2±2.13	91.7±7.37	285±15.4	1.62±0.03	0.45±0.06	2.48±0.46	0.58±0.31
		Total	330–949 (1412)	60.8±4.11	73.9±8.44	87.5±2.25	91.6±7.36	285±15.4	1.62±0.03	0.45±0.06	2.56±0.47	0.60±0.31
Suburban Summer	CHONS	CHON ₁ S ₁	139–438	29.0±4.30	31.9±16.4	62.3±11.3	88.2±12.4	321±10.2	1.71±0.06	0.83±0.09	3.20±0.50	0.17±0.21
		CHON ₂ S ₁	60–111	8.37±1.31	2.29±1.59	8.45±3.55	5.36±3.39	332±29.4	0.76±0.15	0.37±0.09	12.6±2.41	2.50±0.17
		Total	231–558 (895)	40.2±3.41	34.8±16.1	56.3±9.21	73.0±10.2	325±14.9	1.60±0.17	0.77±0.11	4.27±1.73	0.43±0.47
Urban Summer	CHONS	CHON ₁ S ₁	132–359	23.1±4.38	18.4±13.6	74.2±9.76	93.5±9.36	336±30.2	1.67±0.06	0.74±0.06	3.59±1.56	0.29±0.47
		CHON ₂ S ₁	53–114	9.67±1.84	4.30±3.81	3.85±3.53	8.13±3.03	335±16.5	0.75±0.13	0.32±0.15	13.6±3.47	2.59±0.61
		Total	206–458 (787)	33.6±3.56	22.9±12.6	59.7±7.54	89.4±9.89	332±19.2	1.53±0.26	0.69±0.12	4.89±2.64	0.54±0.55
Urban Winter	CHONS	CHON ₁ S ₁	54–578	29.2±7.24	23.2±9.81	68.8±4.50	94.4±3.18	318±9.72	1.63±0.05	0.68±0.07	4.49±1.16	0.59±0.58
		CHON ₂ S ₁	37–87	7.41±2.91	1.99±2.57	12.4±9.35	21.3±16.0	358±12.5	0.74±0.10	0.31±0.09	12.1±1.09	2.49±0.13
		Total	144–694 (1277)	39.2±4.11	26.1±8.44	56.5±6.70	92.0±6.54	322±9.08	1.44±0.24	0.65±0.17	6.02±2.60	0.88±0.70

Table S4. Comparison of H/C_w and O/C_w ratios of CHOS compounds in this study and other studies.

Sample	Location	Season	Extraction solution	H/C _w	O/C _w	Instrument	References
PM _{2.5}	Shanghai (suburb)	Summer	Methanol	1.88±0.06	0.58±0.14	Orbitrap MS	This study
	Shanghai (urban)	Summer		1.81±0.04	0.53±0.11		
		Winter		1.62±0.03	0.45±0.06		
PM _{2.5}	Pearl River Delta		Water	1.67±0.31	0.55 ± 0.17	Orbitrap MS	(Lin et al., 2012)
PM _{2.5}	Cambridge	winter	Water and acetonitrile	1.47	0.47	Orbitrap MS	(Rincón et al., 2012)
		summer		1.50	0.66		
PM _{0.18-1.8}	California	after midnight		1.7±0.05	0.87±0.09	Orbitrap MS	(O'brien et al., 2014)
		morning		1.8±0.1	0.93±0.1		
		afternoon		1.8±0.05	0.82±0.09		
		before midnight		1.8±0.0	0.88±0.05		
TSP	Virginia		Water	1.46±0.35	0.47±0.23	FT-ICR MS	(Willoughby et al., 2014)
			Pyridine	1.54±0.38	0.49±0.31		
			Acetonitrile	1.42±0.36	0.49±0.32		
PM _{2.5}	Beijing	Hazy	DCM	1.55±0.41	0.49±0.26	FT-ICR MS	(Jiang et al., 2016)
		Clear		1.74±0.34	0.62±0.34		
		Hazy	Water	1.64±0.37	0.65±0.28		
		Clear		1.82±0.26	0.75±0.37		
PM _{2.5}	Wuhan	Winter	Methanol	1.68±0.44	0.37±0.25	Orbitrap MS	(Wang et al., 2016)
		Summer		1.75±0.36	0.39±0.23		
	Nanjing	Summer		1.68±0.41	0.43±0.32		
	Shanghai	Winter		1.68±0.46	0.40±0.29		
		Summer		1.68±0.42	0.47±0.31		
PM _{2.5}	Shanghai	Spring	Acetonitrile	1	0.2	Orbitrap MS	(Wang et al., 2017)
		Summer		1.1	0.6		
		Fall		1.2	0.4		
		Winter		1.3	0.2		
PM _{2.5}	Mainz	low-pollution	Acetonitrile /water	1.66	0.78	Orbitrap MS	(Wang et al., 2018)
	Beijing	low-pollution		1.81	0.63		
		high-pollution		1.74	0.51		
PM _{2.5}	Changchun		Acetonitrile /water	1.56±0.11	1.17±0.13	Orbitrap MS	(Wang et al., 2021)
	Shanghai			1.85±0.04	1.41±0.19		
	Guangzhou			1.85±0.02	1.48±0.05		
PM _{2.5}	Guangzhou	Whole year	Methanol	1.77±0.03	0.52±0.07	FT-ICR MS	(Jiang et al., 2022)
PM _{2.5}	Beijing	Winter	Methanol	1.17	0.76	Orbitrap MS	(Wang et al., 2024)
		Summer		1.37	0.60		
	Harbin	Winter		1.20	0.73		
		Summer		1.35	0.60		
	Xi'an	Winter		1.29	0.74		
		Summer		1.45	0.63		
	Chengdu	Winter		1.23	0.76		
		Summer		1.33	0.60		
	Guangzhou	Winter		1.27	0.74		
		Summer		1.43	0.65		
	Wuhan	Winter		1.16	0.77		
		Summer		1.40	0.63		
PM _{2.5}	Anshan	Winter	Water	1.42±0.07	0.45±0.05	FT-ICR MS	(Ning et al., 2025)

