


Supplementary Information Raw data of Ultra-trace elemental determination of Si by means of graphite furnace-atomic absorption spectrometry	 EVONIK Leading Beyond Chemistry
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1. General

1.1 Cook book of the manufacturer

SOLAAR Cookbook
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← →
Einblenden Optionen

Silicon Si

Atomic no.	14	Atomic mass	28.086
Primary wavelength (nm)	251.6	Bandpass (nm)	0.5

Lamp Current		Performance	
normal use	75%	flame characteristic concentration (mg/l)	1.3
best sensitivity	75%	furnace characteristic mass (pg)	21
best precision	100%		

Emission wavelength (nm)	251.6		
Secondary wavelengths (nm)		Sensitivity reduction	
	250.7	2.6 X	
	251.4	3.4 X	
	252.9	3.4 X	
	252.4	3.8 X	
	221.7	4.5 X	
	221.1	10 X	

Flame ([show](#)/[hide details](#))

Furnace ([show](#)/[hide details](#))

Cuvette type	Coated or ELC	Modifier	none recommended
Ash temperature	1300°C	Signal	20 µl of 25 µg/l gives about 0.1 A
Atomise temperature	2600°C		

1. Background absorption and scatter are common
 - use background correction.
2. Silicon has a high risk of contamination
 - take particular care when preparing solutions.
 - use plastic vessels, and avoid the use of glassware.

Figure 1: Original screenshot from the manufacturer's cookbook with respect to ideal Si conditions. Note the indication for the Modifier as "none recommended". Screenshot taken from SOLAAR AA Software cook book, software version: 11,10, spectrometer software version: 1.30, ©1996-2010 by Thermo Fisher Scientific Inc.

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1.2 Preparation of the stock solution

A silane solution containing 25242 µg/g silane, equating to 5.4 mass% SiO₂, was diluted to a solution containing 48.6 µg/L Si (ethanol) and 51.8 µg/L (acetic acid), respectively.

1.3 Optimisation of the graphite furnace temperatures

Table 1: Optimisation of the ashing and atomisation temperatures in ethanol using a matrix-matched standard. Bold horizontal line indicates change between constant parameters, bold values equate the highest signals found for the given varied parameter. Ideal values were 1000°C and 2700°C for ashing and atomisation temperatures, respectively.

Ashing temperature / °C	Atomisation temperature / °C	Signal height	Signal area
800	2700	0.305	0.148
900	2700	0.298	0.147
1000	2700	0.309	0.152
1100	2700	0.276	0.137
1200	2700	0.236	0.117
1300	2700	0.154	0.076
1000	1700	0.002	0.001
1000	1800	0.002	0.001
1000	1900	0.004	0.002
1000	2000	0.008	0.004
1000	2100	0.021	0.012
1000	2200	0.047	0.027
1000	2300	0.083	0.051
1000	2400	0.110	0.090
1000	2500	0.166	0.137
1000	2600	0.245	0.161
1000	2700	0.298	0.153
1000	2700	0.329	0.166
1000	2800	0.322	0.140
1000	2900	0.242	0.105

Table 2: Optimisation of the ashing and atomization temperatures in acetic acid using a matrix-matched standard. Bold horizontal line indicates change between constant parameters, bold values equate the highest signals found for the given varied parameter. Ideal values were 1150°C and 2650°C for ashing and atomisation temperatures, respectively.

Ashing temperature / °C	Atomisation temperature / °C	Signal height	Signal area
800	2700	0.110	0.053
900	2700	0.153	0.074
1100	2700	0.129	0.066
1150	2700	0.137	0.068

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Ashing temperature / °C	Atomisation temperature / °C	Signal height	Signal area
1200	2700	0.127	0.064
1250	2700	0.106	0.050
1150	2600	0.117	0.074
1150	2650	0.138	0.077
1150	2700	0.127	0.064
1150	2750	0.132	0.062
1150	2800	0.131	0.058
1150	2850	0.100	0.043

2. Si in food contact acetic acid

2.1 Calibration & Linearity

Table 3: Calibration data. Slope $m = 0.00376$ L/ μg , intercept $b = 0.0028$, coefficient of correlation $r = 0.9970$, characteristic concentration $\beta_{\text{char.}}(\text{Si}) = 1.1688$ $\mu\text{g/L}$.

