Supporting Information for

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

Yuping Chen[1,2,3], Lingling Xu[1,2*], Xiaolong Fan[1,2], Ziyi Lin[1,2,3], Chen Yang[1,2,3], Gaojie Chen[1,2,3], Ronghua Zheng[1,2], Youwei Hong[1,2], Mengren Li[1,2], Yanru Zhang[4], Jinsheng Chen[1,2*]

[1]State Key Laboratory of Advanced Environmental Technology, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen 361021, China.

[2]Fujian Key Laboratory of Atmospheric Ozone Pollution Prevention, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen 361021, China.

[3]University of Chinese Academy of Sciences, Beijing 100049, China

[4]Xiamen Environmental Monitoring Station, Xiamen 361021, China

* Corresponding author.

E-mail address: Jinsheng Chen (jschen@iue.ac.cn) and Lingling Xu (linglingxu@iue.ac.cn).

Contents of this file

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: UV: 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

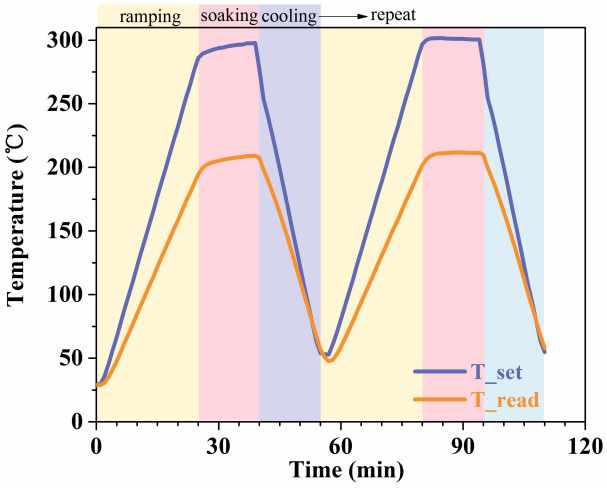


Fig. S1 The set temperature of the instrument (T_set) and actual temperature on the filter (T_read) change with time of the two heating cycles.

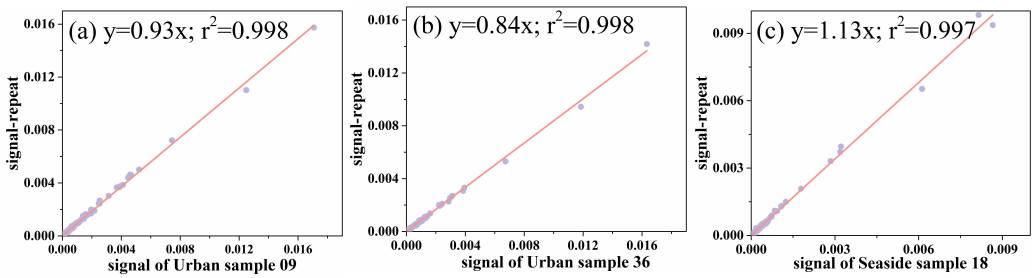


Fig. S2 The correlation of parallel experiments.

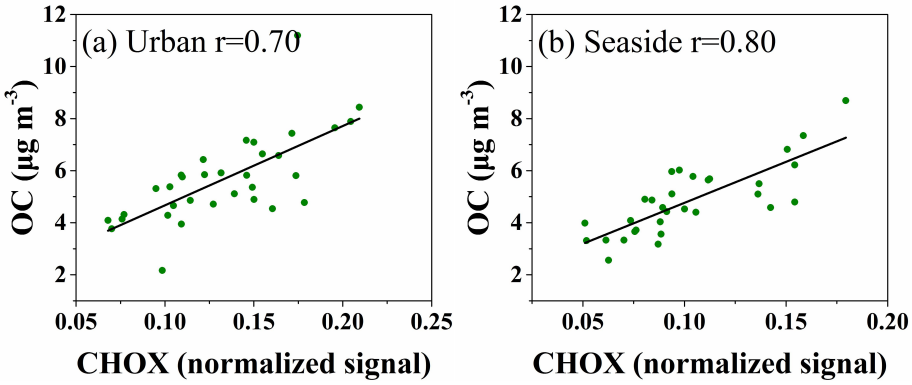


Fig. S3 The correlation between the CHOX signal and OC concentration at the urban (a) and the seaside (b) sites.

