Supplement of

Vertical and seasonal variations in airborne endotoxins in a coastal megacity of North China: insights from 3-hydroxy fatty acids

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Text S1 Chemicals and reagents. The 3-OH-FA standards (C_8, C_9, C_{10}, C_{12}, C_{14}, C_{16} and C_{18}) were purchased from J&K Chemical (Beijing, China), while the rest of the 3-OH-FA standards (C_{11}, C_{13}, C_{15} and C_{17}) were purchased from Shanghai SCR-Biotech Co., Ltd. The information on 3-OH-FAs standards and the method validation is presented in Table S1 and Table S2. 2-chloro-1-methylpyridinium iodide (CMPI), triethylamine (TEA), 2-dimethylaminoethylamine (DMED), formic acid (FA), HPLC-grade acetonitrile (ACN), ethyl acetate (EtOAc), dichloromethane (DCM), methyl tert-butyl ether (MTBE), and HPLC-grade methanol (MeOH) were purchased from Aladdin Chemistry Co. Ltd. (Shanghai, China). The isotope-labeling reagent d_4-DMED, the d_4-DMED-labled saturated fatty acids (C_8 – C_{18}), and the d_4-DMED-labled 3-OH-FA standards (C_8, C_9, C_{10}, C_{12}, C_{14}, C_{16} and C_{18}) were synthesized according to the previous report (Hao et al., 2015).

Table S1. The 3-OH-FAs standards list.

Analytes	Molecular Formula	CAS No.	Abbreviation	M.W.[a]
3-hydroxyoctanoic acid	$C_8H_{16}O_3$	14292-27-4	3-OH-C_8	160.2
3-hydroxynonanoic acid	$C_9H_{18}O_3$	40165-87-5	3-OH-C_9	174.2
3-hydroxydecanoic acid	$C_{10}H_{20}O_3$	14292-26-3	3-OH-C_{10}	188.3
3-hydroxyundecanoic acid	$C_{11}H_{22}O_3$	40165-88-6	3-OH-C_{11}	202.3
3-hydroxydodecanoic acid	$C_{12}H_{24}O_3$	1883-13-2	3-OH-C_{12}	216.3
3-hydroxytridecanoic acid	$C_{13}H_{26}O_3$	32602-69-0	3-OH-C_{13}	230.4
3-hydroxytetradecanoic acid	$C_{14}H_{28}O_3$	28715-21-1	3-OH-C_{14}	244.4
3-hydroxypentadecanoic acid	$C_{15}H_{30}O_3$	32602-70-3	3-OH-C_{15}	258.4
3-hydroxyhexadecanoic acid	$C_{16}H_{32}O_3$	928-17-6	3-OH-C_{16}	272.4
2-hydroxyhexadecanoic acid	$C_{16}H_{32}O_3$	764-67-0	2-OH-C_{16}	272.4
3-hydroxyheptadecanoic acid	$C_{17}H_{34}O_3$	40165-89-7	3-OH-C_{17}	286.4
3-hydroxyoctadecanoic acid	$C_{18}H_{36}O_3$	45261-96-9	3-OH-C_{18}	300.5

Note: [a] Molecular weight

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Table S2. Method validation for target 3-OH-FAs.

Analytes	MRM parameter	Retention time (min)	R^2
3-OH-C_8	231.2→186.2	3.19	0.9995
3-OH-C_9	245.2→200.2	4.14	0.9972
3-OH-C_{10}	259.2→214.2	5.20	0.9986
3-OH-C_{11}	273.2→228.2	6.42	0.9901
3-OH-C_{12}	287.2→242.2	7.63	0.9956
3-OH-C_{13}	301.2→238.2	7.65	0.9947
3-OH-C_{14}	315.2→270.2	9.89	0.9958
3-OH-C_{15}	329.2→284.2	8.84	0.9888
3-OH-C_{16}	343.2→298.2	12.06	0.9931
3-OH-C_{17}	357.2→294.2	13.18	0.9912
3-OH-C_{18}	371.2→326.2	14.10	0.9949