Solution	Concentration / $\mu\text{g/L}$	Extinction at 251.6 nm (Si)
Blank	0.00	0.0046
Standard 1	2.0718	0.0127
Standard 2	4.9206	0.0210
Standard 3	6.9925	0.0277
Standard 4	10.1003	0.0397
Standard 5	15.0209	0.0561
Standard 6	19.9415	0.0757
Standard 7	25.1212	0.1018

2.2 Accuracy & Precision

Table 4: Raw data from the Accuracy and Precision experiments.

Name	Signal height	Signal area	RSD / %	Conc. / $\mu\text{g/L}$	Corrected Conc. / $\mu\text{g/L}$
Blank Avg.	0.005	0.002	23.2		
Blank 1/3	0.004	0.001			
Blank 2/3	0.004	0.002			
Blank 3/3	0.006	0.003			
Standard 1 Avg.	0.014	0.007	9.8	2.0718	
Standard 1 1/3	0.013	0.007			
Standard 1 2/3	0.012	0.006			
Standard 1 3/3	0.013	0.007			
Standard 2 Avg.	0.021	0.011	7.6	4.9206	
Standard 2 1/3	0.021	0.011			

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Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
Standard 2 2/3	0.023	0.011			
Standard 2 3/3	0.019	0.012			
Standard 3 Avg.	0.029	0.016	6.9	6.9925	
Standard 3 1/3	0.028	0.015			
Standard 3 2/3	0.028	0.015			
Standard 3 3/3	0.026	0.013			
Standard 4 Avg.	0.040	0.021	2.4	10.1003	
Standard 4 1/3	0.040	0.021			
Standard 4 2/3	0.039	0.021			
Standard 4 3/3	0.040	0.022			
Standard 5 Avg.	0.057	0.030	3.4	15.0209	
Standard 5 1/3	0.056	0.029			
Standard 5 2/3	0.054	0.027			
Standard 5 3/3	0.057	0.031			
Standard 6 Avg.	0.074	0.038	2.9	19.9415	
Standard 6 1/3	0.076	0.039			
Standard 6 2/3	0.078	0.041			
Standard 6 3/3	0.075	0.039			
Standard 7 Avg.	0.105	0.056	3.3	25.1212	
Standard 7 1/3	0.102	0.055			
Standard 7 2/3	0.098	0.052			
Standard 7 3/3	0.103	0.056			
QC 1 µg/L Avg.	0.031	0.016	6.4	7.5427	1.5085
QC 1 µg/L 1/3	0.033	0.017			
QC 1 µg/L 2/3	0.029	0.016			
QC 1 µg/L 3/3	0.032	0.016			
Sample Avg.	0.017	0.009	31.3	3.7442	0.7488
Sample 1/3	0.014	0.007			
Sample 2/3	0.014	0.007			
Sample 3/3	0.023	0.011			
Sample Avg.	0.014	0.008	2.4	3.0934	0.6187
Sample 1/3	0.040	0.019			
Sample 2/3	0.014	0.008			
Sample 3/3	0.015	0.008			
Sample Avg.	0.015	0.008	12.9	3.1952	0.6390
Sample 1/3	0.014	0.007			