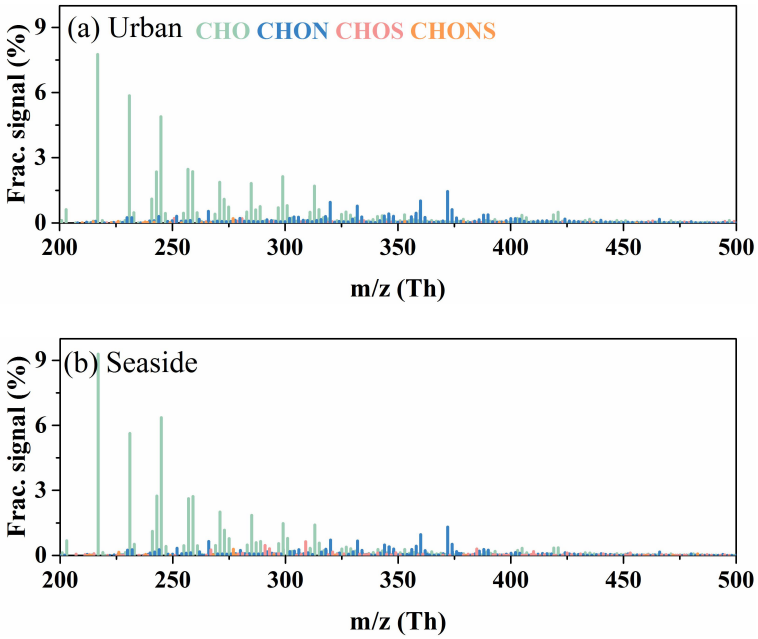


Fig. S4 Mass spectra of the identified compounds (CHO, CHON, CHOS, and CHONS) within the range of m/z 200~500 at the urban (a) and the seaside (b) sites.

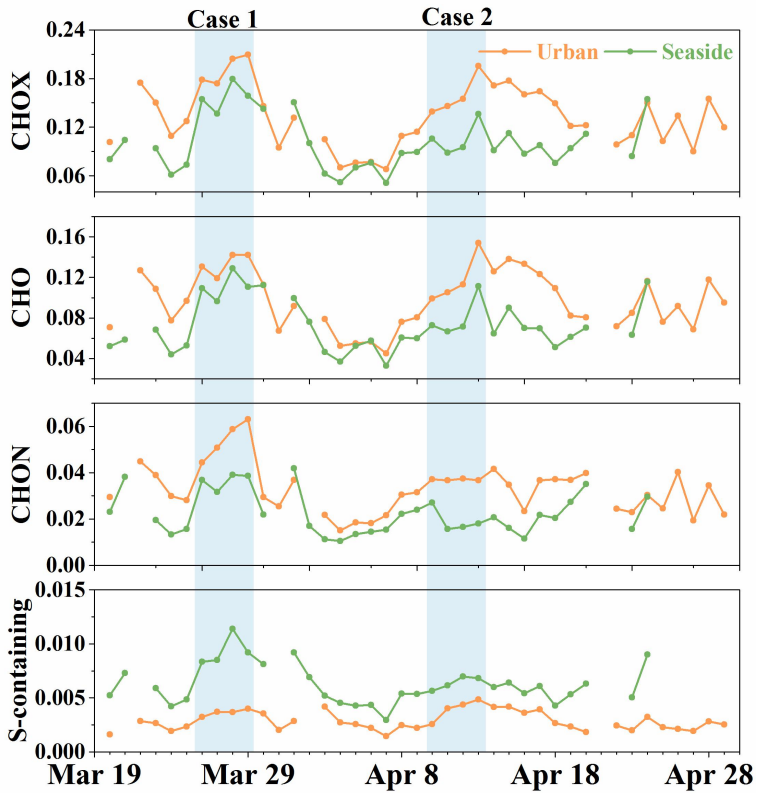


Fig. S5 Temporal variations of CHOX, CHO, CHON, and S-containing compounds (normalized signal) at the urban (a) and the seaside (b) sites.

