Continuous-flow analyses of calcium isotopes using the Neoma MC-ICPMS/MS with H_2 or SF_6

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Supplementary Information

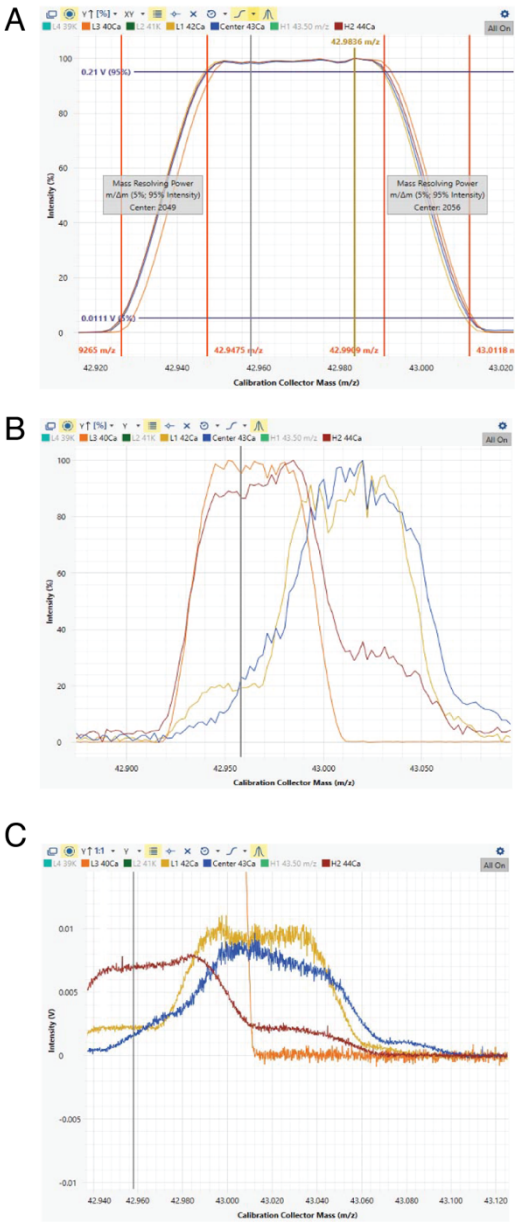

Fig. S1 : A) Peak scan in the low-resolution mode with H_2 of the ICP-Ca Lyon solution at 250 ng mL^{-1} using the set of parameters given in Table 1 showing the peak shape of the different Ca m/z values with the automated calculation of the resolution (mass resolving power) on the edges of the peak. B) Peak scan in the low-resolution mode with H_2 of a HNO_3 0.05M solution in relative intensity (%), showing the interferences on the Ca m/z except the ^{40}Ca m/z. C) Peak scan in the low-resolution mode with H_2 of a HNO_3 0.05M solution in absolute intensity (V), showing that the intensity of the interferences on the ^{42}Ca m/z is very significant, and that, despite positioning the peak centre on the low mass shoulder, the ^{43}Ca m/z is still interfered, highlighting the necessity of blank subtraction.

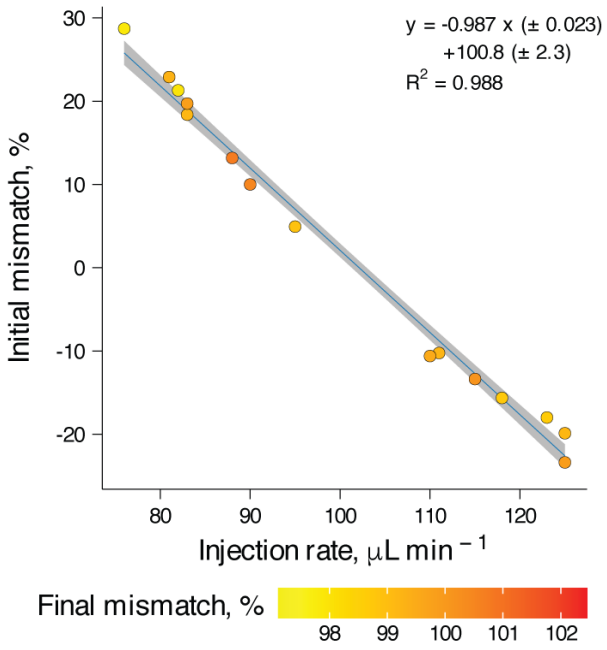

Fig. S2 : Effect of modulating initial mismatch with injection rate on the final mismatch: for an initial mismatch ranging from -20% to +30%, the final corrected mismatch is generally ±2%. A +1% initial mismatch is corrected with -1 µL min^{-1} and a -1% initial mismatch is corrected with +1 µL min^{-1}. Nominal injection rate is 100 µL min^{-1}.

