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Measurement report: Molecular characterization of organic aerosol in coastal environments using offline FIGAERO-I-CIMS

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Table S1

Summary of offline data ($PM_{2.5}$ and chemical compositions) and online data (gaseous pollutants and meteorological parameters) at the urban and the seaside sites (average ± sd).

para	Urban	Seaside
Offline data		
CHO	0.0978±0.0284	0.0729±0.0252
CHON	0.0330±0.0108	0.0226±0.0093
CHOS	0.0023±0.0006	0.0056±0.0016
CHONS	0.0006±0.0003	0.0007±0.0003
OC(μg m^{-3})	5.70±1.64	4.87±1.31
EC	1.57±0.80	0.91±0.42
NO_3^-	5.08±4.65	5.19±4.20
SO_4^{2-}	5.08±3.49	5.89±3.94
NH_4^+	2.81±1.73	3.08±1.58
Cl^-	0.18±0.11	0.18±0.09
$PM_{2.5}$	30.74±11.39	28.93±10.49
Online data (μg m^{-3})		
$PM_{2.5}$	16.67±9.41	16.95±9.36
SO_2	2.52±1.56	2.75±1.95
NO*x*	37.16±25.14	23.72±18.63
O_3	51.47±32.00	69.67±39.81
CO (mg m^{-3})	0.67±0.13	0.42±0.16
UVB (W m^{-2})	7.22±11.46	8.03±12.18
WS (m s^{-1})	0.88±0.46	2.20±1.62
***T* (℃)**	22.5±3.2	22.1±3.0
RH (%)	82±16	92±13

Note: UVB: ultraviolet, WS: wind speed, *T*: temperature, RH: relative humidity.

Table S2

Summary of the intensity-weighted parameter P_w for different type of CHOX.

Parameter (weight)		DBE	DBE/C	O_{eff}/C	OSc	AI_{mod}
CHOX	Urban	3.25	0.56	0.82	0.49	0.17
	Seaside	2.99	0.56	0.85	0.55	0.15
	Urban_C1	3.35	0.54	0.77	0.37	0.17
	Seaside_C1	3.06	0.53	0.80	0.41	0.15
	Urban_C2	3.22	0.57	0.83	0.51	0.18
	Seaside_C2	2.85	0.58	0.91	0.69	0.15
CHO	Urban	3.11	0.59	0.98	0.67	0.18
	Seaside	2.84	0.60	1.04	0.77	0.15
	Urban_C1	3.26	0.57	0.92	0.54	0.19
	Seaside_C1	2.93	0.57	0.97	0.60	0.16
	Urban_C2	3.10	0.59	0.97	0.66	0.19
	Seaside_C2	2.72	0.62	1.08	0.87	0.15
CHON	Urban	3.66	0.47	0.42	-0.08	0.14
	Seaside	3.58	0.47	0.41	-0.11	0.14
	Urban_C1	3.58	0.45	0.43	-0.10	0.12
	Seaside_C1	3.55	0.45	0.42	-0.13	0.13
	Urban_C2	3.68	0.50	0.44	0.02	0.16
	Seaside_C2	3.60	0.51	0.41	-0.01	0.18
S-containing	Urban	3.19	0.59	0.36	1.00	0.10
	Seaside	2.54	0.38	0.33	0.35	0.08
	Urban_C1	3.27	0.62	0.33	1.00	0.10
	Seaside_C1	2.68	0.40	0.30	0.27	0.08
	Urban_C2	3.16	0.60	0.35	1.07	0.10
	Seaside_C2	2.32	0.41	0.35	0.56	0.07