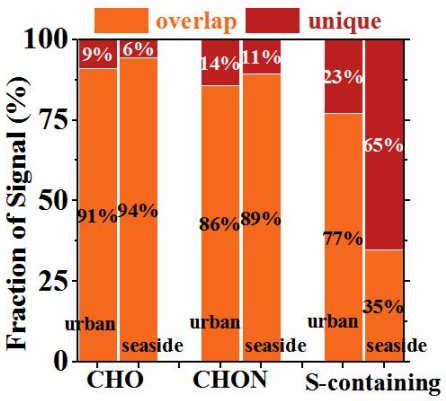


Fig. S6 The fraction of signals from the same chemical formula (overlap) and different chemical formula (remain) compounds identified at the two sites.

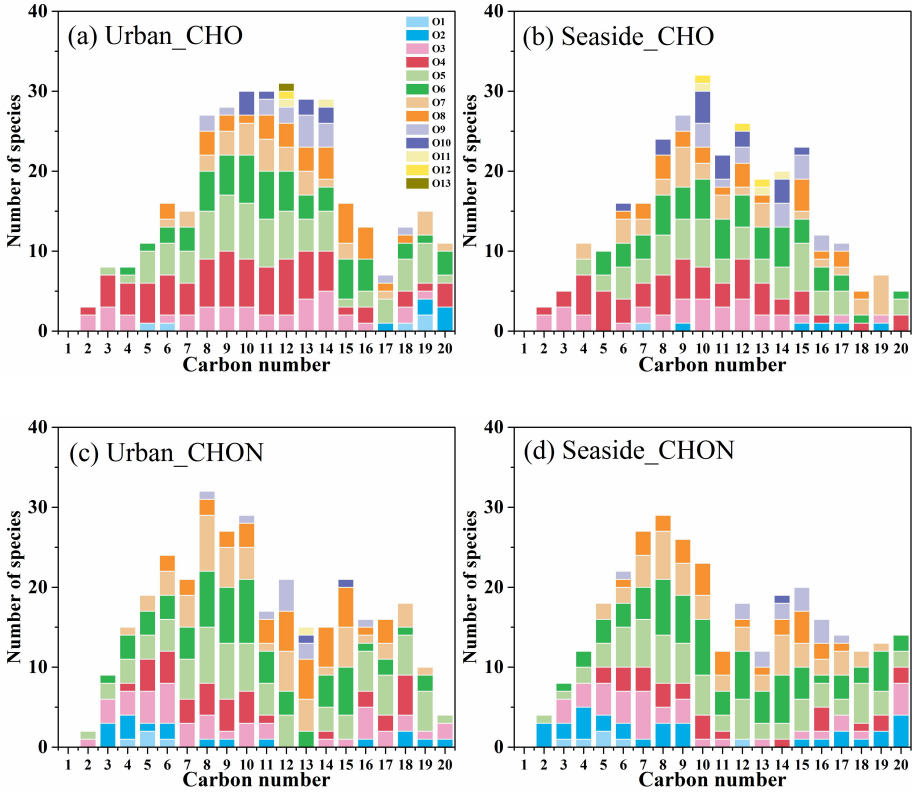


Fig. S7 Number of CHO and CHON categorized by the number of carbon atoms at the urban (a,c) and seaside (b,d) sites.

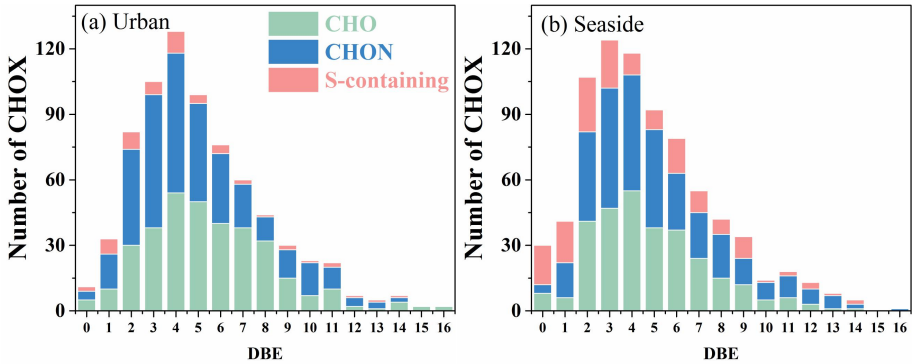


Fig. S8 Number of CHOX categorized by the double bonds equivalent (DBE) at the urban (a) and seaside (b) sites.