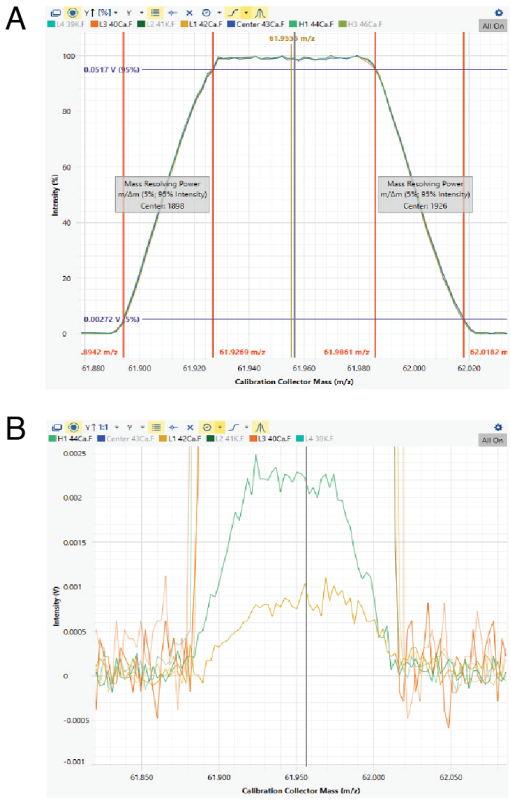

Fig. S3 : A) Peak scan in the low-resolution mode with SF_6 of the ICP-Ca Lyon solution at 500 ng mL^{-1} using the set of parameters given in Table 1 showing the peak shape of the different Ca m/z values with the automated calculation of the resolution (mass resolving power) on the edges of the peak. B) Peak scan in the low-resolution with SF_6 mode of a HNO_3 0.05M solution in absolute intensity (V), showing the absence of any significant interferences on the CaF isotopes.

Table S1 : ^{40}Ca intensity, corresponding noise-to-signal ratio, and Ca isotope compositions in the H_2 mode, according to settings given in Table 1.

Session	Date	[Ca], ng ml^{-1}	^{40}Ca ± 2SD signal, V	n signal	^{40}Ca ± 2SD blank, V	n blank	Noise to signal ratio, %	$\delta^{44/40}Ca$ ± 2 SD, ‰	$\delta^{43/40}Ca$ ± 2 SD, ‰	$\delta^{42/40}Ca$ ± 2 SD, ‰	$\delta^{44/42}Ca$ ± 2 SD, ‰
#55	2025/01	250	142 ± 1.8	33	0.230 ± 0.027	80	0.16	0.000 ± 0.129	-0.009 ± 0.194	0.006 ± 0.067	-0.004 ± 0.135
#56	2025/01	250	145 ± 1.4	53	0.236 ± 0.035	111	0.16	-0.006 ± 0.129	-0.005 ± 0.125	-0.002 ± 0.063	-0.002 ± 0.14
#66	2025/04	250	258 ± 7.0	158	0.452 ± 0.112	351	0.17	0.008 ± 0.143	-0.002 ± 0.116	-0.001 ± 0.101	0.003 ± 0.048
#67	2025/04	250	260 ± 20.0	50	0.376 ± 0.192	89	0.14	0.005 ± 0.125	-0.014 ± 0.103	-0.001 ± 0.094	0.005 ± 0.057
#68	2025/05	250	201 ± 7.5	226	0.495 ± 0.275	431	0.25	0.006 ± 0.113	-0.001 ± 0.137	0.004 ± 0.067	0.002 ± 0.054
#76	2025/10	100	44 ± 1.3	23	0.435 ± 0.045	261	0.98	0.004 ± 0.129	0.009 ± 0.203	0.004 ± 0.087	0.001 ± 0.117
#76	2025/10	250	113 ± 9.1	120	0.435 ± 0.045	261	0.39	0.004 ± 0.091	0.003 ± 0.092	0.002 ± 0.081	0.003 ± 0.072
#76	2025/10	50	22.0 ± 0.11	11	0.435 ± 0.045	261	2	0.003 ± 0.147	-0.018 ± 0.134	-0.003 ± 0.063	0.004 ± 0.176

Table S2: Ca isotope compositions of the CRMs measured in this study. n and N stand for the number of measurements and the number of digested aliquots, respectively.

