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Precise determination of ^{204}Pb-based isotopic ratios in environmental samples by quadrupole inductively coupled plasma mass spectrometry

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Supplementary information

Table S1. Doehlert design for the multivariate optimization of the spray chamber temperature and the sample uptake rate

Run	X_1	X_2	T (°C)	UR (µL/min)
1	0	0	42	200
2	1	0	80	200
3	0.5	0.866	61	300
4	-1	0	4	200
5	-0.5	-0.866	23	100
6	0.5	-0.866	61	100
7	-0.5	0.866	23	300

Table S2. Central composite design for the multivariate optimization of the quadrupoles' parameters

Run	X_1	X_2	X_3	CRO (V)	QRO (V)	CPV (V)
1	-1	-1	-1	-14.9	-7.0	-23.2
2	1	-1	-1	-1.1	-7.0	-23.2
3	-1	1	-1	-14.9	1.0	-23.2
4	1	1	-1	-1.1	1.0	-23.2
5	-1	-1	1	-14.9	-7.0	-4.8
6	1	-1	1	-1.1	-7.0	-4.8
7	-1	1	1	-14.9	1.0	-4.8
8	1	1	1	-1.1	1.0	-4.8
9	-1.73	0	0	-20.0	-3.0	-14.0
10	1.73	0	0	4.0	-3.0	-14.0
11	0	-1.73	0	-8.0	-10.0	-14.0
12	0	1.73	0	-8.0	4.0	-14.0
13	0	0	-1.73	-8.0	-3.0	-30.0
14	0	0	1.73	-8.0	-3.0	2.0

15-20	0	0	0	-8.0	-3.0	-14.0

Table S3. Models' coefficients and their significance (Central composite design)

	Sensitivity (Mcps ppm^{-1})	
Coefficient	**Value**	**p-value**
b_0	102.9	<0.001
b_1	3.16	0.037
b_2	-1.49	0.241
b_3	12.1	<0.001
b_{12}	-1.49	0.361
b_{13}	-8.19	0.003
b_{23}	0.16	0.917
b_{11}	-18.7	<0.001
b_{22}	-4.03	0.012
b_{33}	-19.0	<0.001
Model performance		
%EV [(a)]	82.0	
%CVEV [(b)]	34.7	

Notes: [(a)] explained variance; [(b)] cross-validation explained variance

Table S4. Models' coefficients and their significance (Doehlert design)

	Sensitivity (Mcps ppm^{-1})		Oxides (CeO/Ce)	
Coefficient	**Value**	**p-value**	**Value**	**p-value**
b_0	61.5	<0.001	1.20	0.23
b_1	5.39	<0.001	3.23	<0.001
b_2	24.4	<0.001	0.92	0.12
b_{12}	0.87	0.38	1.10	0.34
b_{11}	14.3	<0.001	3.83	0.01
b_{22}	-6.33	<0.001	-0.68	0.57
Model performance				
%EV [(a)]	99.6		80.9	
%CVEV [(b)]	99.3		68.0	

Notes: [(a)] explained variance; [(b)] cross-validation explained variance