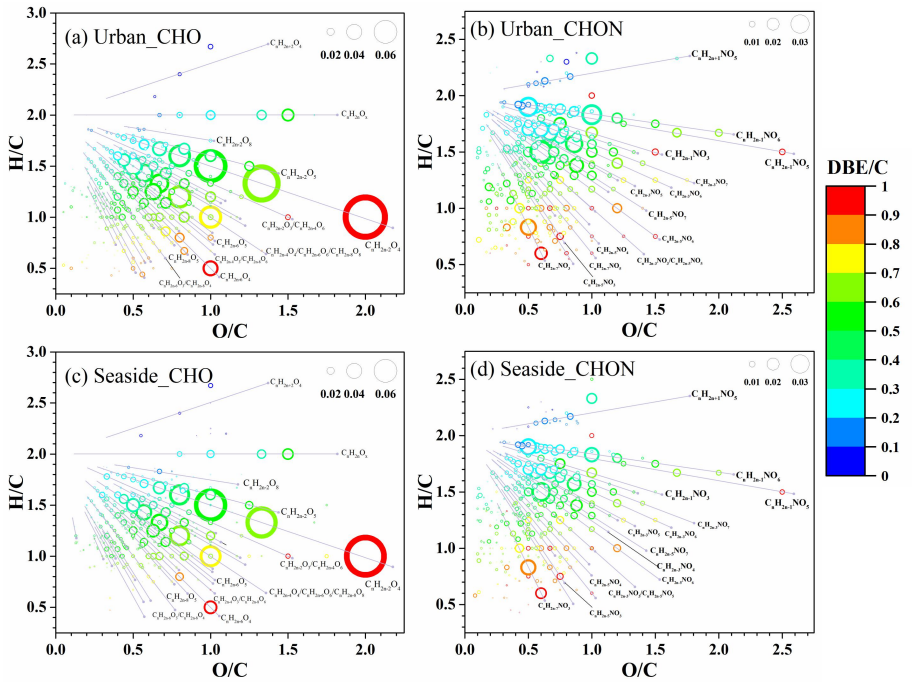


Fig. S9 Van Krevelen (VK) diagram of CHO and CHON. The circle size corresponds to signal intensity and the color scale represents the DBE/C ratio.