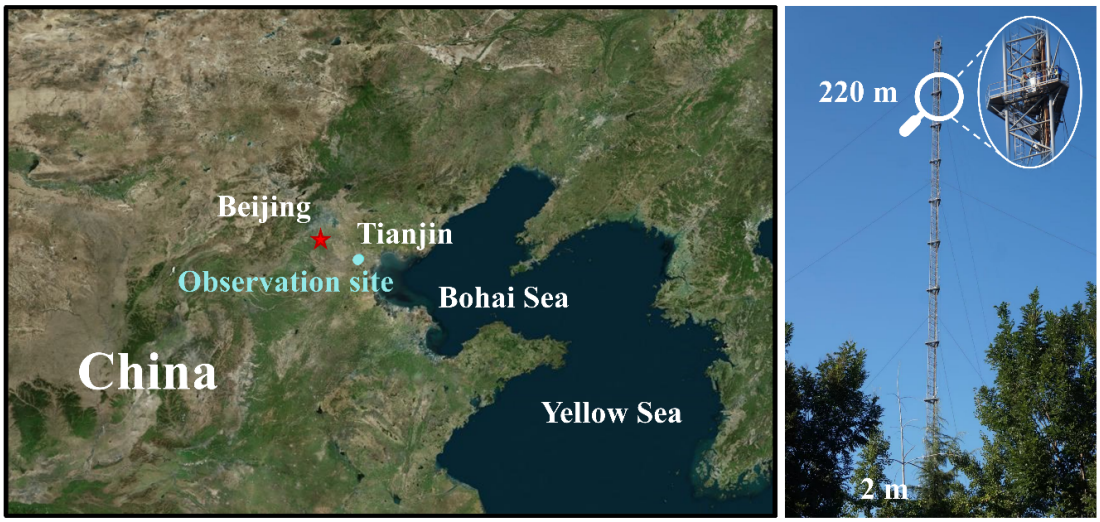

Figure S1. Geographical location of the observation site at the Tianjin Atmospheric Boundary Layer Observatory of the China Meteorological Administration, located at the southern area of urban Tianjin, China (39°08'N; 117°22'E) and sampler setting on the 255-m meteorological tower. The background map is sourced from MeteoInfo (Wang, 2019), and the tower photograph was taken by Libin Wu.

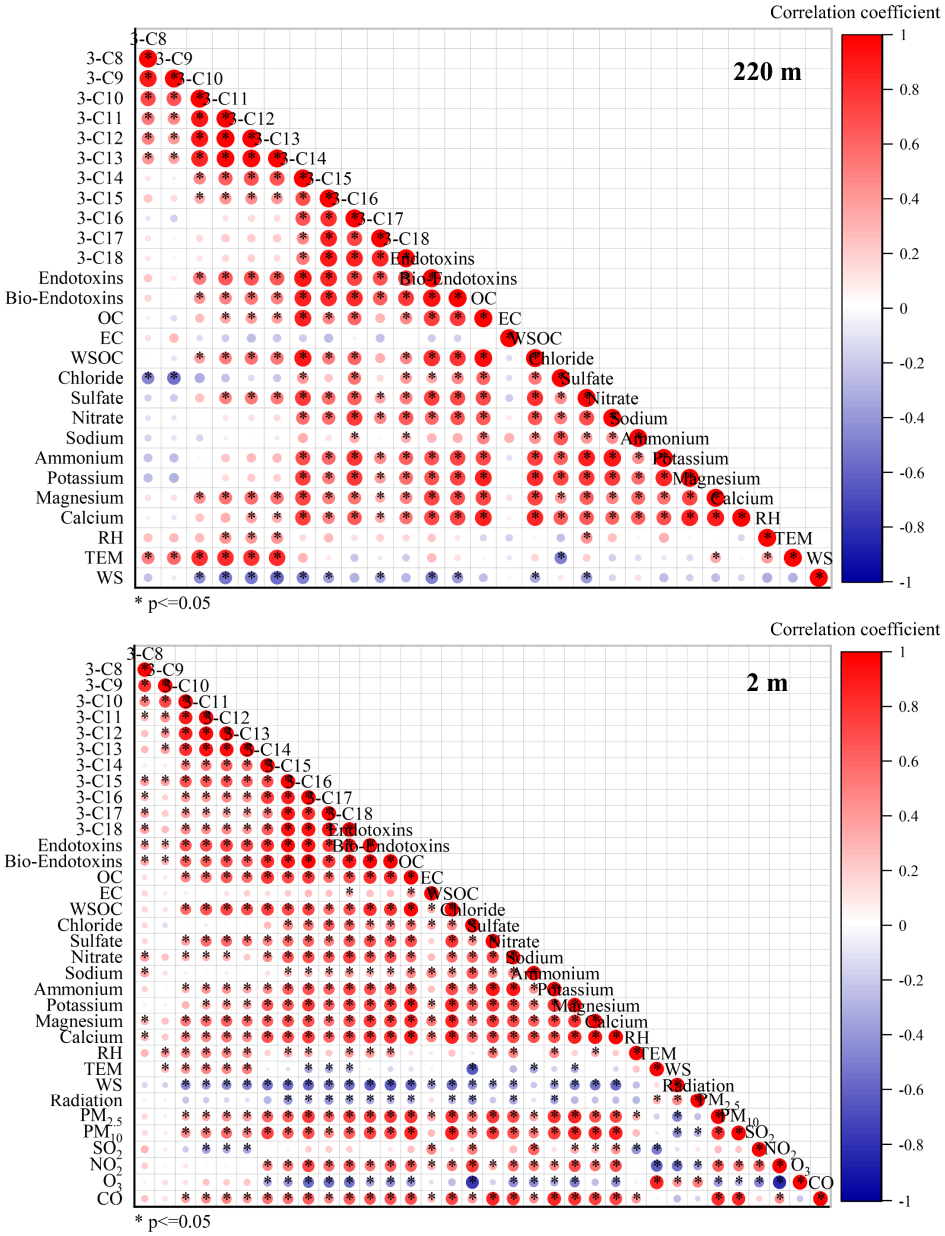

Figure S2. Spearman correlation between concentration of 3-OH-FAs, endotoxins and environmental factors (meteorological parameters, carbonaceous fraction, anions and cations, air pollutants) at different heights.

References

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