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Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
Sample 2/3	0.017	0.008			
Sample 3/3	0.013	0.007			
QC 1 µg/L Avg.	0.032	0.017	0.4	7.8084	1.5617
QC 1 µg/L 1/3	0.225	0.092			
QC 1 µg/L 2/3	0.032	0.017			
QC 1 µg/L 3/3	0.032	0.017			
Sample + 1 µg/L Avg.	0.033	0.017	5.2	8.0828	1.6166
Sample + 1 µg/L 1/3	0.031	0.016			
Sample + 1 µg/L 2/3	0.034	0.017			
Sample + 1 µg/L 3/3	0.035	0.018			
Sample + 1 µg/L Avg.	0.036	0.019	8.9	8.7469	1.7494
Sample + 1 µg/L 1/3	0.034	0.017			
Sample + 1 µg/L 2/3	0.034	0.018			
Sample + 1 µg/L 3/3	0.039	0.020			
Sample + 1 µg/L Avg.	0.034	0.017	2.9	8.2511	1.6502
Sample + 1 µg/L 1/3	0.034	0.018			
Sample + 1 µg/L 2/3	0.033	0.016			
Sample + 1 µg/L 3/3	0.035	0.018			
QC 1 µg/L Avg.	0.036	0.019	1.5	8.7381	1.7476
QC 1 µg/L 1/3	0.036	0.018			
QC 1 µg/L 2/3	0.035	0.019			
QC 1 µg/L 3/3	0.036	0.019			
Sample + 2 µg/L Avg.	0.055	0.028	2.6	13.9178	2.7836
Sample + 2 µg/L 1/3	0.057	0.030			
Sample + 2 µg/L 2/3	0.055	0.028			
Sample + 2 µg/L 3/3	0.054	0.027			
Sample + 2 µg/L Avg.	0.054	0.027	0.4	13.6876	2.7375
Sample + 2 µg/L 1/3	0.054	0.027			
Sample + 2 µg/L 2/3	0.054	0.027			

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Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
Sample + 2 µg/L 3/3	0.055	0.027			
Sample + 2 µg/L Avg.	0.060	0.030	4.0	15.2283	3.0457
Sample + 2 µg/L 1/3	0.063	0.032			
Sample + 2 µg/L 2/3	0.059	0.029			
Sample + 2 µg/L 3/3	0.058	0.029			
QC 1 µg/L Avg.	0.034	0.017	1.8	8.4193	1.6839
QC 1 µg/L 1/3	0.035	0.018			
QC 1 µg/L 2/3	0.034	0.017			
QC 1 µg/L 3/3	0.034	0.017			
Sample + 3 µg/L Avg.	0.077	0.039	0.9	19.7263	3.9453
Sample + 3 µg/L 1/3	0.076	0.039			
Sample + 3 µg/L 2/3	0.078	0.039			
Sample + 3 µg/L 3/3	0.077	0.038			
Sample + 3 µg/L Avg.	0.082	0.041	1.8	20.9570	4.1914
Sample + 3 µg/L 1/3	0.083	0.041			
Sample + 3 µg/L 2/3	0.082	0.041			
Sample + 3 µg/L 3/3	0.080	0.040			
Sample + 3 µg/L Avg.	0.075	0.038	1.7	19.3013	3.8603
Sample + 3 µg/L 1/3	0.077	0.040			
Sample + 3 µg/L 2/3	0.075	0.038			
Sample + 3 µg/L 3/3	0.075	0.037			
QC 1 µg/L Avg.	0.036	0.018	3.4	8.7204	1.7441
QC 1 µg/L 1/3	0.037	0.018			
QC 1 µg/L 2/3	0.036	0.018			
QC 1 µg/L 3/3	0.034	0.018			


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Table 5: Calculations for the Accuracy & Precision experiments.

Name	Accuracy	Precision		
	Recovery Rate / %	Avg. / %	SD / %	RSD / %
Sample + 1 µg/L Avg.	91	97	7	7
Sample + 1 µg/L Avg.	104			
Sample + 1 µg/L Avg.	95			
Sample + 2 µg/L Avg.	102	106	8	8
Sample + 2 µg/L Avg.	100			
Sample + 2 µg/L Avg.	115			
Sample + 3 µg/L Avg.	105	107	6	5
Sample + 3 µg/L Avg.	113			
Sample + 3 µg/L Avg.	103			

2.3 Limit of detection, limit of quantitation

Table 6: Raw data & calculations for the determinations of the LOD and LOQ, respectively, by means of the blank method. Values below the bold line refer to calculations.