Table S5. Comparison of H/C_w and O/C_w ratios of CHONS compounds in this study and other studies.

Sample	Location	Season	Extraction solution	H/C _w	O/C _w	Instrument	References
PM _{2.5}	Shanghai (suburb)	Summer	Methanol	1.60±0.17	0.77±0.11	Orbitrap MS	This study
	Shanghai (urban)	Summer		1.53±0.26	0.69±0.12		
		Winter		1.44±0.24	0.65±0.17		
PM _{2.5}	Pearl River Delta		Water	1.73±0.29	0.81±0.22	Orbitrap MS	(Lin et al., 2012)
PM _{2.5}	Cambridge	Winter	Water and acetonitrile	1.99	0.73	Orbitrap MS	(Rincón et al., 2012)
		Summer		1.65	0.80		
PM _{0.18-1.8}	California	after midnight		1.7±0.0	0.99±0.02	Orbitrap MS	(O'brien et al., 2014)
		morning		1.7±0.0	1.0±0.005		
		afternoon		1.7±0.05	0.92±0.03		
		before midnight		1.7±0.05	0.89±0.09		
TSP	Virginia		Water	1.65±0.20	0.71±0.21	FT-ICR MS	(Willoughby et al., 2014)
			Pyridine	1.52±0.28	0.64±0.23		
			Acetonitrile	1.27±0.29	0.45±0.25		
PM _{2.5}	Beijing	Hazy	DCM	1.57±0.37	0.69±0.31	FT-ICR MS	(Jiang et al., 2016)
		Clear		1.75±0.31	0.76±0.27		
		Hazy	Water	1.51±0.37	0.70±0.32		
		Clear		-	-		
PM _{2.5}	Wuhan	Winter	Methanol	1.58±0.46	0.35±0.13	Orbitrap MS	(Wang et al., 2016)
		Summer		1.69±0.34	0.40±0.17		
	Nanjing	Summer		1.69±0.35	0.44±0.21		
	Shanghai	Winter		1.64±0.52	0.42±0.27		
		Summer		1.64±0.47	0.53±0.38		
PM _{2.5}	Shanghai	Spring	Acetonitrile	1.5	0.2	Orbitrap MS	(Wang et al., 2017)
		Summer		1.5	0.4		
		Fall		1.6	0.3		
		Winter		1.5	0.4		
PM _{2.5}	Mainz	Low pollution	Acetonitrile/water	1.54	0.91	Orbitrap MS	(Wang et al., 2018)
	Beijing	Low pollution		1.57	0.81		
		High pollution		1.56	0.59		
PM _{2.5}	Changchun		Acetonitrile/water	1.35±0.02	1.07±0.11	Orbitrap MS	(Wang et al., 2021)
	Shanghai			1.56±0.03	1.00±0.13		
	Guangzhou			1.56±0.04	0.82±0.03		
PM _{2.5}	Guangzhou	Whole year	Methanol	1.72±0.03	0.72±0.06	FT-ICR MS	(Jiang et al., 2022)
PM _{2.5}	Beijing	Winter	Methanol	1.15	1.02	Orbitrap MS	(Wang et al., 2024)
		Summer		1.28	0.96		
	Harbin	Winter		1.30	1.08		
		Summer		1.26	0.98		
	Xi'an	Winter		1.26	1.04		
		Summer		1.39	0.99		
	Chengdu	Winter		1.17	1.02		
		Summer		1.34	0.91		
	Guangzhou	Winter		1.20	1.02		
		Summer		1.51	0.82		
	Wuhan	Winter		1.12	1.06		
		Summer		1.49	1.00		
PM _{2.5}	Anshan	Winter	Water	1.43±0.09	0.55±0.07	FT-ICR MS	(Ning et al., 2025)