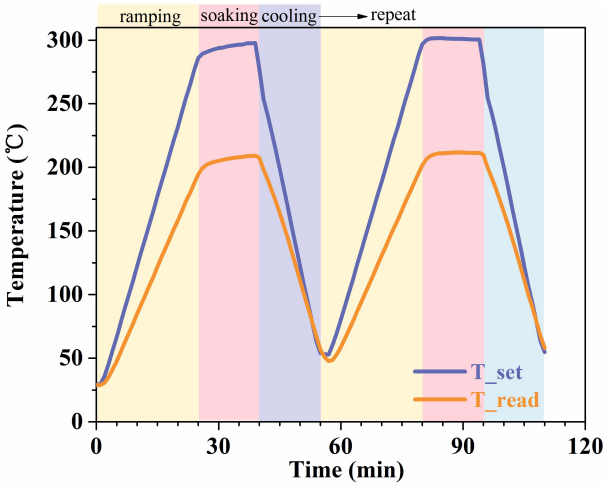


Fig. S1 The set temperature of the instrument (T_set) and actual temperature on the filter (T_read) change with time of the two heating cycles.

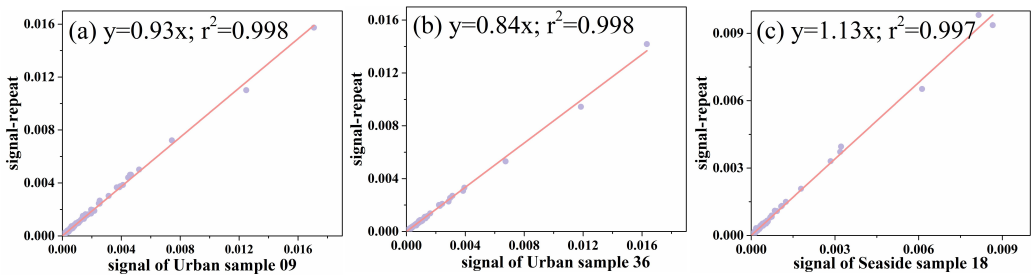


Fig. S2 The correlation of parallel experiments.

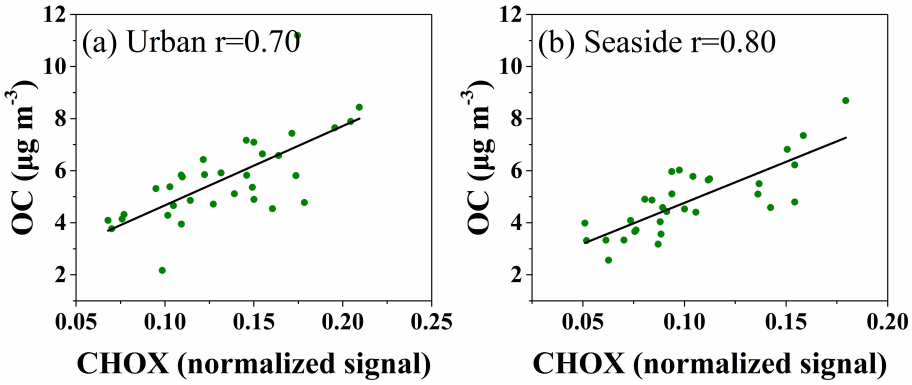


Fig. S3 The correlation between the CHOX signal and OC concentration at the urban (a) and the seaside (b) sites.

