

Supplementary Information

Measurement Report: Molecular Dynamics of Organic Aerosol in the Wintertime East China Sea Driven by East Asian Outflows

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Table S1. Gradient Separation of LC

Time	Methanol	Water	Remarks
0.5 min	5%	95%	linear
0.5-27 min	95%	5%	
27-27.1 min	5%	95%	

Table S2. Basic information of the three periods.

	Unit	MBGA	PE_North	PE_East
Temperature	°C	11.8	8.8	9.0
RH	%	89.1	71.7	55.5
DSWRF	Wm ⁻¹	234.6	449.7	933.6
O ₃ _Path	µg/m ³	--	50.9	62.8
SO ₂ _Path	µg/m ³	--	21.9	16.3
NO ₂ _Path	µg/m ³	--	46.7	60.1
Ox_path	µg/m ³	--	94.6	120.6
Na ⁺	µg/m ³	0.2	1.3	1.3
NH ₄ ⁺	µg/m ³	0.3	11.5	14.6
K ⁺	µg/m ³	0.1	0.9	1.3
Mg ²⁺	µg/m ³	0.03	0.2	0.3
Ca ²⁺	µg/m ³	0.2	0.5	1.7
Cl ⁻	µg/m ³	0.3	1.7	2.2
NO ₃ ⁻	µg/m ³	0.8	14.5	29.5
SO ₄ ²⁻	µg/m ³	1.3	17.3	9.8
NO ₃ ⁻ /nss-SO ₄ ²⁻		0.6	0.8	3.2
SOR_Path		0.04	0.4	0.4
NOR_Path		0.02	0.2	0.3
ALWC	µg/m ³	6.0	42.6	29.0
ALWC/PM _{2.5}		1.4	0.8	0.4

OC	$\mu\text{g}/\text{m}^3$	0.6	4.6	9.4
EC	$\mu\text{g}/\text{m}^3$	0.2	0.6	1.0

Table S3. Summary of molecular characteristic of organic aerosol compositions.

Subgroup	Sample	DBE	DBE $\geq$ 4	X _c < 2.5	2.5 $\leq$ X _c < 2.71	X _c $\geq$ 2.71	O _{sc}	O(N)/C	H/C	O/N<2	O/N $\geq$ 3	O/S	O/S $\geq$ 4
ESI+			%	%	%	%				%	%	%	%
	MBGA	8.54 $\pm$ 7.95	74.34	41.59	17.7	40.71	-0.8 $\pm$ 0.68	0.24 $\pm$ 0.18	1.28 $\pm$ 0.54				
	PE_North	9.07 $\pm$ 6.61	83.43	25.41	37.02	37.57	-0.63 $\pm$ 0.72	0.25 $\pm$ 0.25	1.13 $\pm$ 0.53				
CHO	PE_East	9.75 $\pm$ 7.13	85.01	34.7	30.8	34.5	-0.61 $\pm$ 0.63	0.24 $\pm$ 0.2	1.09 $\pm$ 0.52				
	MBGA	8.04 $\pm$ 8.38	59.63	63.64	10.16	26.2	-1.08 $\pm$ 0.67	0.25 $\pm$ 0.2	1.59 $\pm$ 0.59	50.53	30.21		
	PE_North	9.35 $\pm$ 9.16	63.67	61.2	8.47	30.34	-0.9 $\pm$ 0.82	0.28 $\pm$ 0.25	1.46 $\pm$ 0.64	47.62	33.51		
CHON	PE_East	8.84 $\pm$ 9.01	62.32	61.26	7.73	31.01	-0.99 $\pm$ 0.7	0.26 $\pm$ 0.22	1.51 $\pm$ 0.61	52.46	31.4		
	MBGA	11.02 $\pm$ 7.34	85.94	32.81	28.13	39.06	-0.93 $\pm$ 0.57	0.15 $\pm$ 0.14	1.24 $\pm$ 0.47			2.48 $\pm$ 2.43	20.31
	PE_North	9.56 $\pm$ 7.37	76.04	48.96	17.71	33.33	-0.94 $\pm$ 0.67	0.16 $\pm$ 0.16	1.27 $\pm$ 0.54			2.39 $\pm$ 2.34	16.67
CHOS	PE_East	9.75 $\pm$ 7.87	82.84	48.52	22.49	28.99	-0.99 $\pm$ 0.65	0.17 $\pm$ 0.21	1.34 $\pm$ 0.49			2.7 $\pm$ 2.83	21.89
	MBGA	9.84 $\pm$ 8.51	74.15	55.1	12.24	32.65	-1.08 $\pm$ 0.72	0.19 $\pm$ 0.2	1.45 $\pm$ 0.61	68.03	17.01	3.03 $\pm$ 2.96	29.25
	PE_North	11.78 $\pm$ 9.21	78.29	45.74	11.24	43.02	-0.9 $\pm$ 0.71	0.18 $\pm$ 0.19	1.27 $\pm$ 0.62	63.57	22.09	2.79 $\pm$ 3.14	23.26
CHONS	PE_East	12.65 $\pm$ 9.56	74.67	44.06	6.33	49.6	-0.87 $\pm$ 0.71	0.17 $\pm$ 0.17	1.21 $\pm$ 0.69	62.8	22.96	2.51 $\pm$ 2.53	22.43
CHN	MBGA	11.23 $\pm$ 7.83	92.98	7.02	24.56	68.42	-1.25 $\pm$ 0.48	1.25 $\pm$ 0.48	0.12 $\pm$ 0.07				