Table S6. Molecular information and their relative abundance of isoprene-derived organosulfates detected at Shanghai. Noted the formulas in the Table S5–S10 were from the summarization of recent studies and the reference in (Bruggemann et al., 2020; Ye et al., 2020; Zhu et al., 2019; Wang et al., 2019).

Molecular formula	m/z [M-H] [−]	DBE	Relative peak area (%)		
			Suburban Summer	Urban Summer	Urban Winter
C ₂ H ₆ O ₅ S	140.9863	0	3.05	3.67	3.62
C ₃ H ₄ O ₈ S	198.9554	2	0.53	0.47	1.35
C ₃ H ₆ O ₆ S	168.9812	1	6.93	5.14	12.58
C ₃ H ₆ O ₇ S	184.9761	1	0.18	0.49	2.64
C ₃ H ₆ O ₈ S	200.9711	1	0.74	0.25	1.07
C ₃ H ₆ O ₉ S	216.9660	1	1.25	0.88	3.00
C ₃ H ₈ O ₆ S	170.9969	0	0.08	0.02	0.21
C ₄ H ₆ O ₅ S	164.9863	2	3.27	2.73	2.68
C ₄ H ₆ O ₆ S	180.9812	2	3.32	1.53	3.80
C ₄ H ₈ O ₅ S	167.0020	1	4.22	2.44	6.01
C ₄ H ₈ O ₆ S	182.9969	1	16.51	11.79	12.95
C ₄ H ₈ O ₇ S	198.9918	1	2.62	3.52	0.30
C ₄ H ₈ O ₈ S	214.9867	1	0.06	0.07	0.55
C ₄ H ₈ O ₉ S	230.9816	1	0.21	0.13	0.82
C ₅ H ₈ O ₆ S	194.9969	2	8.06	6.02	9.75
C ₅ H ₈ O ₇ S	210.9918	2	4.48	1.14	6.63
C ₅ H ₈ O ₈ S	226.9867	2	1.63	2.87	1.63
C ₅ H ₈ O ₁₁ S	274.9715	2	1.23	0.89	2.35
C ₅ H ₁₀ O ₅ S	181.0176	1	5.72	5.69	20.68
C ₅ H ₁₀ O ₆ S	197.0125	1	10.57	9.76	17.33
C ₅ H ₁₀ O ₇ S	213.0074	1	2.94	1.88	3.10
C ₅ H ₁₀ O ₈ S	229.0024	1	5.63	0.13	0.44
C ₅ H ₁₂ O ₆ S	199.0282	0	0.31	0.25	0.66
C ₅ H ₁₂ O ₇ S	215.0231	0	16.41	7.75	10.32
C ₅ H ₁₂ O ₈ S	231.0180	0	1.32	0.98	2.45
C ₇ H ₁₀ O ₆ S	221.0125	3	1.62	1.09	3.80
C ₇ H ₁₀ O ₇ S	237.0074	3	5.42	3.17	5.66
C ₈ H ₁₂ O ₆ S	235.0282	3	0.56	0.46	2.36
C ₈ H ₁₂ O ₇ S	251.0231	3	8.20	4.66	13.64
C ₈ H ₁₄ O ₅ S	221.0489	2	3.52	2.42	11.83
C ₈ H ₁₄ O ₆ S	237.0438	2	13.77	9.04	21.72
C ₈ H ₁₄ O ₇ S	253.0387	2	33.92	17.88	20.05
C ₈ H ₁₄ O ₈ S	269.0337	2	6.85	1.49	6.20
C ₈ H ₁₄ O ₁₀ S	301.0235	2	0.10	0.24	0.61
C ₉ H ₁₆ O ₇ S	267.0544	2	50.43	25.62	35.43