Name	Value
Blank 1	0.0039
Blank 2	0.0048
Blank 3	0.0050
Blank 4	0.0048
Blank 5	0.0041
Blank 6	0.0035
Blank 7	0.0028
Blank 8	0.0038
Blank 9	0.0034
Blank 10	0.0044
Mean	0.0041
Standard deviation	0.0007
Concentrating factor	5
LOD / µg/L	0.565
LOQ / µg/L	1.883
LOD WRT concentrating factor / µg/L	0.113
LOQ WRT concentrating factor / µg/L	0.377

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2.4 Stability of solution

Table 7: Raw data for the Stability of Solution.

Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
Blank Avg.	0.004	0.002	5.7	0.000	
Blank 1/3	0.004	0.002			
Blank 2/3	0.003	0.002			
Blank 3/3	0.004	0.002			
Standard 1 Avg.	0.016	0.008	2.2	2.056	
Standard 1 1/3	0.016	0.008			
Standard 1 2/3	0.017	0.008			
Standard 1 3/3	0.016	0.009			
Standard 2 Avg.	0.029	0.015	7.7	4.882	
Standard 2 1/3	0.027	0.014			
Standard 2 2/3	0.031	0.016			
Standard 2 3/3	0.028	0.015			
Standard 3 Avg.	0.035	0.019	7.4	6.938	
Standard 3 1/3	0.033	0.018			
Standard 3 2/3	0.036	0.020			
Standard 3 3/3	0.064	0.033			
Standard 4 Avg.	0.048	0.025	12.7	10.021	
Standard 4 1/3	0.055	0.028			
Standard 4 2/3	0.045	0.024			
Standard 4 3/3	0.045	0.024			
Standard 5 Avg.	0.061	0.033	4.5	14.904	
Standard 5 1/3	0.065	0.035			
Standard 5 2/3	0.060	0.032			
Standard 5 3/3	0.060	0.031			
Standard 6 Avg.	0.079	0.042	2.0	20.043	
Standard 6 1/3	0.077	0.042			
Standard 6 2/3	0.080	0.043			
Standard 6 3/3	0.079	0.042			
Standard 7 Avg.	0.099	0.054	1.2	25.182	
Standard 7 1/3	0.101	0.055			
Standard 7 2/3	0.099	0.054			
Standard 7 3/3	0.098	0.053			
QC 1 µg/L Avg.	0.039	0.021	0.4	8.465	1.693


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Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
QC 1 µg/L 1/3	0.039	0.022			
QC 1 µg/L 2/3	0.039	0.021			
QC 1 µg/L 3/3	0.039	0.021			
Sample Avg.	0.025	0.013	14.7	4.595	0.919
Sample 1/3	0.028	0.015			
Sample 2/3	0.034	0.018			
Sample 3/3	0.022	0.012			
Sample Avg.	0.021	0.011	21.4	3.480	0.696
Sample 1/3	0.020	0.011			
Sample 2/3	0.017	0.008			
Sample 3/3	0.026	0.014			
Sample Avg.	0.019	0.010	21.3	2.807	0.561
Sample 1/3	0.021	0.011			
Sample 2/3	0.014	0.007			
Sample 3/3	0.020	0.011			
QC 1 µg/L Avg.	0.033	0.018	2.1	6.880	1.376
QC 1 µg/L 1/3	0.034	0.018			
QC 1 µg/L 2/3	0.033	0.017			
QC 1 µg/L 3/3	0.032	0.018			
Sample + 2 µg/L Avg.	0.049	0.026	2.6	11.128	2.226
Sample + 2 µg/L 1/3	0.050	0.026			
Sample + 2 µg/L 2/3	0.048	0.026			
Sample + 2 µg/L 3/3	0.047	0.026			
Sample + 2 µg/L Avg.	0.049	0.026	9.3	11.275	2.255
Sample + 2 µg/L 1/3	0.046	0.023			
Sample + 2 µg/L 2/3	0.048	0.025			
Sample + 2 µg/L 3/3	0.054	0.028			
Sample + 2 µg/L Avg.	0.050	0.026	1.8	11.533	2.307
Sample + 2 µg/L 1/3	0.051	0.027			
Sample + 2 µg/L 2/3	0.049	0.025			
Sample + 2 µg/L 3/3	0.050	0.026			
QC 1 µg/L Avg.	0.036	0.019	2.1	7.700	1.540

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Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
QC 1 µg/L 1/3	0.036	0.019			
QC 1 µg/L 2/3	0.036	0.018			
QC 1 µg/L 3/3	0.037	0.020			

Table 8: Calculations for the Stability of Solution.