	PE_North	12.35±7.3	95.05	4.95	14.85	80.2	-1.08±0.44	1.08±0.44	0.11±0.06				
	PE_East	10.7±7.25	95.58	4.42	24.15	71.43	-1.03±0.47	1.03±0.47	0.11±0.08				
ESI-													
	MBGA	3.69±3.91	34.95	82.52	10.68	6.8	-1.05±0.77	0.3±0.32	1.65±0.35				
	PE_North	4.09±3.83	41.41	71.21	17.17	11.62	-0.98±0.8	0.29±0.32	1.55±0.44				
CHO	PE_East	4.47±3.77	47.76	65.04	19.72	15.24	-0.89±0.78	0.29±0.3	1.46±0.5				
	MBGA	5.82±4.58	65.88	67.06	15.29	17.65	-1.14±0.74	0.23±0.2	1.6±0.43	61.18	24.71		
	PE_North	6.99±5.4	74.27	62.62	14.08	23.3	-0.9±0.71	0.25±0.17	1.39±0.53	51.94	29.61		
CHON	PE_East	7.12±5.43	81.34	62.88	15.62	21.5	-0.52±0.8	0.34±0.22	1.2±0.53	35.9	46.65		
	MBGA	2.49±3.1	28.21	89.74	7.69	2.56	-1.53±0.4	0.22±0.18	1.97±0.28			2.12±1.73	25.64
	PE_North	1.4±2.38	18.95	93.68	4.21	2.11	-1.35±0.7	0.34±0.31	2.04±0.33			2.6±1.89	40
CHOS	PE_East	1.78±2.9	22.73	92.61	5.11	2.27	-1.39±0.6	0.29±0.23	1.98±0.37			2.74±2.17	40.34
	MBGA	8.56±7.79	65.63	56.25	12.5	31.25	-1.03±0.95	0.24±0.26	1.51±0.63	62.5	21.88	4.47±5.45	34.38
	PE_North	8.29±7.26	71.01	53.62	15.94	30.43	-0.95±0.93	0.26±0.28	1.46±0.64	69.57	18.84	4.05±5.2	27.54
CHONS	PE_East	9.41±8.82	74.17	49.17	16.67	34.17	-0.79±0.92	0.32±0.33	1.43±0.62	61.67	29.17	4.39±5.42	30.83

Table S4. The fraction of potential aromatics with a benzene/naphthalene/anthracene/pyrene core structure. FN: formula number. RI: relative intensity.

FN/RI (%)		MBGA+	PE_North+	PE_East+	MBGA-	PE_North-	PE_East-
CHO	<2.5	41.59/27.11	25.41/26.68	34.7/30.86	82.52/86.44	71.21/81.68	65.04/77.02
	$2.50 \leq X_c < 2.71$	17.7/27.84	37.02/53	30.8/46.4	10.68/8.97	17.17/11.34	19.72/13.75
	$2.71 \leq X_c < 2.80$	15.93/33.68	9.94/10.14	14.37/10.63	2.91/3.06	8.08/5.96	10.77/7.89
	$2.80 \leq X_c < 2.83$	3.54/0.38	4.97/1.72	6.37/1.97	0.97/0.99	2.02/0.82	1.83/0.92
	$2.83 \leq X_c < 2.92$	21.24/10.99	22.65/8.46	13.76/10.14	2.91/0.54	1.52/0.21	2.64/0.43
	<2.5	63.64/79.1	61.2/82.93	61.26/76.85	67.06/78.75	62.62/81.77	62.88/84.84
	$2.50 \leq X_c < 2.71$	10.16/10.66	8.47/4.84	7.73/10.11	15.29/10.33	14.08/7.9	15.62/8.24
	$2.71 \leq X_c < 2.80$	7.75/1.3	4.23/1.83	7.63/4.61	5.88/7.67	5.34/3.57	8.72/3.82
CHON	$2.80 \leq X_c < 2.83$	2.14/0.22	3.88/0.54	3/0.42	4.71/1.23	1.94/0.75	2.03/0.38
	$2.83 \leq X_c < 2.92$	16.31/8.73	22.22/9.86	20.39/8.01	7.06/2.02	16.02/6.02	10.75/2.72
CHOS	<2.5	32.81/34.34	48.96/40.63	48.52/53.83	89.74/96.62	93.68/98.81	92.61/98.55
	$2.50 \leq X_c < 2.71$	28.13/32.93	17.71/26.37	22.49/20.54	7.69/2.9	4.21/0.94	5.11/1.15
	$2.71 \leq X_c < 2.80$	15.63/27.58	9.38/18.69	10.65/10.77	2.56/0.48	2.11/0.25	1.14/0.18

	$2.80 \leq X_c < 2.83$	9.38/1.56	8.33/6.74	3.55/5.78	0/0	0/0	0/0
	$2.83 \leq X_c < 2.92$	14.06/3.6	15.63/7.58	14.79/9.08	0/0	0/0	1.14/0.12
	< 2.5	55.1/75.2	45.74/31.34	44.06/38.05	56.25/83.32	53.62/82.82	49.17/67.52
	$2.50 \leq X_c < 2.71$	12.24/2.76	11.24/35.87	6.33/3.82	12.5/7.5	15.94/7.73	16.67/19.04
	$2.71 \leq X_c < 2.80$	9.52/6.39	10.85/9.27	8.71/20.18	3.13/0.7	4.35/1.97	10/3.81
	$2.80 \leq X_c < 2.83$	6.12/2.03	6.2/14.12	6.33/6.61	6.25/2.25	7.25/1.34	4.17/0.74
CHONS	$2.83 \leq X_c < 2.92$	17.01/13.61	25.97/9.4	34.56/31.33	21.88/6.24	18.84/6.13	20/8.89

Table S5. The fraction of oxidation state of organic molecules. FN: formula number. RI: relative intensity.