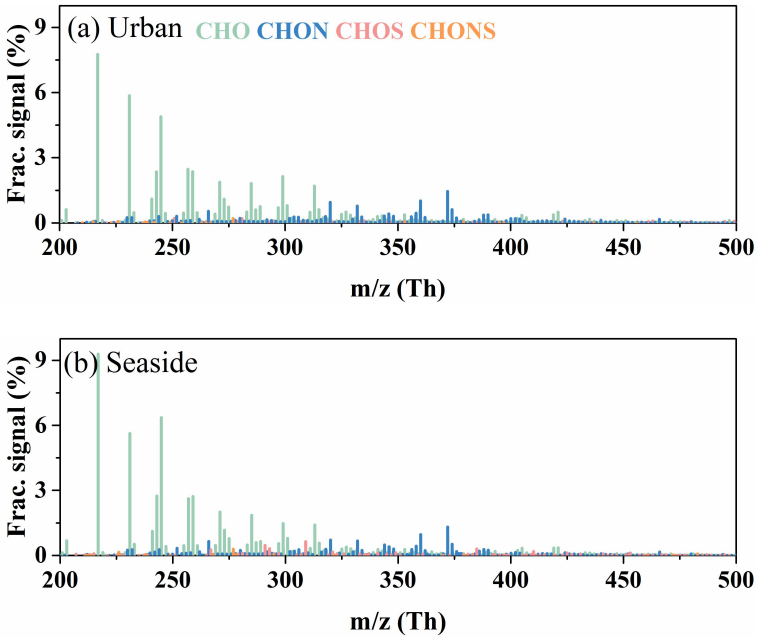


Fig. S4 Mass spectra of the identified compounds (CHO, CHON, CHOS, and CHONS) within the range of m/z 200~500 at the urban (a) and the seaside (b) sites.

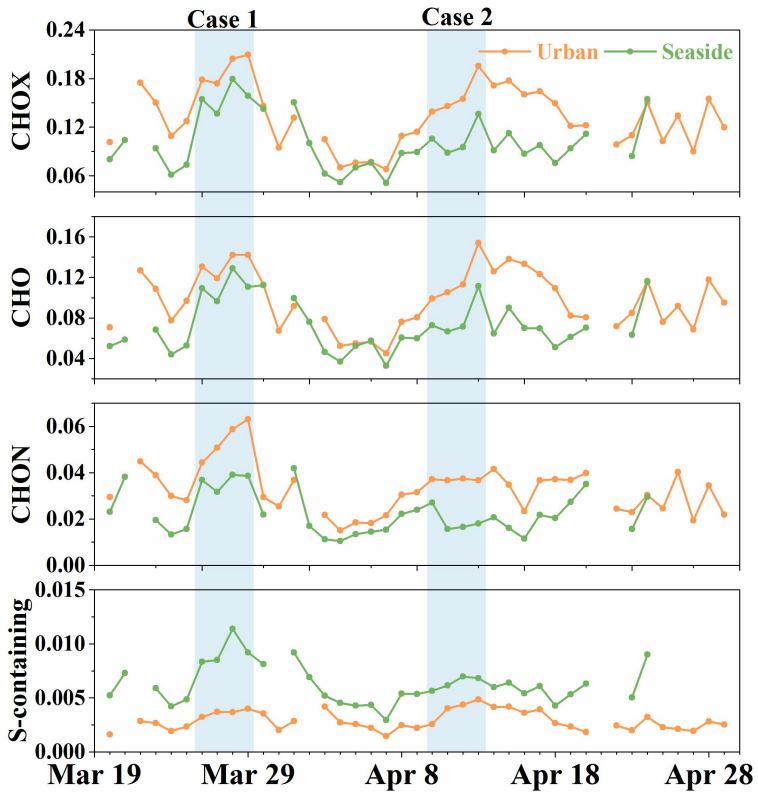


Fig. S5 Temporal variations of CHOX, CHO, CHON, and S-containing compounds (normalized signal) at the urban (a) and the seaside (b) sites.

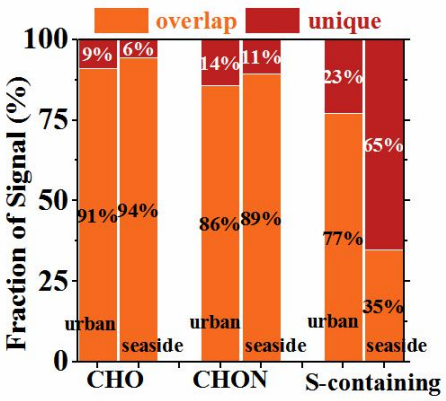


Fig. S6 The fraction of signals from the same chemical formula (overlap) and different chemical formula (remain) compounds identified at the two sites.