Name	Accuracy	Precision		
	Recovery Rate / %	Avg. / %	SD / %	RSD / %
Sample + 2 µg/L Avg.	72	74	2	3
Sample + 2 µg/L Avg.	74			
Sample + 2 µg/L Avg.	76			

3. Si in food contact ethanol

3.1 Calibration & Linearity

Table 9: Calibration data. Slope $m = 0.00551$ L/µg, intercept $b = 0.0056$, coefficient of correlation $r = 0.9986$, characteristic concentration $\beta_{\text{char.}}(\text{Si}) = 0.7991$ µg/L. Data below the bold line were used for the Accuracy & Precision experiments starting from the 2 µg/L standard addition. Here, slope $m = 0.00546$ L/µg, intercept $b = 0.0073$, coefficient of correlation $r = 0.9999$, characteristic concentration $\beta_{\text{char.}}(\text{Si}) = 0.8066$ µg/L.

Solution	Concentration / µg/L	Extinction at 251.6 nm (Si)
Blank	0	0.003
Standard 1	1.9425	0.016
Standard 2	5.0989	0.035
Standard 3	7.0414	0.044
Standard 4	9.9551	0.061
Standard 5	15.0540	0.092
Standard 6	19.9101	0.118
Standard 7	25.0091	0.139
Blank	0	0.006
Standard 1	1.9425	0.018
Standard 2	5.0989	0.036
Standard 3	7.0414	0.046
Standard 4	9.9551	0.061
Standard 5	15.0540	0.090
Standard 6	19.9101	0.116
Standard 7	25.0091	0.143

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3.2 Accuracy & Precision

Table 10: Raw data from the Accuracy and Precision experiments. Data below the bold line correspond to analyses made on a later day.

Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
Blank Avg.	0.003	0.001	45.0	0	
Blank 1/3	0.004	0.001			
Blank 2/3	0.002	0.000			
Blank 3/3	0.002	0.001			
Standard 1 Avg.	0.016	0.009	9.0	1.9425	
Standard 1 1/3	0.017	0.010			
Standard 1 2/3	0.021	0.010			
Standard 1 3/3	0.015	0.007			
Standard 2 Avg.	0.035	0.019	7.8	5.0989	
Standard 2 1/3	0.045	0.022			
Standard 2 2/3	0.037	0.019			
Standard 2 3/3	0.034	0.018			
Standard 3 Avg.	0.044	0.023	1.2	7.0414	
Standard 3 1/3	0.045	0.023			
Standard 3 2/3	0.044	0.023			
Standard 3 3/3	0.044	0.023			
Standard 4 Avg.	0.061	0.031	1.2	9.9551	
Standard 4 1/3	0.060	0.031			
Standard 4 2/3	0.061	0.031			
Standard 4 3/3	0.062	0.032			
Standard 5 Avg.	0.092	0.047	1.1	15.0540	
Standard 5 1/3	0.091	0.047			
Standard 5 2/3	0.091	0.047			
Standard 5 3/3	0.093	0.048			
Standard 6 Avg.	0.118	0.062	3.0	19.9101	
Standard 6 1/3	0.120	0.062			
Standard 6 2/3	0.120	0.062			
Standard 6 3/3	0.114	0.061			
Standard 7 Avg.	0.139	0.074	0.8	25.0091	
Standard 7 1/3	0.139	0.073			
Standard 7 2/3	0.140	0.074			
Standard 7 3/3	0.138	0.073			
QC 1 µg/L Avg.	0.039	0.020	1.7	6.0846	1.2169