$C_{10}H_{20}O_{10}S$	331.0704	1	0.04	0.05	0.05
$C_{10}H_{22}O_{10}S$	333.0861	0	0.23	0.14	0.19
$C_{12}H_{18}O_8S$	321.0650	4	3.48	2.60	2.80
$C_{12}H_{20}O_6S$	291.0908	3	1.96	1.58	5.50
$C_{15}H_{32}O_{13}S$	451.1491	0	0.49	0.23	1.76
$C_5H_{11}NO_7S$	228.0183	1	6.49	3.88	13.11
$C_5H_{11}NO_8S$	244.0133	1	1.22	0.81	3.78
$C_5H_{11}NO_9S$	260.0082	1	15.82	9.21	2.20
$C_5H_9NO_{10}S$	273.9874	2	29.00	11.79	0.96
$C_5H_{10}N_2O_{11}S$	304.9933	2	0.43	0.09	0.78
$C_8H_{13}NO_{12}S$	346.0086	3	0.18	0.11	1.32

Table S7. Molecular information and their relative abundance of monoterpene-derived organosulfates detected at Shanghai.

Precursor group	Molecular formula	m/z [M-H] ⁻	DBE	Relative peak area (%)		
				Suburban Summer	Urban Summer	Urban Winter
Monoterpene	C ₃ H ₆ O ₈ S	200.9711	1	0.76	0.42	1.36
	C ₅ H ₈ O ₈ S	226.9867	2	1.63	2.87	1.63
	C ₅ H ₁₀ O ₈ S	229.0024	1	0.27	0.13	0.44
	C ₅ H ₁₂ O ₆ S	199.0282	0	0.36	0.25	0.66
	C ₅ H ₁₂ O ₇ S	215.0231	0	0.27	0.18	0.72
	C ₆ H ₁₂ O ₄ S	179.0384	1	1.77	2.05	18.69
	C ₆ H ₁₂ O ₆ S	211.0282	1	20.30	14.53	45.85
	C ₆ H ₁₂ O ₈ S	243.0180	1	0.66	0.67	0.28
	C ₇ H ₈ O ₈ S	250.9867	4	0.60	0.64	0.36
	C ₇ H ₁₀ O ₈ S	253.0024	3	5.13	1.45	2.13
	C ₇ H ₁₂ O ₆ S	223.0282	2	7.69	7.49	17.66
	C ₇ H ₁₂ O ₉ S	271.0129	2	0.71	0.60	1.12
	C ₇ H ₁₄ O ₆ S	225.0438	1	16.39	10.65	37.45
	C ₈ H ₁₀ O ₈ S	265.0024	4	0.54	0.76	1.25
	C ₈ H ₁₂ O ₇ S	251.0231	3	8.20	4.66	13.64
	C ₈ H ₁₂ O ₈ S	267.0180	3	14.90	11.52	3.32
	C ₈ H ₁₄ O ₆ S	237.0438	2	13.77	9.04	21.72
	C ₈ H ₁₄ O ₇ S	253.0387	2	33.92	17.88	20.05
	C ₈ H ₁₄ O ₉ S	285.0286	2	0.45	0.07	0.29
	C ₈ H ₁₈ O ₆ S	241.0751	0	0.86	0.42	6.28
	C ₈ H ₁₈ O ₈ S	273.0650	0	0.85	0.57	3.42
	C ₉ H ₈ O ₇ S	258.9918	6	0.66	0.42	5.70
	C ₉ H ₁₀ O ₅ S	229.0176	5	1.87	1.59	6.47
	C ₉ H ₁₀ O ₆ S	245.0125	5	1.06	0.90	7.25
	C ₉ H ₁₂ O ₇ S	263.0231	4	2.04	1.49	1.71
	C ₉ H ₁₂ O ₉ S	295.0129	4	0.60	1.17	0.56
	C ₉ H ₁₄ O ₆ S	249.0438	3	2.84	2.91	6.79
	C ₉ H ₁₄ O ₇ S	265.0387	3	17.95	6.82	15.11
	C ₉ H ₁₄ O ₈ S	281.0337	3	13.86	6.20	9.50
	C ₉ H ₁₄ O ₉ S	297.0286	3	3.25	0.22	1.43
	C ₉ H ₁₆ O ₄ S	219.0697	2	0.58	0.54	4.01
	C ₉ H ₁₆ O ₅ S	235.0646	2	15.59	11.36	38.59
	C ₉ H ₁₆ O ₆ S	251.0595	2	26.01	17.22	49.34
	C ₉ H ₁₆ O ₇ S	267.0544	2	50.43	25.62	35.43
	C ₉ H ₁₆ O ₈ S	283.0493	2	9.53	5.02	17.32
	C ₉ H ₁₆ O ₉ S	299.0442	2	0.72	0.34	0.41
	C ₉ H ₁₈ O ₄ S	221.0853	1	3.14	2.32	15.43