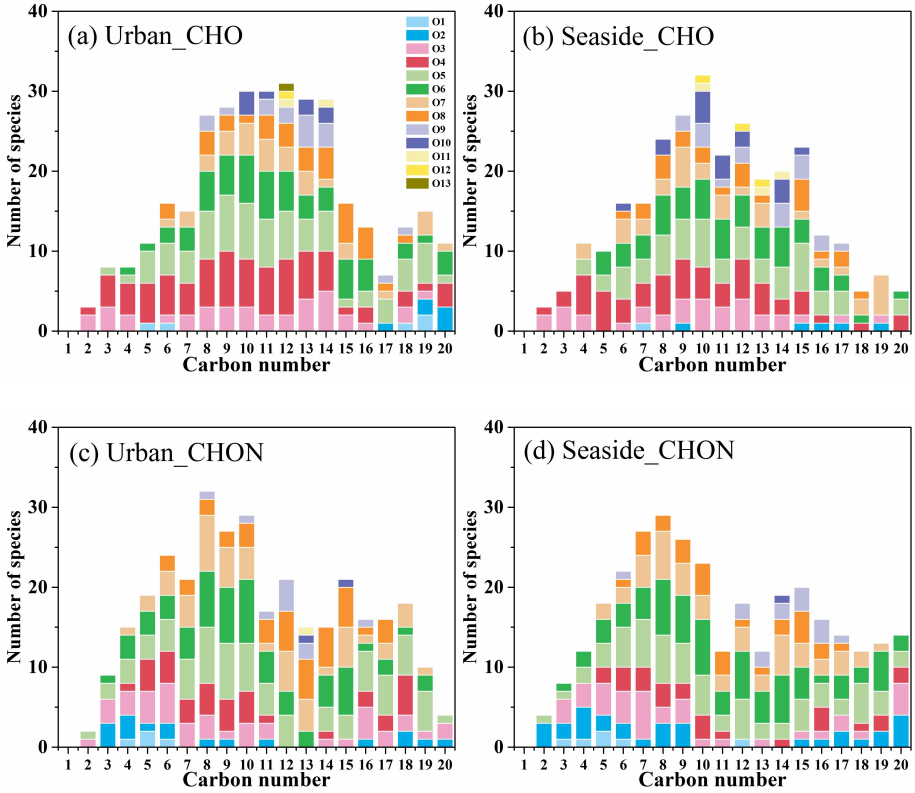
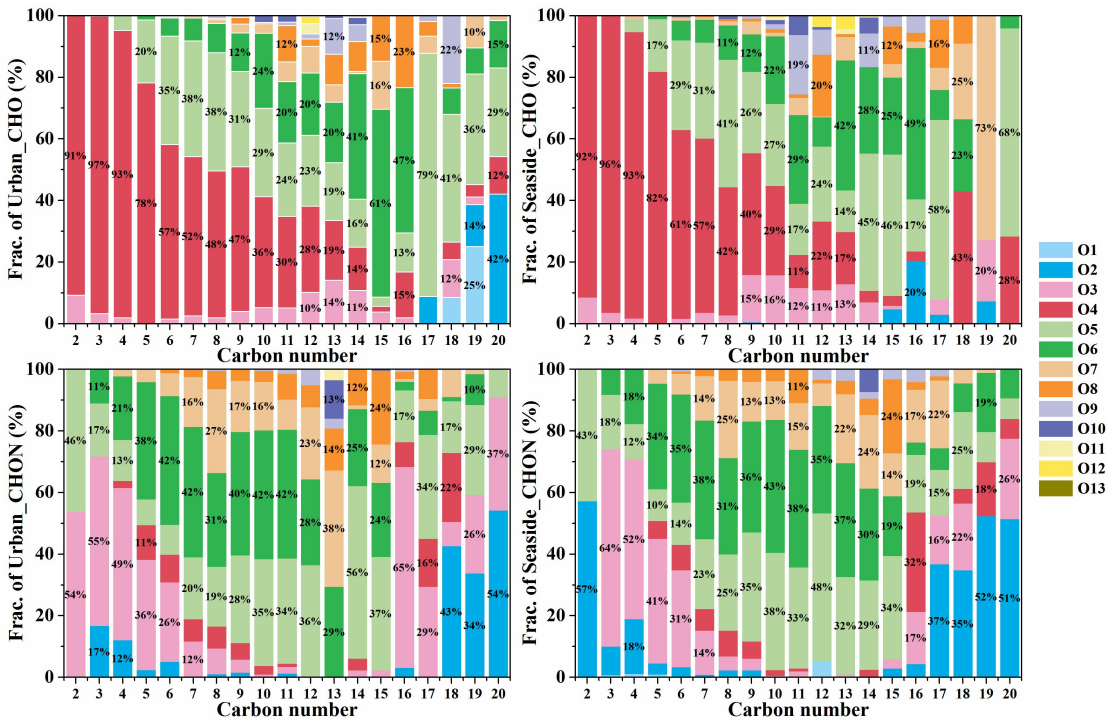