CRM ID	$\delta^{44/40}Ca$ ± 2 SD, ‰	$\delta^{43/40}Ca$ ± 2 SD, ‰	$\delta^{42/40}Ca$ ± 2 SD, ‰	$\delta^{44/42}Ca$ ± 2 SD, ‰	n	N
BCR-184	-1.40 ± 0.15	-1.20 ± 0.06	-0.68 ± 0.09	-0.74 ± 0.057	3	1
BCR-186	-0.34 ± 0.01	-0.30 ± 0.24	-0.13 ± 0.00	-0.22 ± 0.048	2	1
BCR-380R	-2.30 ± 0.03	-1.70 ± 0.08	-1.20 ± 0.07	-1.1 ± 0.035	3	2
BCR-383	-1.21 ± 0.08	-1.11 ± 0.04	-0.77 ± 0.03	-0.65 ± 0.01	3	1
ERM-CD281	-1.50 ± 0.18	-1.20 ± 0.11	-0.77 ± 0.13	-0.75 ± 0.1	8	2
ERM-CE464	0.41 ± 0.17	0.02 ± 0.01	0.19 ± 0.04	0.23 ± 0.08	2	1
IAPSO	0.87 ± 0.11	0.67 ± 0.10	0.49 ± 0.07	0.39 ± 0.065	6	2
SRM-1400	-2.20 ± 0.17	-1.70 ± 0.14	-1.10 ± 0.11	-1.1 ± 0.1	39	7
SRM-1515	-0.69 ± 0.19	-0.54 ± 0.15	-0.37 ± 0.11	-0.31 ± 0.15	6	2
SRM-1573	-1.43 ± 0.03	-1.11 ± 0.09	-0.67 ± 0.06	-0.56 ± 0.02	2	1
SRM-1577c	0.08 ± 0.13	0.081± 0.20	0.09 ± 0.03	-0.029 ± 0.1	3	1
Tort-3	0.63 ± 0.14	0.32 ± 0.21	0.33 ± 0.10	0.3 ± 0.058	7	2

Table S3 : ^{40}CaF intensity, corresponding noise-to-signal ratio, and CaF isotope compositions in the SF_6 mode, according to settings given in Table 1.

Session	Date	[Ca], ng ml^{-1}	^{40}CaF ± 2SD signal, V	n signal	^{40}CaF ± 2SD blank, V	n blank	Noise to signal ratio, %	$\delta^{44/40}CaF$ ± 2 SD, ‰	$\delta^{42/40}CaF$ ± 2 SD, ‰	$\delta^{44/42}CaF$ ± 2 SD, ‰
#9	2024/05	500	62.6 ± 0.9	46	0.098± 0.055	61	0.16	-0.002 ± 0.149	-0.005 ± 0.089	-0.004 ± 0.103
#9	2024/05	250	31.0 ± 0.9	88	0.072± 0.009	140	0.23	-0.011 ± 0.150	-0.006 ± 0.094	-0.007 ± 0.102
#24	2024/11	250	23.7 ± 0.2	16	0.095± 0.004	23	0.40	0.002 ± 0.124	0.003 ± 0.080	-0.001 ± 0.110
#24	2024/11	500	45.1 ± 5.7	73	0.101 ± 0.013	73	0.22	-0.001± 0.132	-0.002 ± 0.088	0.000 ± 0.087
#38	2025/01	500	34.7 ± 2.0	32	0.055 ± 0.007	64	0.16	-0.001 ± 0.099	-0.005 ± 0.097	0.001 ± 0.123
#39	2025/01	500	32.7 ± 2.2	54	0.060 ± 0.002	105	0.18	-0.007 ± 0.137	-0.000 ± 0.097	0.002± 0.137