Sesquiterpene	C ₉ H ₁₈ O ₆ S	253.0751	1	20.61	15.06	36.02
	C ₉ H ₁₈ O ₇ S	269.0700	1	10.32	3.59	13.60
	C ₉ H ₂₀ O ₄ S	223.1010	0	8.85	15.47	24.86
	C ₁₀ H ₁₀ O ₅ S	241.0176	6	0.52	0.43	2.51
	C ₁₀ H ₁₀ O ₇ S	273.0074	6	0.64	0.63	7.89
	C ₁₀ H ₁₂ O ₆ S	259.0282	5	2.24	1.77	3.61
	C ₁₀ H ₁₄ O ₄ S	229.0540	4	2.60	1.36	2.74
	C ₁₀ H ₁₄ O ₆ S	261.0438	4	2.03	1.06	1.93
	C ₁₀ H ₁₄ O ₁₁ S	341.0184	4	0.02	0.01	0.07
	C ₁₀ H ₁₆ O ₄ S	231.0697	3	4.41	2.37	7.80
	C ₁₀ H ₁₆ O ₅ S	247.0646	3	6.46	4.07	16.45
	C ₁₀ H ₁₆ O ₆ S	263.0595	3	12.82	6.54	18.43
	C ₁₀ H ₁₆ O ₇ S	279.0544	3	47.47	23.30	67.24
	C ₁₀ H ₁₆ O ₈ S	295.0493	3	14.38	4.44	13.00
	C ₁₀ H ₁₆ O ₉ S	311.0442	3	5.90	0.87	1.02
	C ₁₀ H ₁₆ O ₁₀ S	327.0391	3	2.37	2.09	1.34
	C ₁₀ H ₁₈ O ₅ S	249.0802	2	11.99	8.76	25.14
	C ₁₀ H ₁₈ O ₆ S	265.0751	2	17.15	9.58	31.55
	C ₁₀ H ₁₈ O ₇ S	281.0700	2	52.91	25.09	31.85
	C ₁₀ H ₁₈ O ₈ S	297.0650	2	13.43	5.27	14.93
	C ₁₀ H ₁₈ O ₉ S	313.0599	2	5.11	2.04	1.52
	C ₁₀ H ₂₀ O ₅ S	251.0959	1	56.42	29.99	118.32
	C ₁₀ H ₂₀ O ₆ S	267.0908	1	11.76	6.89	23.91
	C ₁₀ H ₂₀ O ₇ S	283.0857	1	6.66	2.38	13.58
	C ₁₀ H ₂₂ O ₄ S	237.1166	0	4.85	7.18	24.18
	C ₁₀ H ₂₂ O ₅ S	253.1115	0	0.89	0.77	7.12
	C ₁₁ H ₁₆ O ₇ S	291.0544	4	1.23	1.21	1.80
	C ₁₁ H ₁₈ O ₈ S	309.0650	3	7.95	2.27	8.40
	C ₁₂ H ₁₂ O ₆ S	283.0282	7	0.34	0.21	0.39
	C ₁₄ H ₂₂ O ₇ S	333.1013	4	2.74	1.63	2.41
	C ₁₄ H ₂₂ O ₈ S	349.0963	4	1.85	1.77	2.12
	C ₁₄ H ₂₄ O ₅ S	303.1272	3	2.09	0.84	4.99
	C ₁₄ H ₂₄ O ₆ S	319.1221	3	3.10	1.59	3.43
	C ₁₄ H ₂₄ O ₈ S	351.1119	3	3.15	2.78	6.31
	C ₁₅ H ₂₄ O ₇ S	347.1170	4	7.90	3.96	4.85
	C ₁₅ H ₂₄ O ₈ S	363.1119	4	1.62	1.17	3.38
	C ₁₅ H ₂₆ O ₅ S	317.1428	3	1.33	0.34	6.19
	C ₁₅ H ₂₆ O ₆ S	333.1377	3	1.93	0.84	3.48
	C ₁₆ H ₂₈ O ₇ S	363.1483	3	2.28	1.28	2.86
	C ₁₆ H ₂₈ O ₈ S	379.1432	3	6.96	2.19	4.10
	C ₂₀ H ₃₂ O ₅ S	383.1898	5	3.66	1.48	1.96
	C ₂₀ H ₃₄ O ₅ S	385.2054	4	0.67	0.23	1.06