Fig. S7 Number of CHO and CHON categorized by the number of carbon atoms at the urban (a,c) and seaside (b,d) sites.



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60 **Fig. S8 Signal intensity proportion of CHO and CHON categorized by the number of carbon**

61 **atoms at the urban (a, c) and seaside (b, d) sites.**

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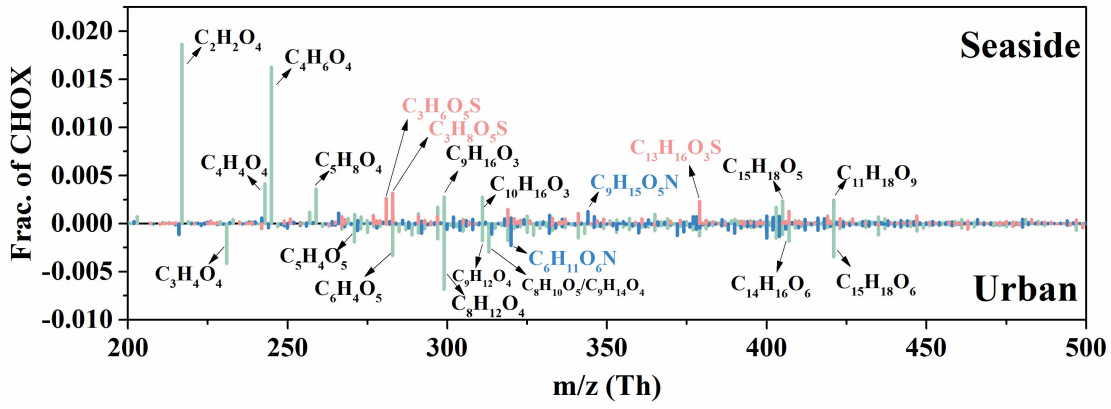

63

64 **Fig. S9 Mass spectrum of CHOX species signal proportion difference between urban and**

65 **coastal sites.**

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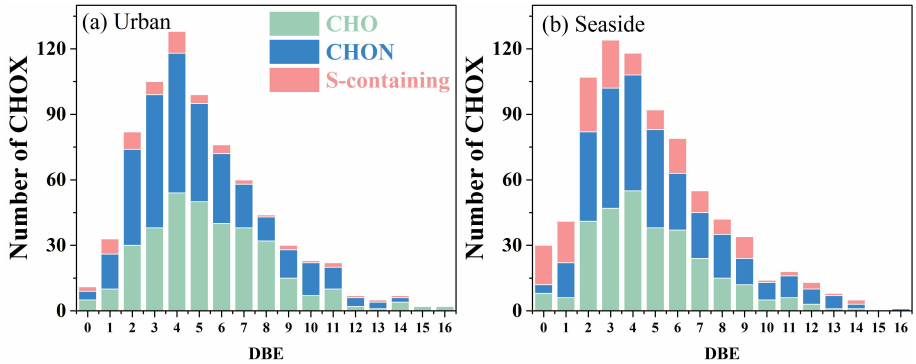

Fig. S10 Number of CHOX categorized by the double bonds equivalent (DBE) at the urban (a) and seaside (b) sites.