	FN/RI	LV-OOA+	SV-OOA+	BBOA+	HOA+	Other+	LV-OOA-	SV-OOA-	BBOA-	HOA-	Other-
	MBGA	12.45/6.19	13.83/16.81	32.08/34.51	2.36/12.39	39.28/30.09	3.37/6.8	3.2/10.68	28.45/44.66	7.8/8.74	57.17/29.13
	PE_North	16.99/5.52	29.21/29.28	19.53/22.1	19.22/13.26	15.05/29.83	0.7/6.57	9.15/21.72	31.99/38.38	6.95/9.6	51.22/23.74
CHO	PE_East	6.79/4.11	37.86/34.09	25.66/19.51	17.65/13.96	12.04/28.34	2.74/0	18.2/9.69	28.93/34.04	7.01/45.39	43.11/10.87
	MBGA	0.04/0.53	20.52/9.63	20.76/23.26	20.69/17.91	37.98/48.66	2.19/3.53	9.04/11.76	32.42/20	25.14/27.06	31.22/37.65
	PE_North	1.18/3.53	5/9.7	15.53/19.4	11.29/14.46	67.01/52.91	18.69/8.74	26.69/25.24	18.17/21.36	13.71/16.99	22.75/27.67
CHON	PE_East	1.07/2.32	16.16/12.75	20.29/21.16	11.13/18.65	51.35/45.12	33.76/25.15	40.66/30.63	11.39/19.88	4.45/10.55	9.74/13.79
	MBGA	0/0	12.72/10.94	43.94/26.56	13.42/23.44	29.93/39.06	0/0	4.57/7.69	23.79/20.51	4.23/12.82	67.41/58.97
	PE_North	0.47/3.13	38.6/14.58	35.53/20.83	12.74/25	12.66/36.46	0.14/1.05	4.6/12.63	47.94/31.58	5.43/5.26	41.89/49.47
CHOS	PE_East	0.75/1.18	22.59/13.61	40.09/26.63	25.24/26.63	11.32/31.95	0.18/1.7	5.5/13.64	56.33/40.91	3.68/1.7	34.31/42.05
	MBGA	0.67/0.68	6.17/9.52	13.07/21.09	20.21/17.69	59.89/51.02	1.2/3.13	6.05/6.25	6.94/12.5	19.62/21.88	66.19/56.25
	PE_North	0.39/1.94	12.68/11.63	52.13/20.16	4.76/10.47	30.03/55.81	0.46/1.45	10.66/17.39	9.22/15.94	21.25/17.39	58.41/47.83
CHONS	PE_East	1.14/2.11	12.12/8.18	27.81/14.25	6.73/9.76	52.21/65.7	1.87/5.83	26.94/18.33	21.52/24.17	5.89/10	43.77/41.67

Table S6. Stoichiometric ranges of van Kervelen classes.

Signal	Class	H/C	O/C
I	Lipids-like	1.5-2.0	0-0.3
II	Aliphatic/peptides-like	1.5-2.2	0.3-0.67
III	Carbohydrates-like	1.5-2.5	0.67-1
IV	Unsaturated hydrocarbons	0.67-1.5	<0.1
V	CRAMs-like structures	0.67-1.5	0.1-0.67
VI	Aromatic structures	0.2-0.67	<0.67
VII	Highly oxygenated compounds	0.6-1.5	0.67-1.0

Table S7. The fraction of organic molecules assigned by stoichiometric ranges. FN: formula number. RI: relative intensity. Note: The range of each area is given in Table S3, and Type-1 to Type-7 in this table and Figure S6 correspond to I to VII, respectively.

%	CHO			CHON			CHOS			CHONS		
FN/RI	MBGA	PE_North	PE-East	MBGA	PE_North	PE-East	MBGA	PE_North	PE-East	MBGA	PE_North	PE-East
Type-												
1+	14.36/21.24	12.25/16.02	10.93/17.04	26.61/24.33	24.6/24.87	22.11/23.96	19.99/23.44	22.24/36.73	27.75/37.28	61.25/36.73	18.68/29.07	21.84/29.82
Type-												
2+	7.54/9.73	12.68/4.97	10.31/6.78	24.09/16.84	7.37/9.7	16.11/10.82	8.47/6.25	3.31/3.06	7.75/2.96	3.86/8.16	1.78/4.26	2.32/3.17

Type-													
3+	0.1/0.88	0.09/0.55	0.11/0.62	0.03/0.27	0.93/1.94	1.46/2.32	0/0	0/0	0.05/0.59	0.57/1.36	0.45/1.16	0.31/0.53	
Type-													
4+	0.57/7.08	7.18/9.94	3.9/6.98	3.31/10.16	4.15/11.11	5.33/12.27	51.69/34.38	27.16/22.45	34.17/25.44	10.55/14.29	42.55/17.44	22.34/15.04	
Type-													
5+	55.3/40.71	28.79/34.81	41.45/37.78	12/18.72	14.19/21.34	21.62/20.39	11.73/26.56	36.62/22.45	18.22/17.75	9.12/15.65	16.25/17.05	13/14.78	
Type-													
6+	18.55/10.62	34.34/24.31	30.36/26.69	5.63/7.49	4.41/9.35	4.23/11.4	7.22/6.25	7.68/13.27	3.61/7.1	4.45/12.93	10.83/19.38	25.2/28.5	
Type-													
7+	0/0	0.09/0.55	0.19/1.03	0.14/1.34	0.17/1.41	0.32/0.97	0/0	0.46/1.02	0.91/1.18	1.07/2.72	0.7/1.55	0.71/1.85	
Other+	3.59/9.73	4.58/8.84	2.76/3.08	28.18/20.86	44.19/20.28	28.81/17.87	0.9/3.13	2.54/1.02	7.53/7.69	9.14/8.16	8.76/10.08	14.27/6.33	
Type-													
1-	73.18/58.25	74.1/58.08	66.86/47.56	44.65/56.47	30.03/43.69	12.23/24.54	30.59/41.03	41.47/26.32	39.8/27.27	21.09/31.25	22.5/26.09	14.24/25	
Type-													
2-	2.97/8.74	3.2/10.1	3.85/7.11	14.92/8.24	9.94/5.83	4.16/4.87	35.05/20.51	18.53/18.95	25.16/27.27	7.85/9.38	7.71/7.25	8.23/6.67	
Type-													
3-	0/0	0/0	0.04/0.2	0/0	0/0	0/0	0.71/2.56	4.5/7.37	1.33/3.41	0/0	3.98/4.35	34.21/5.83	