	$C_{20}H_{34}O_9S_2$	481.1571	4	0.14	0.01	0.23
Terpene	$C_{10}H_{17}NO_7S$	294.0653	3	352.88	158.71	531.63
	$C_9H_{15}NO_8S$	296.0446	3	24.04	19.32	55.92
	$C_{10}H_{17}NO_8S$	310.0602	3	28.79	13.28	30.43
	$C_9H_{15}NO_9S$	312.0395	3	8.53	4.14	12.81
	$C_{10}H_{17}NO_9S$	326.0551	3	59.04	19.53	21.00
	$C_{10}H_{19}NO_9S$	328.0708	2	10.60	5.05	17.91
	$C_9H_{17}NO_{10}S$	330.0500	2	22.12	9.87	6.22
	$C_{10}H_{17}NO_{10}S$	342.0500	3	54.93	18.18	42.47
	$C_{10}H_{16}N_2O_{10}S$	355.0453	4	1.03	0.67	2.14
	$C_{15}H_{25}NO_7S$	362.1279	4	34.29	12.63	37.31
	$C_{10}H_{18}N_2O_{11}S$	373.0559	3	1.15	0.64	1.73
	$C_{14}H_{25}NO_9S$	382.1177	3	2.88	2.01	6.77
	$C_{10}H_{18}N_2O_{12}S$	389.0508	3	1.03	0.23	1.45

Table S8. Molecular information and their relative abundance of other biogenic VOCs-derived organosulfates (2-Methyl-3-Buten-2-ol; 2-E-pentenal, 2-E-hexenal, 3-Z-hexenal, cis-3-hexen-1-ol, and β -caryophyllene) detected at Shanghai.

Molecular formula	m/z [M-H] ⁻	DBE	Relative peak area (%)		
			Suburban Summer	Urban Summer	Urban Winter
C ₃ H ₆ O ₆ S	168.9812	1	6.93	5.14	12.58
C ₃ H ₆ O ₇ S	184.9761	1	0.18	0.49	2.64
C ₄ H ₁₀ O ₅ S	169.0176	0	3.84	5.57	4.77
C ₅ H ₁₂ O ₆ S	199.0282	0	0.36	0.25	0.66
C ₅ H ₁₀ O ₇ S	213.0074	1	2.94	1.88	3.1
C ₅ H ₁₀ O ₈ S	229.0024	1	0.23	0.13	0.44
C ₆ H ₁₀ O ₆ S	209.0125	2	11.25	5.78	14.19
C ₆ H ₁₂ O ₆ S	211.0282	1	20.3	14.53	45.85
C ₉ H ₁₆ O ₆ S	251.0595	2	26.01	17.22	49.34
C ₉ H ₁₈ O ₇ S	269.0700	1	10.32	3.59	13.6
C ₁₄ H ₂₄ O ₅ S	303.1272	3	2.09	0.84	4.99
C ₁₄ H ₂₄ O ₆ S	319.1221	3	3.1	1.59	3.43
C ₁₄ H ₂₂ O ₇ S	333.1013	4	2.74	1.63	2.41
C ₁₄ H ₂₂ O ₈ S	349.0963	4	1.85	1.77	2.12
C ₁₄ H ₂₄ O ₈ S	351.1119	3	3.15	2.78	6.31
C ₁₅ H ₂₆ O ₅ S	317.1428	3	1.33	0.34	6.19
C ₁₅ H ₂₆ O ₆ S	333.1377	3	1.93	0.84	3.48
C ₁₅ H ₂₄ O ₇ S	347.117	4	7.9	3.96	4.85
C ₁₅ H ₂₄ O ₈ S	363.1119	4	1.62	1.17	3.38
C ₁₆ H ₂₈ O ₇ S	363.1483	3	2.28	1.28	2.86
C ₁₆ H ₂₈ O ₈ S	379.1432	3	6.96	2.19	4.1
C ₁₄ H ₂₅ NO ₉ S	382.1177	3	2.88	2.01	6.77
C ₁₅ H ₂₅ NO ₇ S	362.1279	4	34.29	12.63	37.31

Table S9. Molecular information and their relative abundance of aromatic-derived organosulfates detected at Shanghai.