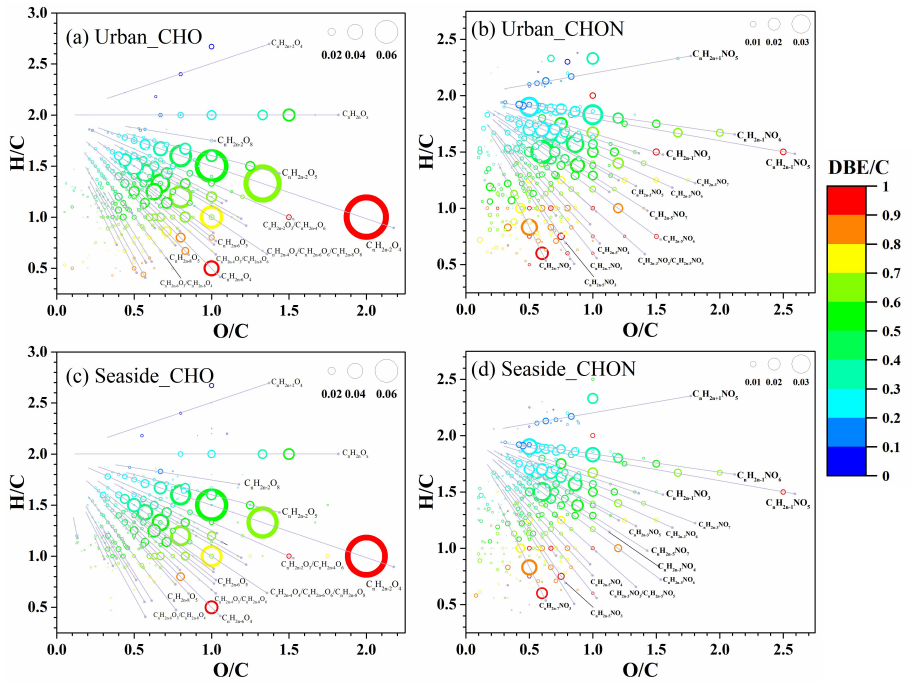

Fig. S11 Van Krevelen (VK) diagram of CHO and CHON. The circle size corresponds to signal intensity and the color scale represents the DBE/C ratio.