Type-												
4-	1.51/2.91	1.15/2.53	1.89/3.46	1.89/8.24	0.65/3.88	0.45/3.04	0/0	0/0	0.43/1.7	4.01/18.75	3.25/20.29	7.87/21.67
Type-												
5-	13.1/22.33	16.22/23.74	18.9/27.85	35.13/23.53	52.64/33.5	70.96/46.86	1.84/5.13	1.15/3.16	1.57/3.98	10.15/21.88	8.67/20.29	11.97/15.83
Type-												
6-	0/0	1.86/5.05	4.2/8.13	0/0	3.32/9.71	3.98/11.16	0/0	0/0	0.08/0.57	1.19/12.5	0.72/11.59	2.72/12.5
Type-												
7-	0/0	0/0	0.05/0.2	0/0	1.05/2.43	4.84/5.27	0/0	0.29/2.11	0/0	0/0	0.26/1.45	0.51/2.5
Other	9.23/7.77	3.47/0.51	4.22/5.49	3.41/3.53	2.36/0.97	3.37/4.26	31.81/30.77	34.06/42.11	31.62/35.8	55.72/6.25	52.9/8.7	20.25/10

Table S8. The fractions of volatility organic compounds. FN: formula number. RI: relative intensity.

ESI+	FN/RI	MBGA (%)	PE_North (%)	PE_East (%)
CHO	IVOC	30.97/32.57	33.7/46.6	34.5/44.11
	SVOC	23.01/14.52	18.78/9.85	19.51/9.61
	LVOC	23.01/35.29	22.65/25.8	19.51/28.04
	ELVOC	23.01/17.62	24.86/17.75	26.49/18.24
CHON	IVOC	2.94/1.8	4.94/2.25	5.8/2.55
	SVOC	12.83/14.09	13.93/15.63	14.3/18.43
	LVOC	36.1/52.28	29.81/49.9	26.57/40.44
	ELVOC	48.13/31.83	51.32/32.22	53.33/38.58
CHOS	IVOC	0/0	5.21/7.42	3.55/2.13
	SVOC	14.06/29.02	17.71/28.85	17.75/25.25
	LVOC	42.19/56.23	40.63/44.27	35.5/46.08
	ELVOC	43.75/14.75	36.46/19.46	43.2/26.53
CHONS	IVOC	20.41/25.25	20.41/25.25	17.15/28.44
	SVOC	14.29/10.27	14.29/10.27	16.36/27.05
	LVOC	21.09/22.44	21.09/22.44	18.47/20.27
	ELVOC	44.22/42.05	44.22/42.05	48.02/24.23
CHN	IVOC	19.3/21.79	28.71/28.34	53.06/82.26
	SVOC	19.3/25.95	24.75/40.46	23.13/9.83
	LVOC	45.61/49.37	19.8/10.93	11.9/4.98
	ELVOC	15.79/2.89	26.73/20.27	11.9/2.93
ESI-	FN/RI	MBGA (%)	PE_North (%)	PE_East (%)
CHO	IVOC	49.51/31.67	53.03/41.72	53.25/42.26
	SVOC	39.81/57.36	32.83/45.68	34.96/48.32
	LVOC	3.88/8.04	8.59/9.47	7.52/7.5
	ELVOC	6.8/2.93	5.56/3.13	4.27/1.92
CHON	IVOC	3.53/4.33	6.8/30.03	7.71/39.87
	SVOC	36.47/46.98	40.29/36.63	49.7/40.15
	LVOC	17.65/13.57	20.39/9.94	20.89/6.28
	ELVOC	42.35/35.12	32.52/23.39	21.7/13.7
CHOS	IVOC	20.51/15.63	21.05/18.59	21.02/13.2
	SVOC	30.77/67.21	49.47/64.62	53.41/70.77
	LVOC	20.51/10.37	16.84/13.45	13.64/12.95
	ELVOC	28.21/6.79	12.63/3.35	11.93/3.08
CHONS	IVOC	12.5/8.93	23.19/11.42	20.83/19.65
	SVOC	18.75/4.05	10.14/4.52	10.83/6.82
	LVOC	21.88/20.11	23.19/24.31	24.17/19.91
	ELVOC	46.88/66.91	43.48/59.76	44.17/53.62

Table S9. Summary of PM_{2.5} concentration and volatility in different areas.