Molecular formula	m/z [M-H] ⁻	DBE	Relative peak area (%)		
			Suburban Summer	Urban Summer	Urban Winter
C ₆ H ₆ O ₄ S	172.9914	4	0.56	0.31	1.18
C ₇ H ₆ O ₄ S	184.9914	5	0.23	0.28	1.18
C ₇ H ₆ O ₅ S	200.9863	5	2.26	1.70	8.29
C ₇ H ₈ O ₄ S	187.0071	4	0.55	0.71	3.01
C ₈ H ₆ O ₆ S	228.9812	6	0.51	0.35	5.74
C ₈ H ₈ O ₄ S	199.0071	5	0.71	0.43	1.37
C ₈ H ₈ O ₅ S	215.0020	5	3.22	2.61	7.46
C ₈ H ₁₀ O ₄ S	201.0227	4	1.01	2.73	4.73
C ₉ H ₈ O ₅ S	227.0020	6	0.22	0.06	1.89
C ₉ H ₁₀ O ₅ S	229.0176	5	1.87	1.59	6.47
C ₉ H ₁₂ O ₄ S	215.0384	4	0.62	0.75	1.70
C ₉ H ₁₂ O ₅ S	231.0333	4	0.67	0.65	2.24
C ₁₀ H ₁₀ O ₆ S	257.0125	6	0.19	0.26	7.13
C ₁₀ H ₁₀ O ₇ S	273.0074	6	0.64	0.63	7.89
C ₁₀ H ₁₂ O ₇ S	275.0231	5	0.10	0.05	0.57
C ₁₁ H ₁₂ O ₇ S	287.0231	6	1.04	0.58	3.75
C ₁₁ H ₁₄ O ₇ S	289.0387	5	0.13	0.19	0.28
C ₆ H ₅ NO ₆ S	217.9765	5	0.07	0.13	0.45
C ₁₀ H ₁₁ NO ₇ S	288.0183	6	0.54	0.59	3.30
C ₁₀ H ₁₁ NO ₈ S	304.0133	6	0.01	0.07	0.38
C ₁₀ H ₁₁ NO ₉ S	320.0082	6	0.17	#DIV/0!	0.59
C ₁₀ H ₁₇ NO ₉ S	326.0551	3	59.04	19.53	21.00
C ₁₁ H ₁₃ NO ₈ S	318.0289	6	0.08	0.09	0.23
C ₁₁ H ₁₃ NO ₉ S	334.0238	6	0.11	0.07	0.14
C ₁₂ H ₁₅ NO ₈ S	332.0446	6	0.02	0.06	0.19
C ₁₂ H ₁₅ NO ₁₀ S	364.0344	6	0.04	0.09	0.18

Table S10. Molecular information and their relative abundance of long-chain alkanes-derived organosulfates detected at Shanghai.

Molecular formula	m/z [M-H] ⁻	DBE	Relative peak area (%)		
			Suburban Summer	Urban Summer	Urban Winter
C ₇ H ₁₄ O ₅ S	209.0489	1	22.41	18.24	76.35
C ₇ H ₁₆ O ₄ S	195.0697	0	2.42	4.03	35.49
C ₈ H ₁₈ O ₄ S	209.0853	0	11.64	16.55	95.01
C ₉ H ₁₆ O ₇ S	267.0544	2	50.43	25.62	35.43
C ₉ H ₁₈ O ₅ S	237.0802	1	18.64	17.03	62.95
C ₉ H ₁₈ O ₇ S	269.0700	1	10.32	3.59	13.60
C ₉ H ₁₈ O ₈ S	285.0650	1	0.31	0.15	0.29
C ₉ H ₂₀ O ₈ S	287.0806	0	0.23	0.09	0.98
C ₁₀ H ₁₆ O ₈ S	295.0493	3	14.38	4.44	13.00
C ₁₀ H ₁₈ O ₆ S	265.0751	2	17.15	9.58	31.55
C ₁₀ H ₁₈ O ₇ S	281.0700	2	52.91	25.09	31.85
C ₁₀ H ₁₈ O ₈ S	297.0650	2	13.43	5.27	14.93
C ₁₀ H ₂₀ O ₅ S	251.0959	1	56.42	29.99	118.32
C ₁₀ H ₂₀ O ₆ S	267.0908	1	11.76	6.89	23.91
C ₁₀ H ₂₀ O ₈ S	299.0806	1	0.32	0.15	0.33
C ₁₂ H ₂₀ O ₇ S	307.0857	3	6.37	1.44	10.26
C ₁₂ H ₂₄ O ₅ S	279.1272	1	88.32	47.93	201.25
C ₁₂ H ₂₆ O ₄ S	265.1479	0	64.32	98.49	59.52
C ₇ H ₁₅ NO ₈ S	272.0446	1	2.85	1.92	10.07
C ₈ H ₁₅ NO ₉ S	300.0395	2	9.38	5.00	15.91
C ₉ H ₁₇ NO ₇ S	282.0653	2	1.49	1.36	9.15
C ₉ H ₁₇ NO ₈ S	298.0602	2	7.46	3.68	24.95
C ₉ H ₁₇ NO ₉ S	314.0551	2	10.14	5.80	19.40
C ₉ H ₁₇ NO ₁₀ S	330.0500	2	22.12	9.87	6.22
C ₁₀ H ₁₉ NO ₈ S	312.0759	2	22.81	8.72	47.88
C ₁₀ H ₁₉ NO ₉ S	328.0708	2	10.60	5.05	17.91
C ₁₀ H ₁₉ NO ₁₀ S	344.0657	2	8.11	3.58	11.03
C ₁₀ H ₁₉ NO ₁₁ S	360.0606	2	0.79	0.45	1.81

