



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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S1. Chemicals and reagents. The 3-OH-FA standards (C₈, C₉, C₁₀, C₁₂, C₁₄, C₁₆ and C₁₈) were purchased from J&K Chemical (Beijing, China), while the rest of the 3-OH-FA standards (C₁₁, C₁₃, C₁₅ and C₁₇) 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-labeled saturated fatty acids (C₈ – C₁₈), and the *d*₄-DMED-labeled 3-OH-FA standards (C₈, C₉, C₁₀, C₁₂, C₁₄, C₁₆ and C₁₈) were synthesized according to the previous report (Hao et al., 2015).

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

Analyte	Molecular Formula	CAS No.	Abbreviation	M.W. ^a
3-hydroxyoctanoic acid	C ₈ H ₁₆ O ₃	14292-27-4	3-OH-C ₈	160.2
3-hydroxynonanoic acid	C ₉ H 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

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

Analyte	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

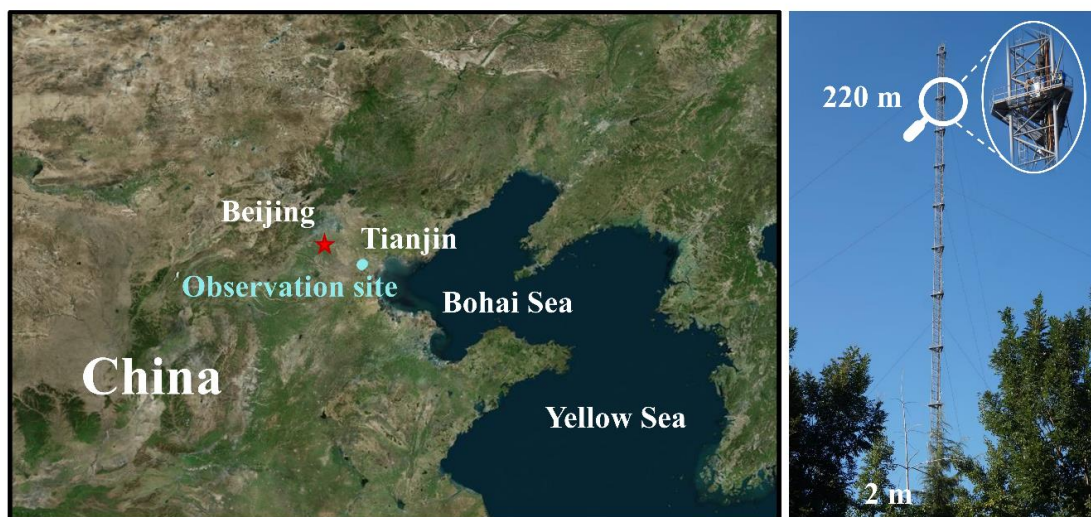


Figure S1. Geographical location of the observation site at the Tianjin Atmospheric Boundary Layer Observatory of the China Meteorological Administration, located at the southern area of urban Tianjin, China (39°08'N; 117°22'E) and sampler setting on the 255-m meteorological tower. The background map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

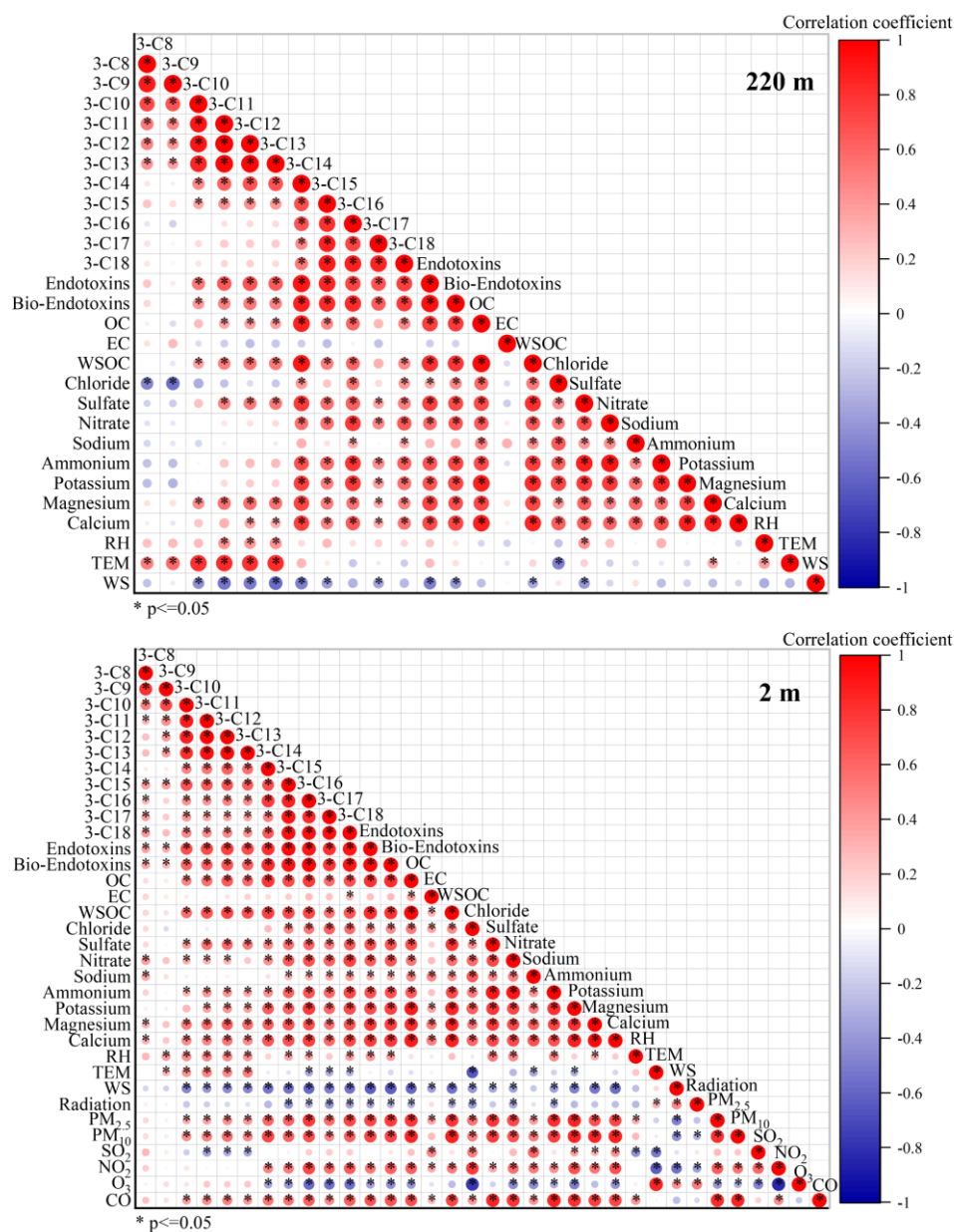


Figure S2. Spearman correlation between concentration of 3-OH-FAs, endotoxins and environmental factors (meteorological parameters, carbonaceous fraction, anions and cations, air pollutants) at different heights. The circle diameter is proportional to correlation coefficient and that asterisks mark significant correlations at $p \leq 0.05$. TEM, temperature; WS, wind speed; RH, relative humidity.

30 **References**

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