Site	PM _{2.5}	Log ₁₀ (C ₀)
Unit	μg/m ³	/μgm ⁻³
Mainz	15.75	0.94
Beijing_Low	39.83	1.62
Xi'an	48.20	1.69
Hong Kong	60.67	2.49
Chengdu	99.67	2.51
Guangzhou	129.33	2.50
Shanghai	148.33	2.58
Beijing_High	242.00	2.90
HNI_MBGA	4.42	-3.26
HNI_PE_North	55.72	-2.47
HNI_PE_East	76.67	-2.43

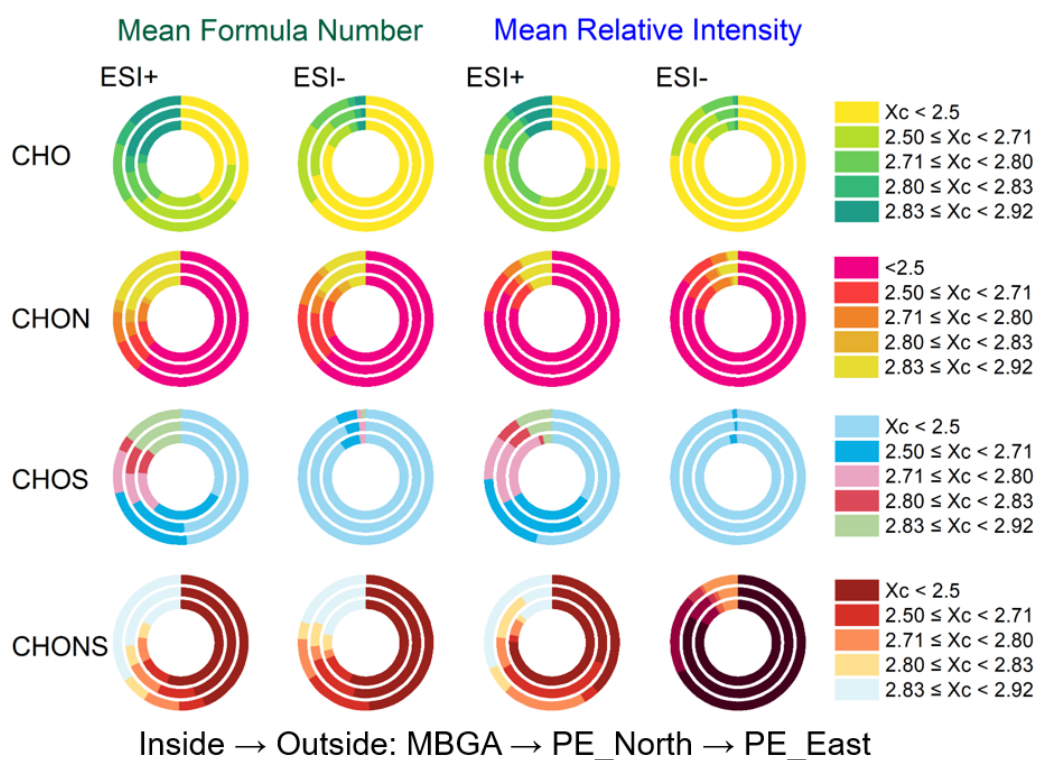


Figure S1. Statistic on the fractions of organic compounds with different X_c values in different subgroups across the three periods in terms of formula number and relative intensity.

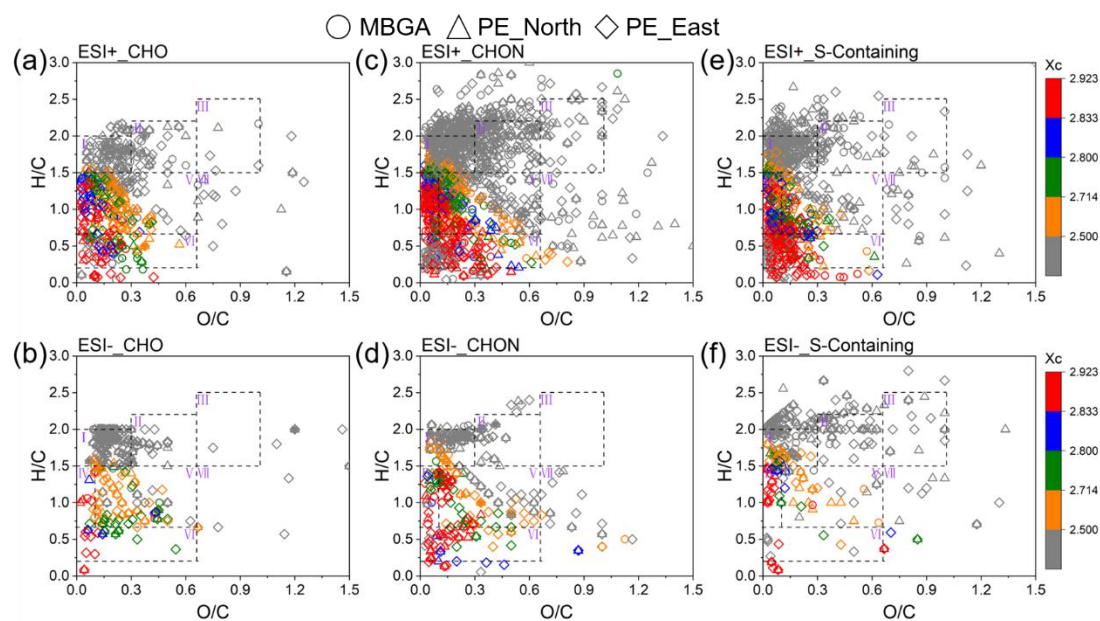


Figure S2. Van Kervelen (VK) diagrams of all detected compounds for (a-b) CHO, (c-d) CHON, and (e-f) S-containing subgroups in ESI+ and ESI-.