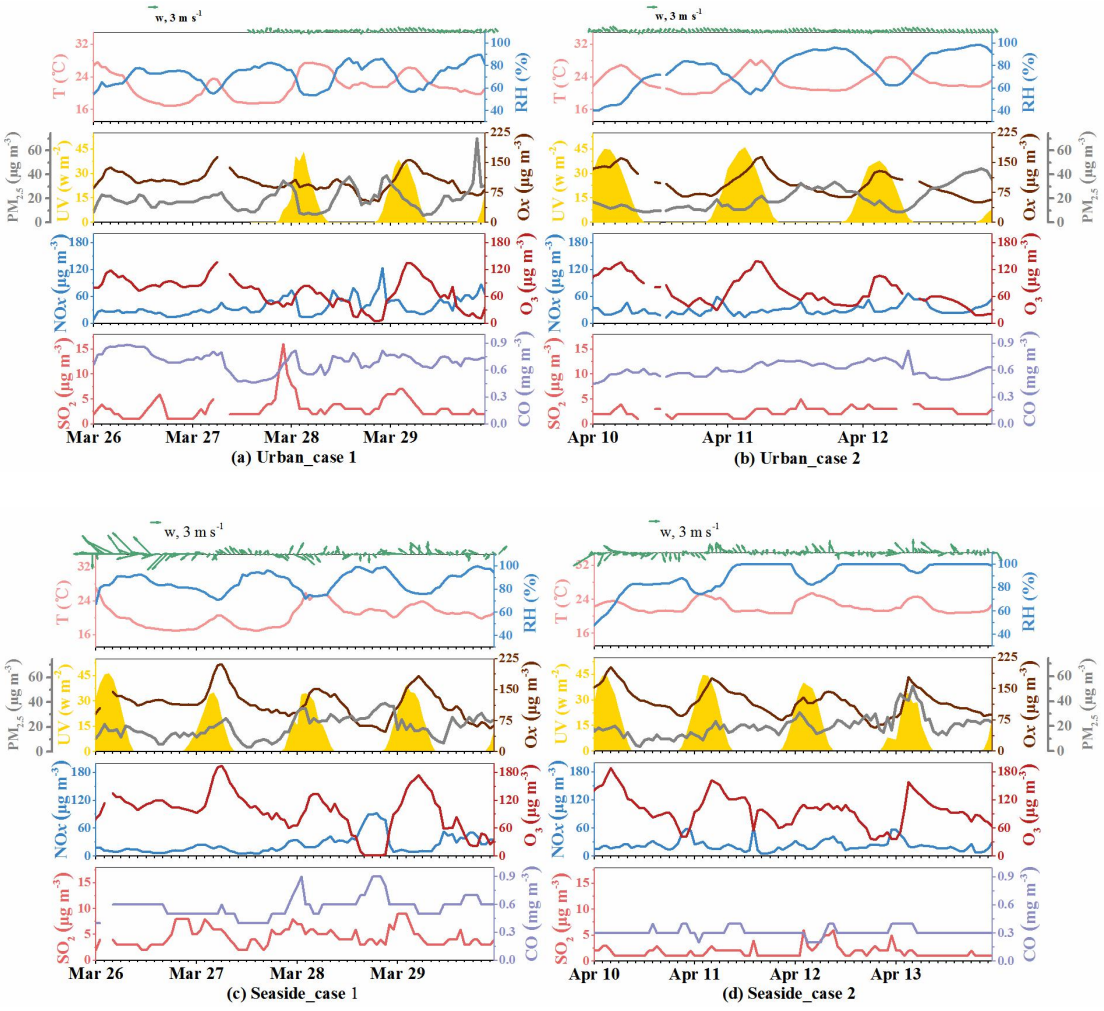


Fig. S10 Temporal variations of online data (meteorological parameters, gaseous pollutants, and $PM_{2.5}$) during different case at the urban (a, b) and the seaside (c, d) sites.

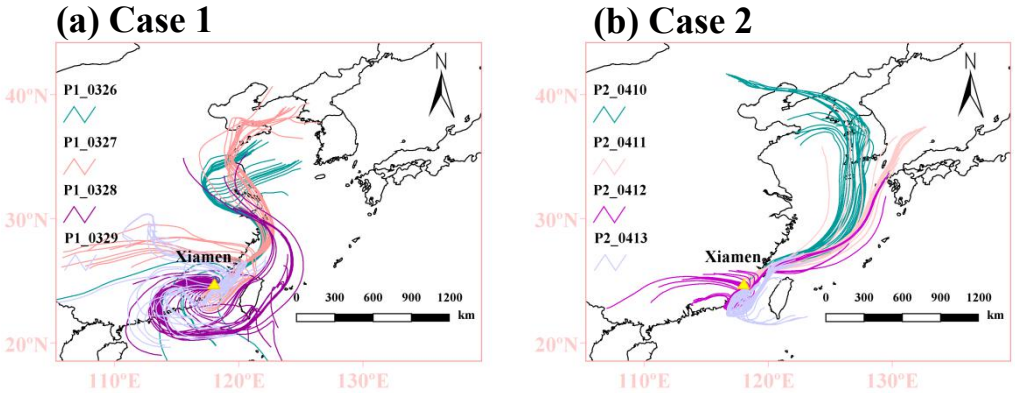


Fig. S11 72 h backward trajectory at the height of 500 m day by day during Case 1 (a) and Case 2 (b).