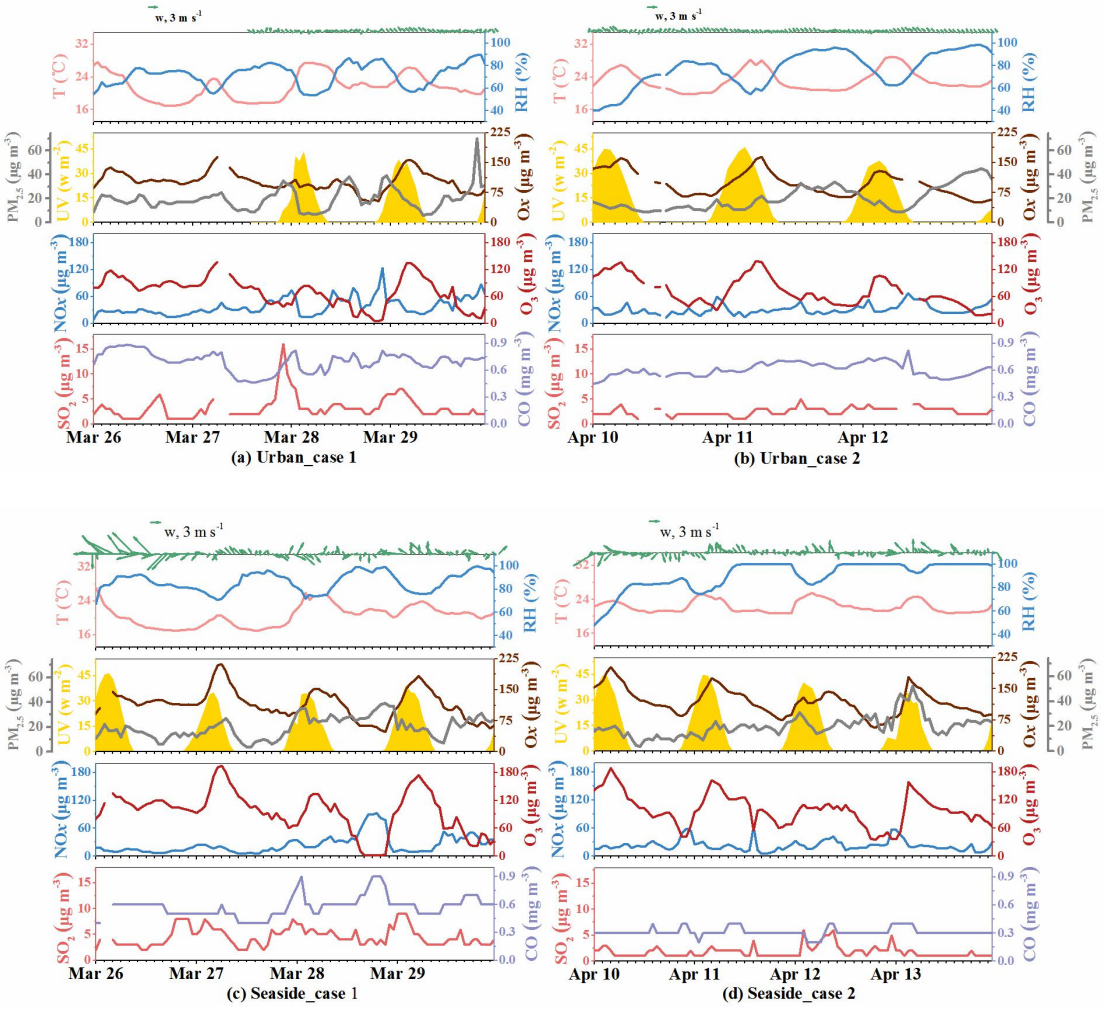

Fig. S12 Temporal variations of online data (meteorological parameters, gaseous pollutants, and $PM_{2.5}$) during different case at the urban (a, b) and the seaside (c, d) sites.

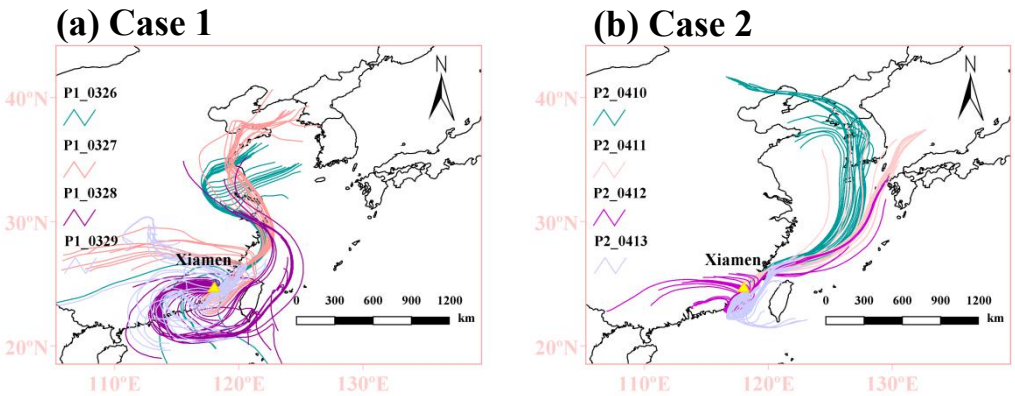

Fig. S13 72 h backward trajectory at the height of 500 m day by day during Case 1 (a) and Case 2 (b).