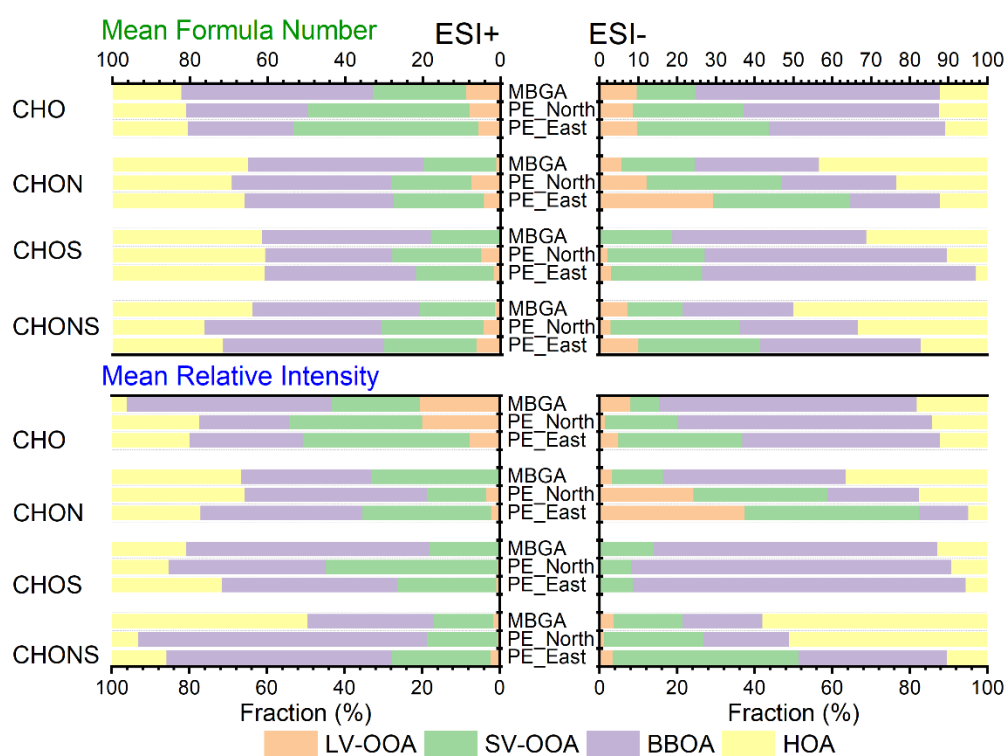


Figure S3. The fraction of LV-OOA, SV-OOA, BBOA and HOA in different subgroups across the three periods in terms of formula number and relative intensity.

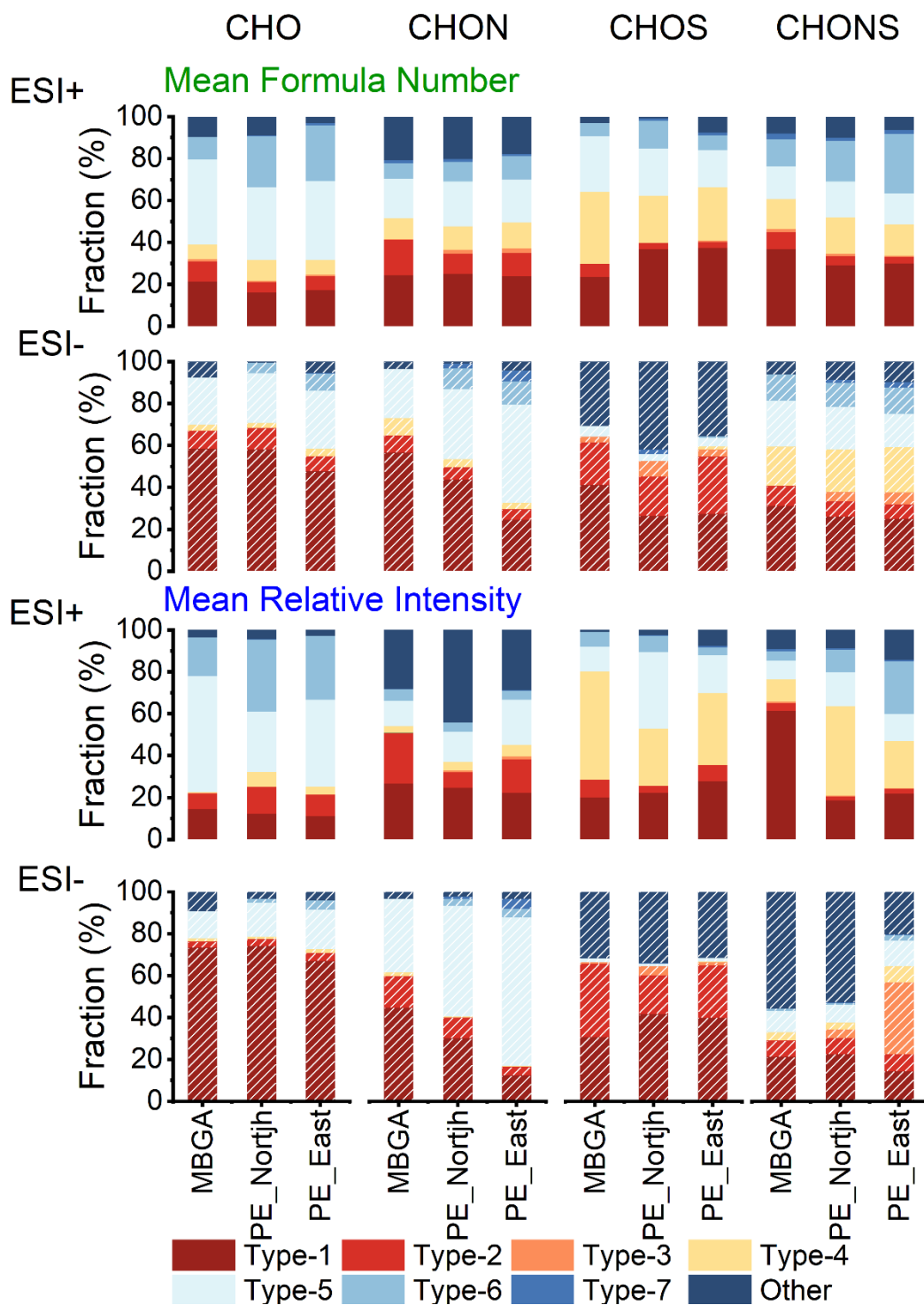


Figure S4. The fraction of various organic compounds classes in different subgroups across the three periods in terms of formula number and relative intensity. The range of each area is given in Table S6, and Type-1 to Type-7 in this figure correspond to I to VII, respectively.