Table S11. Summary of molecular characteristics of CHOS compounds detected in our field samples and source samples, as the MS data are obtained from Cui et al. (2019) and Tang et al. (2020).

Source samples	Formula number	MW _w	H/C _w	O/C _w	O/S _w	DBE _w	% of Xc _c ≥2.5	% of (4s+3n)/o ≤1
BBOA1(Musa)	444	360	1.52	0.47	6.21	4.76	43	88
BBOA2(Hevea)	174	396	1.35	0.40	5.97	7.68	59	86
CCOA1(Anthracite)	549	323	1.01	0.40	5.40	8.55	82	95
CCOA2(Bituminous coal)	463	340	0.99	0.31	4.64	9.90	94	85
Tunnel aerosol	635	325	1.74	0.59	6.79	2.75	23	96
Vehicle emission	112	441	1.31	0.25	4.47	9.54	71	75
Excavator-idling(diesel)	1004	353	1.61	0.38	5.81	4.18	58	96
Excavator-moving(diesel)	334	326	1.51	0.46	5.20	3.58	49	98
Excavator-working(diesel)	631	342	1.63	0.36	5.44	4.00	55	93
Diesel-vessel	334	306	1.66	0.40	5.14	3.47	50	95
Heavy-fuel-oil-vessel	1110	311	1.48	0.36	4.77	4.85	71	83
Suburban summer	1069	300	1.88	0.58	5.21	2.06	7	86
Urban summer	1127	302	1.81	0.53	5.12	2.18	10	85
Urban winter	1412	285	1.62	0.45	4.98	2.56	18	92

Table S12. Summary of molecular characteristics of CHONS compounds detected in our field samples and source samples, as the MS data are obtained from Cui et al. (2019) and Tang et al. (2020).

Source samples	Formula number	MW _w	H/C _w	O/C _w	O/S _w	DBE _w	% of X _c ≥2.5	% of (4s+3n)/o ≤1
BBOA1(Musa)	371	379	1.55	0.50	7.21	4.98	64	64
BBOA2(Hevea)	65	411	1.56	0.50	7.51	4.79	69	63
CCOA1(Anthracite)	767	340	0.98	0.52	6.49	8.99	97	47
CCOA2(Bituminous coal)	293	308	0.97	0.49	5.82	8.04	93	29
Tunnel aerosol	410	340	1.81	0.90	8.73	2.78	29	91
Vehicle emission	17	400	1.17	0.72	8.59	6.92	59	47
Excavator-idling(diesel)	310	325	1.47	0.41	5.59	5.18	65	42
Excavator-moving(diesel)	117	298	1.62	0.48	5.17	5.55	64	9
Excavator-working(diesel)	260	323	1.47	0.40	5.41	5.26	69	27
Diesel-vessel	13	461	1.50	0.36	6.74	9.38	38	46
Heavy-fuel-oil-vessel	398	343	1.35	0.39	5.68	6.35	86	28
Suburban summer	895	325	1.60	0.77	7.54	4.27	11	73
Urban summer	787	332	1.53	0.69	6.98	4.89	15	89
Urban winter	1277	322	1.44	0.65	6.44	6.02	21	92

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