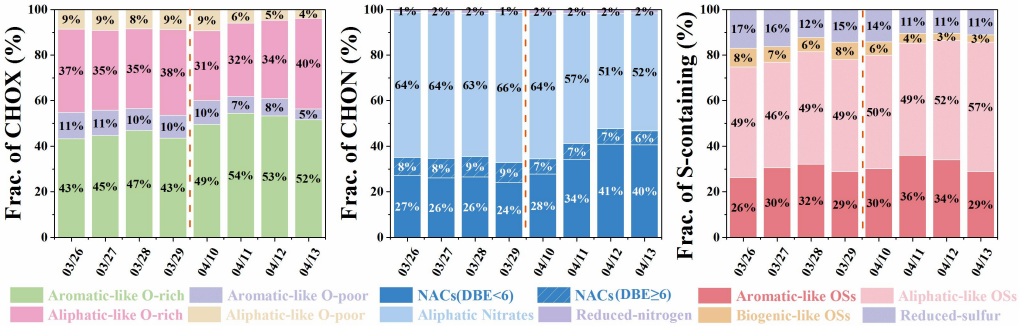


Fig. S12 Fraction distribution of seaside CHOX signal intensity categorized by different parameter (AI_{mod}, DBE，H/C, and O/C) during Case 1 and Case 2.

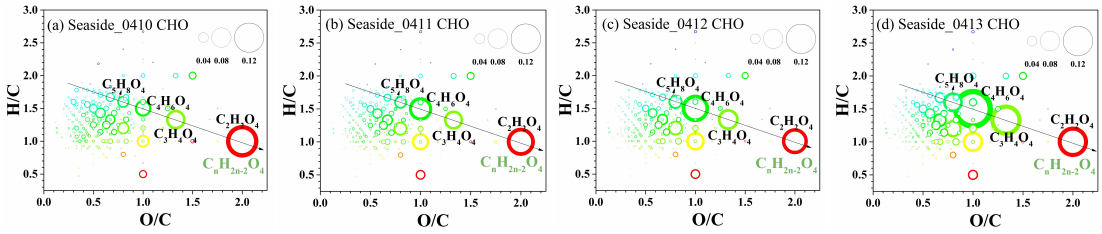
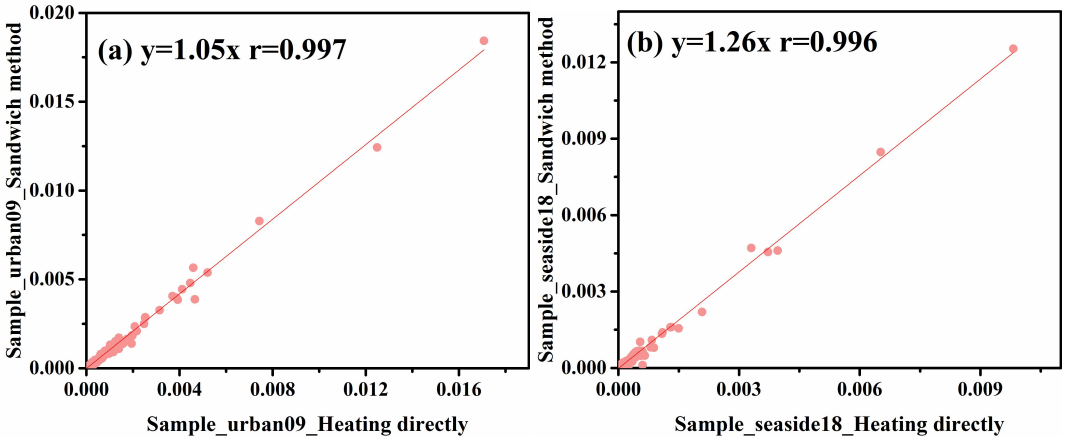


Fig. S13 The van Krevelen (VK) diagram of seaside CHO (i–l) day by day during case 2. The circle size corresponds to signal intensity and the color scale represents the DBE/C ratio.

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. S14), 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.



93

94 **Fig. S14 The correlation of the same sample through two methods.**