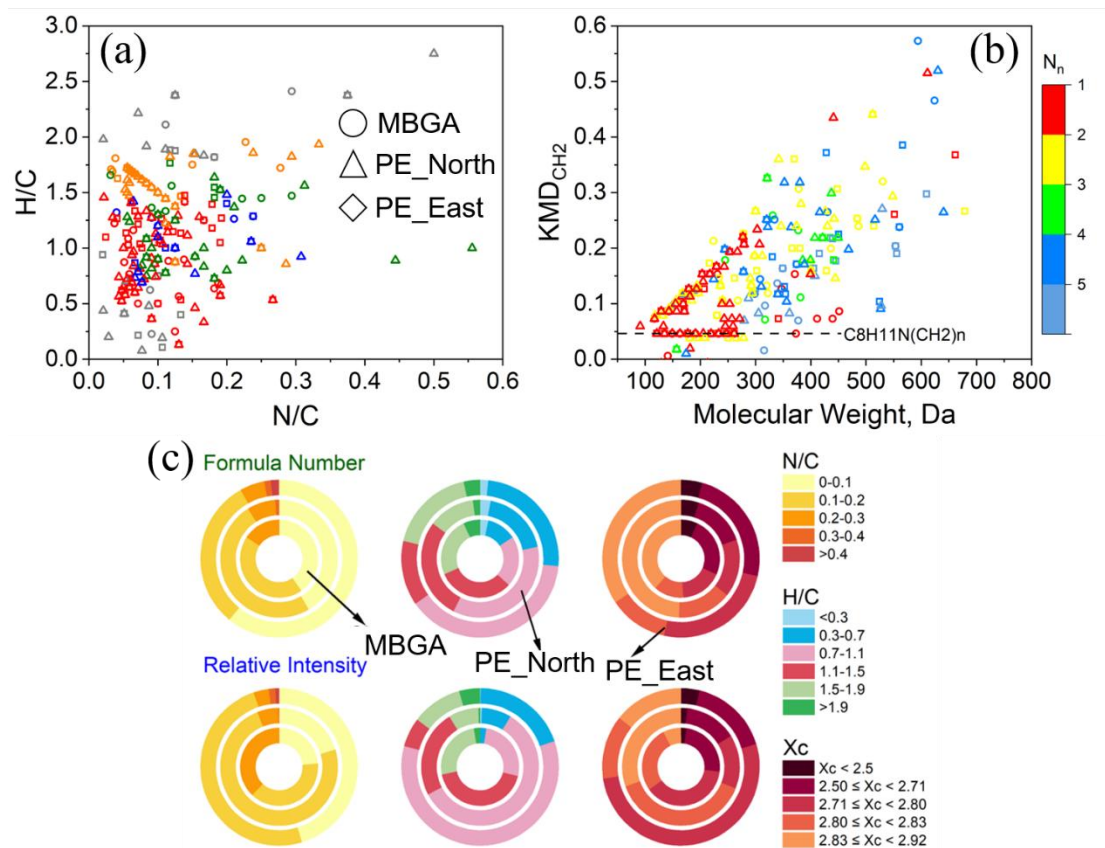


Figure S5. (a) Distribution of N/C versus H/C, (b) CH₂-Kendrick diagrams of CHN⁺, and (c) statistics on N/C, H/C, and X_c.