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Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
QC 1 µg/L 1/3	0.038	0.020			
QC 1 µg/L 2/3	0.039	0.020			
QC 1 µg/L 3/3	0.040	0.020			
Sample Avg.	0.009	0.004	6.1	0.6480	0.1296
Sample 1/3	0.051	0.020			
Sample 2/3	0.009	0.003			
Sample 3/3	0.010	0.004			
Sample Avg.	0.010	0.004	12.5	0.8418	0.1684
Sample 1/3	0.009	0.004			
Sample 2/3	0.011	0.005			
Sample 3/3	0.011	0.005			
Sample Avg.	0.011	0.005	14.6	0.9992	0.1998
Sample 1/3	0.013	0.007			
Sample 2/3	0.010	0.004			
Sample 3/3	0.010	0.004			
QC 1 µg/L Avg.	0.047	0.024	7.7	7.4528	1.4906
QC 1 µg/L 1/3	0.049	0.025			
QC 1 µg/L 2/3	0.043	0.022			
QC 1 µg/L 3/3	0.049	0.024			
Sample + 1 µg/L Avg.	0.033	0.016	16.4	4.9827	0.9965
Sample + 1 µg/L 1/3	0.029	0.015			
Sample + 1 µg/L 2/3	0.031	0.016			
Sample + 1 µg/L 3/3	0.039	0.018			
Sample + 1 µg/L Avg.	0.031	0.015	1.9	4.6740	0.9348
Sample + 1 µg/L 1/3	0.032	0.015			
Sample + 1 µg/L 2/3	0.031	0.014			
Sample + 1 µg/L 3/3	0.032	0.016			
Sample + 1 µg/L Avg.	0.029	0.015	1.7	4.3047	0.8609
Sample + 1 µg/L 1/3	0.029	0.015			
Sample + 1 µg/L 2/3	0.029	0.016			
Sample + 1 µg/L 3/3	0.030	0.015			
QC 1 µg/L Avg.	0.050	0.025	4.1	8.0461	1.6092
QC 1 µg/L 1/3	0.051	0.025			
QC 1 µg/L 2/3	0.048	0.025			
QC 1 µg/L 3/3	0.051	0.026			
Blank Avg.	0.006	0.004	42.5	0	

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Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
Blank 1/3	0.007	0.003			
Blank 2/3	0.004	0.002			
Blank 3/3	0.009	0.005			
Standard 1 Avg.	0.018	0.009	17.8	1.9425	
Standard 1 1/3	0.021	0.011			
Standard 1 2/3	0.015	0.008			
Standard 1 3/3	0.017	0.009			
Standard 2 Avg.	0.036	0.019	3.6	5.0989	
Standard 2 1/3	0.034	0.020			
Standard 2 2/3	0.036	0.018			
Standard 2 3/3	0.036	0.020			
Standard 3 Avg.	0.046	0.025	3.1	7.0414	
Standard 3 1/3	0.046	0.025			
Standard 3 2/3	0.048	0.026			
Standard 3 3/3	0.045	0.025			
Standard 4 Avg.	0.061	0.033	1.4	9.9551	
Standard 4 1/3	0.062	0.033			
Standard 4 2/3	0.060	0.033			
Standard 4 3/3	0.062	0.034			
Standard 5 Avg.	0.090	0.049	1.4	15.0540	
Standard 5 1/3	0.092	0.050			
Standard 5 2/3	0.089	0.049			
Standard 5 3/3	0.090	0.049			
Standard 6 Avg.	0.116	0.064	0.7	19.9101	
Standard 6 1/3	0.116	0.064			
Standard 6 2/3	0.117	0.064			
Standard 6 3/3	0.117	0.064			
Standard 7 Avg.	0.143	0.079	2.0	25.0091	
Standard 7 1/3	0.146	0.080			
Standard 7 2/3	0.140	0.078			
Standard 7 3/3	0.142	0.078			
QC 1 µg/L Avg.	0.042	0.023	8.7	6.4136	1.2827
QC 1 µg/L 1/3	0.043	0.023			
QC 1 µg/L 2/3	0.046	0.024			
QC 1 µg/L 3/3	0.038	0.021			
Sample + 2 µg/L Avg.	0.064	0.034	6.8	10.3303	2.0661