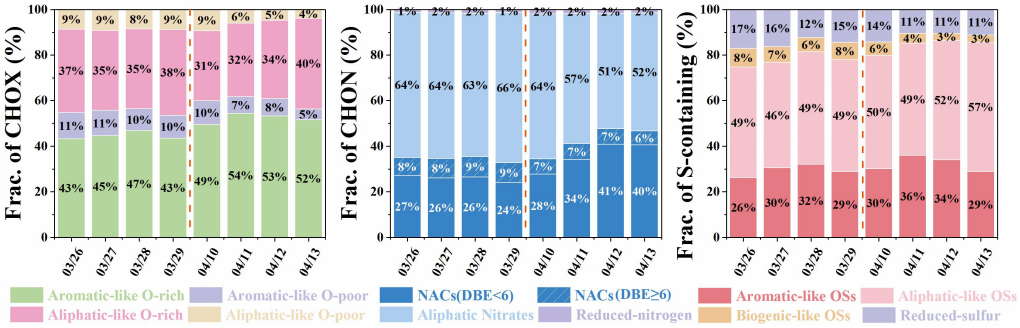

Fig. S14 Fraction distribution of seaside CHOX signal intensity categorized by different parameter (AI_{mod}, DBE，H/C, and O/C) during Case 1 and Case 2.

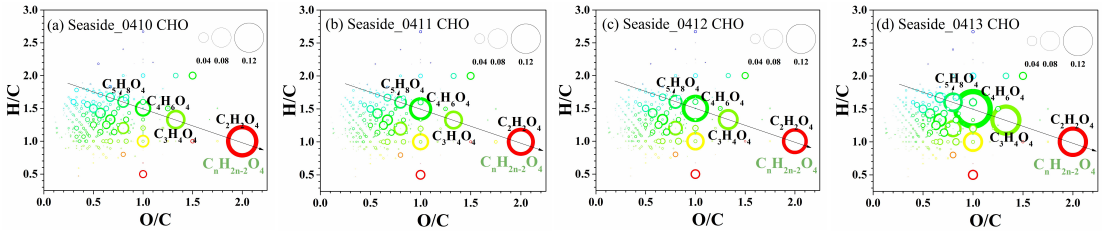

Fig. S15 The van Krevelen (VK) diagram of seaside CHO (i–l) day by day during case 2. The circle size corresponds to signal intensity and the color scale represents the DBE/C ratio.

Text S1: Comparison of methods

However, the method of filter membrane with a larger area might bring about the problem of insufficient pyrolysis. Therefore, we compared the results of two methods (heating directly and sandwich method) for measuring the same sample and found a good correlation between the two methods, with a slope close to 1 (Fig. S16), proving that the results of this method are reliable. Heating directly: an area (1.85 cm^2) of the sample filters was punched off and placed manually one by one in the dedicated filter holder of the FIGAERO directly. Sandwich method: an area (0.50 cm^2) of the sample filters was punched off and placed them between two pre-baked Zefluorr® Teflon filters, installed into the FIGAERO filter holder.

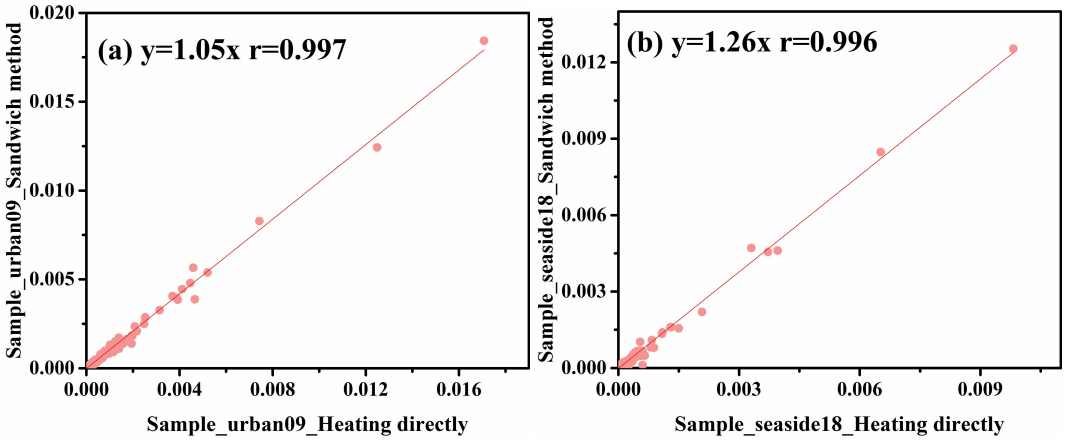

Fig. S16 The correlation of the same sample through two methods.