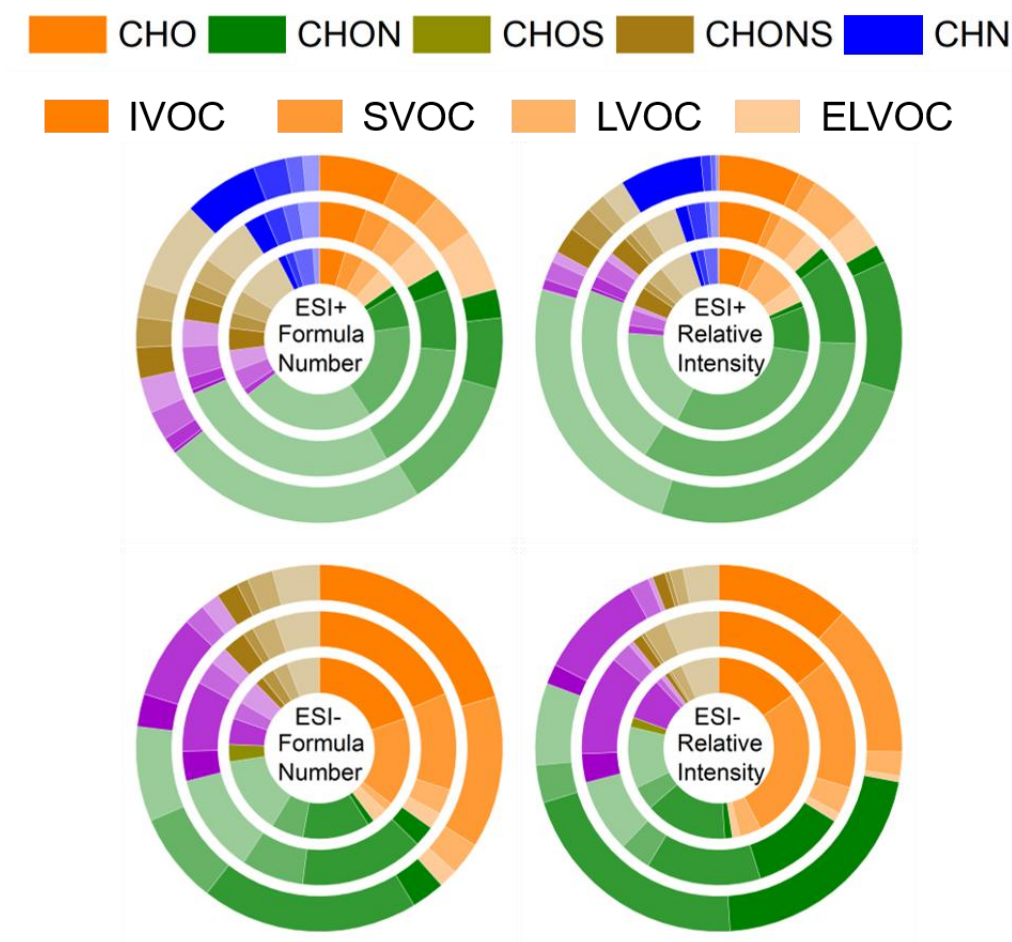


Figure S6. The fraction of organic molecules with different volatility in different subgroups across the three periods in terms of formula number and relative intensity (inside $\rightarrow$ outside: MBGA $\rightarrow$ PE_North $\rightarrow$ PE_East).

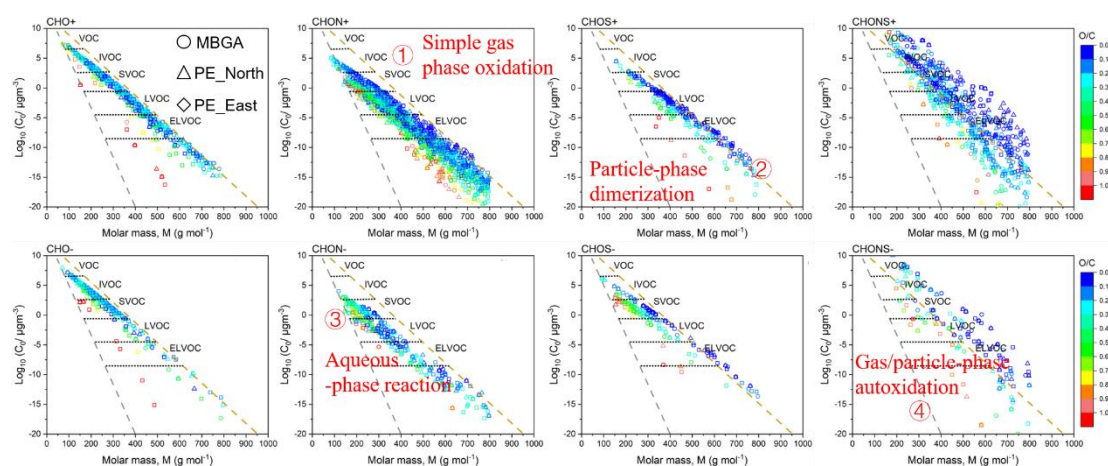


Figure S7. Molecular corridors of molecular weight versus saturation mass concentration (C_0) for organic compounds in CHO, CHON, CHOS and CHONS subgroups.

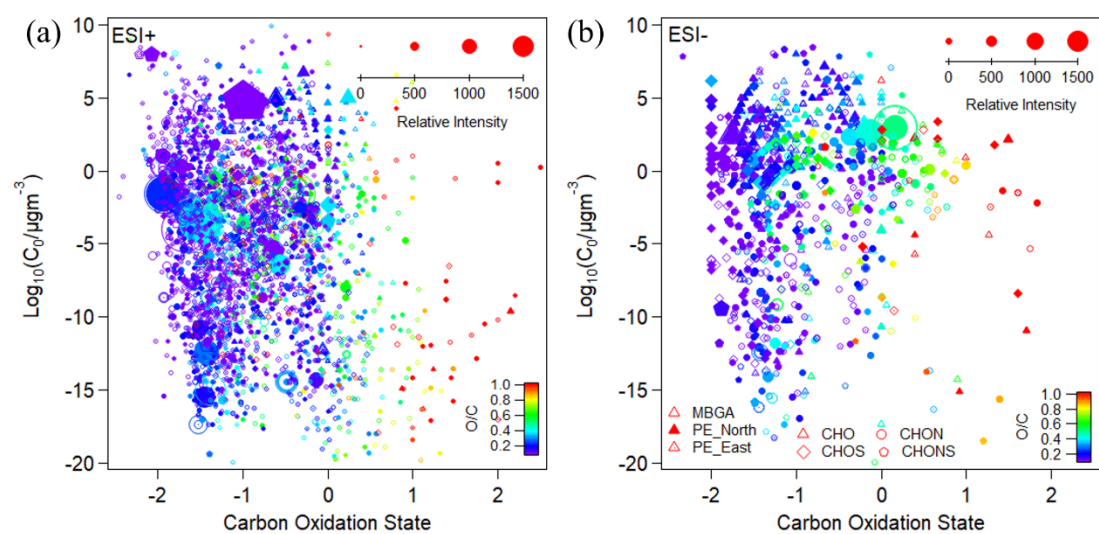


Figure S8. Scatter plots of carbon oxidation state versus saturation mass concentration (C_0) for organic compounds in (a) ESI+ and (b) ESI- mode.