Supplementary Information

Raw data of

**Ultra-trace elemental determination of Si by means of graphite
furnace-atomic absorption spectrometry**



Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
Sample + 2 µg/L 1/3	0.069	0.036			
Sample + 2 µg/L 2/3	0.060	0.032			
Sample + 2 µg/L 3/3	0.062	0.033			
Sample + 2 µg/L Avg.	0.077	0.041	3.2	12.6950	2.5390
Sample + 2 µg/L 1/3	0.074	0.040			
Sample + 2 µg/L 2/3	0.076	0.041			
Sample + 2 µg/L 3/3	0.079	0.043			
Sample + 2 µg/L Avg.	0.058	0.031	3.1	9.2915	1.8583
Sample + 2 µg/L 1/3	0.056	0.030			
Sample + 2 µg/L 2/3	0.060	0.031			
Sample + 2 µg/L 3/3	0.058	0.031			
QC 1 µg/L Avg.	0.045	0.023	8.2	6.8963	1.3793
QC 1 µg/L 1/3	0.047	0.023			
QC 1 µg/L 2/3	0.041	0.022			
QC 1 µg/L 3/3	0.047	0.024			
Sample + 3 µg/L Avg.	0.093	0.049	0.3	15.6096	3.1219
Sample + 3 µg/L 1/3	0.093	0.049			
Sample + 3 µg/L 2/3	0.093	0.049			
Sample + 3 µg/L 3/3	0.092	0.048			
Sample + 3 µg/L Avg.	0.078	0.041	1.3	12.8844	2.5769
Sample + 3 µg/L 1/3	0.077	0.041			
Sample + 3 µg/L 2/3	0.077	0.041			
Sample + 3 µg/L 3/3	0.079	0.042			
Sample + 3 µg/L Avg.	0.077	0.041	1.1	12.8233	2.5647
Sample + 3 µg/L 1/3	0.076	0.041			
Sample + 3 µg/L 2/3	0.077	0.041			
Sample + 3 µg/L 3/3	0.078	0.043			
QC 1 µg/L Avg.	0.043	0.022	7.0	6.5419	1.3084
QC 1 µg/L 1/3	0.044	0.022			
QC 1 µg/L 2/3	0.040	0.021			
QC 1 µg/L 3/3	0.045	0.024			


Supplementary Information Raw data of Ultra-trace elemental determination of Si by means of graphite furnace-atomic absorption spectrometry	 EVONIK Leading Beyond Chemistry
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Table 11: Calculations for the Accuracy & Precision experiments.

Name	Accuracy	Precision		
	Recovery Rate / %	Avg. / %	SD / %	RSD / %
Sample + 1 µg/L Avg.	90	82	9	11
Sample + 1 µg/L Avg.	84			
Sample + 1 µg/L Avg.	72			
Sample + 2 µg/L Avg.	102	106	20	19
Sample + 2 µg/L Avg.	127			
Sample + 2 µg/L Avg.	88			
Sample + 3 µg/L Avg.	103	89	12	14
Sample + 3 µg/L Avg.	82			
Sample + 3 µg/L Avg.	81			

3.3 Limit of detection, limit of quantitation

Table 12: Raw data & calculations for the determinations of the LOD and LOQ, respectively, by means of the blank method. Values below the bold line refer to calculations.

Name	Value
Blank 1	0.0048
Blank 2	0.0036
Blank 3	0.0026
Blank 4	0.0039
Blank 5	0.0037
Blank 6	0.0030
Blank 7	0.0032
Blank 8	0.0040
Blank 9	0.0036
Blank 10	0.0032
Mean	0.0036
Standard deviation	0.0006
Concentrating factor	5
LOD / µg/L	0.333
LOQ / µg/L	1.110
LOD WRT concentrating factor / µg/L	0.067
LOQ WRT concentrating factor / µg/L	0.222

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3.4 Stability of solution

Table 13: Raw data for the Stability of Solution.

Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
Blank Avg.	0.005	0.003	6.5	0	
Blank 1/3	0.006	0.003			
Blank 2/3	0.005	0.003			
Blank 3/3	0.238	0.091			
Standard 1 Avg.	0.024	0.012	16.3	1.9717	
Standard 1 1/3	0.029	0.014			
Standard 1 2/3	0.023	0.011			
Standard 1 3/3	0.021	0.010			
Standard 2 Avg.	0.038	0.019	2.5	5.1757	
Standard 2 1/3	0.037	0.018			
Standard 2 2/3	0.039	0.019			
Standard 2 3/3	0.039	0.020			
Standard 3 Avg.	0.052	0.026	12.1	7.1474	
Standard 3 1/3	0.059	0.028			
Standard 3 2/3	0.047	0.024			
Standard 3 3/3	0.049	0.024			
Standard 4 Avg.	0.062	0.031	2.2	9.8584	
Standard 4 1/3	0.061	0.030			
Standard 4 2/3	0.061	0.030			
Standard 4 3/3	0.063	0.032			
Standard 5 Avg.	0.094	0.047	4.1	15.0341	
Standard 5 1/3	0.092	0.046			
Standard 5 2/3	0.098	0.049			
Standard 5 3/3	0.092	0.046			
Standard 6 Avg.	0.115	0.059	3.7	19.9633	
Standard 6 1/3	0.112	0.057			
Standard 6 2/3	0.112	0.058			
Standard 6 3/3	0.120	0.060			
Standard 7 Avg.	0.136	0.070	1.9	24.8926	
Standard 7 1/3	0.138	0.070			
Standard 7 2/3	0.138	0.071			
Standard 7 3/3	0.133	0.069			
QC 1 µg/L Avg.	0.046	0.024	16.9	6.7494	1.3499


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Raw data of

Ultra-trace elemental determination of Si by means of graphite furnace-atomic absorption spectrometry



Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
QC 1 µg/L 1/3	0.043	0.023			
QC 1 µg/L 2/3	0.041	0.022			
QC 1 µg/L 3/3	0.055	0.026			
Sample Avg.	0.024	0.012	20.4	2.4435	0.4887
Sample 1/3	0.021	0.010			
Sample 2/3	0.022	0.011			
Sample 3/3	0.030	0.014			
Sample Avg.	0.021	0.009	6.8	1.8183	0.3637
Sample 1/3	0.022	0.010			
Sample 2/3	0.020	0.009			
Sample 3/3	0.089	0.035			
Sample Avg.	0.026	0.011	42.1	2.7400	0.5480
Sample 1/3	0.014	0.007			
Sample 2/3	0.035	0.016			
Sample 3/3	0.028	0.012			
QC 1 µg/L Avg.	0.042	0.020	58.3	5.9888	1.1978
QC 1 µg/L 1/3	0.018	0.009			
QC 1 µg/L 2/3	0.041	0.021			
QC 1 µg/L 3/3	0.068	0.029			
Sample + 2 µg/L Avg.	0.084	0.041	1.6	14.1172	2.8234
Sample + 2 µg/L 1/3	0.085	0.040			
Sample + 2 µg/L 2/3	0.083	0.041			
Sample + 2 µg/L 3/3	0.086	0.042			
Sample + 2 µg/L Avg.	0.064	0.031	5.7	10.1078	2.0216
Sample + 2 µg/L 1/3	0.061	0.029			
Sample + 2 µg/L 2/3	0.063	0.031			
Sample + 2 µg/L 3/3	0.068	0.032			
Sample + 2 µg/L Avg.	0.053	0.026	1.7	7.9355	1.5871
Sample + 2 µg/L 1/3	0.054	0.027			
Sample + 2 µg/L 2/3	0.052	0.026			
Sample + 2 µg/L 3/3	0.052	0.026			
QC 1 µg/L Avg.	0.042	0.020	35.7	5.8148	1.1630

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Name	Signal height	Signal area	RSD / %	Conc. / µg/L	Corrected Conc. / µg/L
QC 1 µg/L 1/3	0.033	0.016			
QC 1 µg/L 2/3	0.033	0.018			
QC 1 µg/L 3/3	0.059	0.026			

Table 14: Calculations for the Stability of Solution.

Name	Accuracy	Precision		
	Recovery Rate / %	Avg. / %	SD / %	RSD / %
Sample + 2 µg/L Avg.	102	106	20	19
Sample + 2 µg/L Avg.	127			
Sample + 2 µg/L Avg.	88			