PM$_{2.5}$-bound silicon-containing secondary organic aerosols (Si-SOA) in Beijing ambient air

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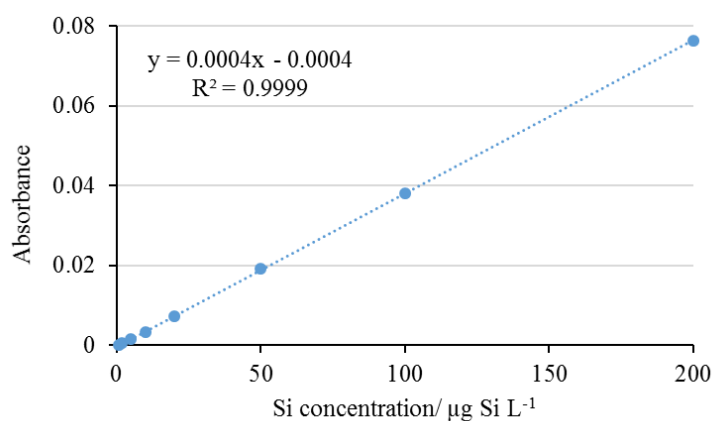
Fig. S1 Calibration curve of silicon standard measured by UV/Vis
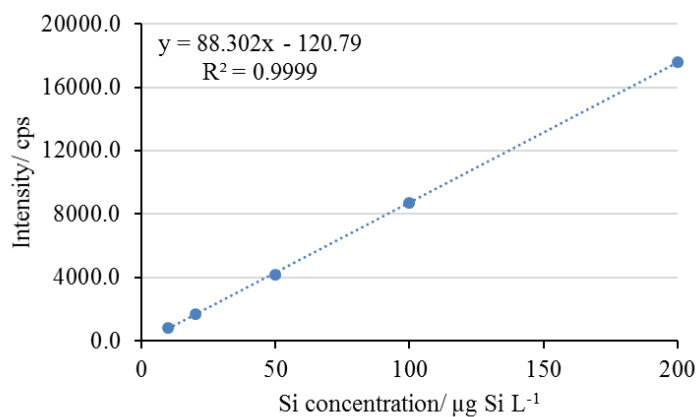
Fig. S2 Calibration curve of silicon standard measured by ICP-OES

Table S1 The detection limits (DL), calibration curve, spike recovery and repeatability of Si measured by UV/Vis and ICP-OES

Instrument		DL		Calibration curve		Spike recovery %	relative standard deviation for 3 consecutive test %	relative standard deviation for repeatability %
		Con. in water (µg L^{-1})	Conc. in air (ng m^3)	Conc. Range (µg L^{-1})	R^2			
UV/Vis	Standard	1.4	0.6	1-200	0.9999	100.0~109.9	1.2 (0.0 ~ 3.1)	-

	Sample			_ª	-	-	2.0 (0.1 ~ 7.8)	8.8 (0.1 ~ 16.2)
ICP-OES	Standard	4.8	2.0	10-200	0.9999	110.3~116.2	3.0 (0.6~8.7)	-
	Sample			-	-	-	2.0 (0.2~8.8)	10.5 (4.8~16.9)

[a] Not available;

Table S2 Organic Si standard- Heptamethylcyclotetrasiloxan-2-ol (D3D^{OH}) measured by UV/Vis

Concentrations/µg L^{-1}	Absorbance (average of 3 tests)	Calculated Si concentrations using UV/Vis calibration curve
469	0.000067	<DL
469	0.000167	<DL
710	0.000200	<DL

"Uncertainty budget of the SO-Si analysis

The combined standard uncertainty of SO-Si in percentage (u_{or}) was calculated using the combined standard uncertainty of total water-soluble Si (u_t) and total water-soluble inorganic Si (u_{in}) according to the following equation:

$$u_{or} = \sqrt{u_t{}^2 + u_{in}{}^2} \tag{1}$$

while the combined standard uncertainties of u_t and u_{in} were calculated using all components and the law of propagation of uncertainty according to the following equation:

$$u_t \ or \ u_{in} = \sqrt{u(extract)^2 + u(DL)^2 + u(cali)^2 + u(blank)^2 + u(repli)^2} \tag{2}$$

Where u(extract) is the uncertainty of extraction recovery, u(DL) is the uncertainty of detection limits, which is calculated as the DL divided by the average concentration of all samples. u(blank) is the uncertainty of blanks, which is calculated as the mean value of each blank divided by the average concentration of all samples. u(cali) is the systematic error which is the average difference between the true value and the analyzed value as a percentage of the true value. u(repli) is the uncertainty from replicates analyses, calculated as the relative standard deviation of the results. All values are provided in percentages.

Table S3. uncertainties for the calculation of u_{or}

parameters	uncertainties/ %		
	total water-soluble Si	total water-soluble inorganic Si	total water-soluble organic Si (SO-Si)
Extraction recovery	13.1	4.5	-
detection limit	8.9	9.3	-
calibration	2.8	1.0	-
blank	13.0	4.1	-
replicate	10.5	8.8	-

(repeatability)			
u_t	23.2	-	-
u_{in}	-	14.2	-
u_{or}	-	-	27.2

As shown in Table S3, higher uncertainties exist in blanks and DLs. This could limit the method application in some samples with low Si concentrations. As mentioned in the manuscript, the Si concentrations on 11th and 12th August were replaced with 0.5DLs due to below DL levels."