Supplementary Information (SI) for Journal of Analytical Atomic Spectrometry.

Advances in high-precision lithium isotopic measurements with the Neoma^{TM} MC-ICP-MS

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Supplementary materials

I. MicroFAST Isotope I autosampler (*Elemental Scientific Inc*. (ESI), Omaha, USA): dual-loop wash optimization

Classical dual loop system:

The dual-loop injection system of the microFAST Isotope I autosampler is composed of two loops (A and B), two syringes, and two four-way valves (P4 and P4F).

- Step 1: The sample 1 solution (yellow pathway) contained in loop A is injected into the nebulizer for analysis, while loop B is simultaneously rinsed with the working solution (blue pathway in Figure. S1).
- Step 2: Loop A continues to deliver sample 1 to the nebulizer (yellow pathway), while loop B loads the next sample 2 solution (green pathway).
- Step 3: The two four-way valves switch positions, allowing sample 2 in loop B to be injected into the nebulizer (green pathway), while loop A is rinsed with the working solution (blue pathway).
- Step 4: The valves switch again loop B continues to inject sample 2 into the nebulizer (green pathway), while loop A loads the new sample 3 solution (green pathway).

This alternating sequence ensures a continuous sample introduction cycle, where one loop injects while the other is simultaneously cleaned and prepared, thereby maximizing analytical throughput

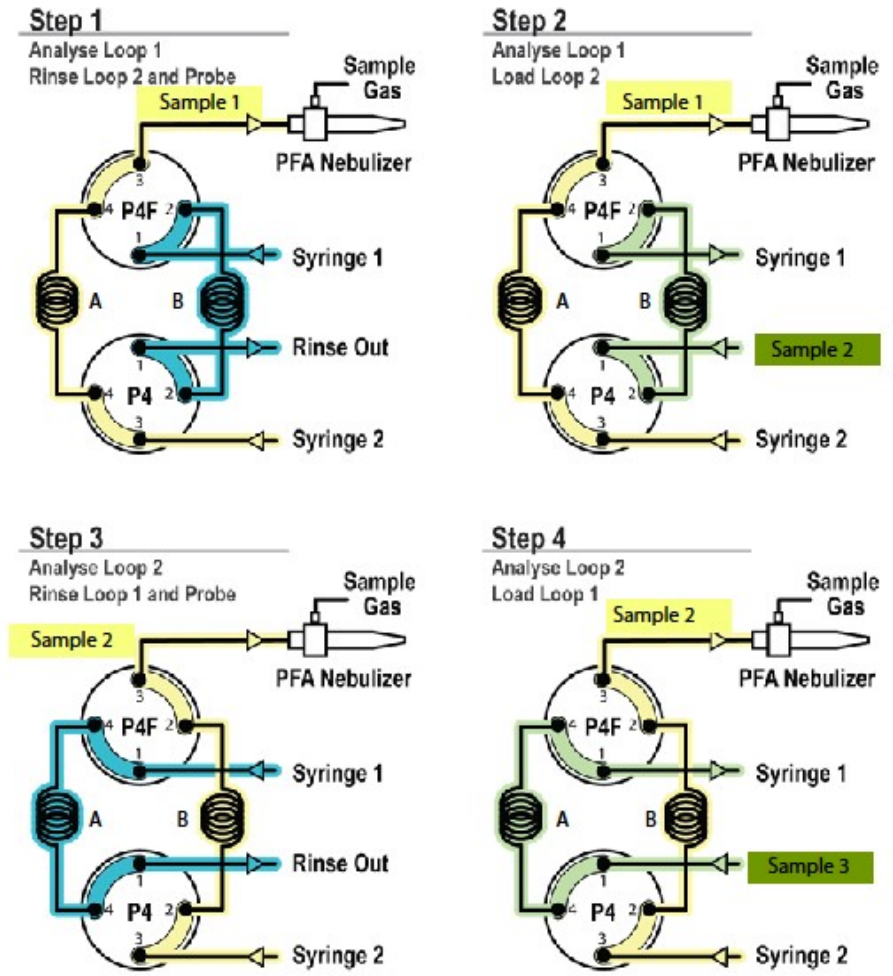


Figure S1: Schematic representation of the dual-loop dual-loop microFAST Isotope I autosampler sequence enabling continuous sample loading and analyses. Modified from https://www.icpms.com/products/autosamplers-for-icp-icpms/

When coupled with the standard Sample Standard Bracketing (SSB) method, the alternating dual-loop operation of the dual-loop microFAST Isotope I autosampler revealed a potential source of bias for Li isotopic measurement. In the conventional SSB sequence ($Blank_1$–$LSVEC_1$–$Blank_2$–$Sample_1$–$Blank_3$–$LSVEC_2$–$Blank_4$–$Sample_2$, etc.), the blanks are consistently analyzed in the same loop (configuration 1), while both standards and samples are injected through the other loop. This asymmetric use of the loops may introduce small but systematic bias in measured δ^7Li values, ultimately affecting reproducibility (see Figure 2 main text), likely due to different rinsing (washing) times.

To overcome this limitation, we implemented a modified SSB sequence ($Blank_1$–$Blank_2$–$LSVEC_1$–$Blank_3$–$Blank_4$–$Sample_1$–$Blank_5$–$Blank_6$–$LSVEC_2$, etc.), incorporating two blanks before each standard or sample analysis. This approach alternates the injection of standards and samples between loops A

and B, ensuring balanced use of both loops for all solution types. As shown in Figure 2 (main text), this configuration proved more suitable for low-level lithium analyses (≤ 3ppb) and improved the reproducibility of lithium isotope measurements. (See Figure 2 main text).

Configuration 1: Conventional SSB sequence

Blank → Loop A

Standard (LSVEC) → Loop B

Blank → Loop A

Sample → Loop B

(Repeat for all n samples)

Configuration 2 Modified (alternating-loop) SSB sequence

Blank 1 → Loop A

Blank 2 → Loop B

Standard (LSVEC) → Loop A

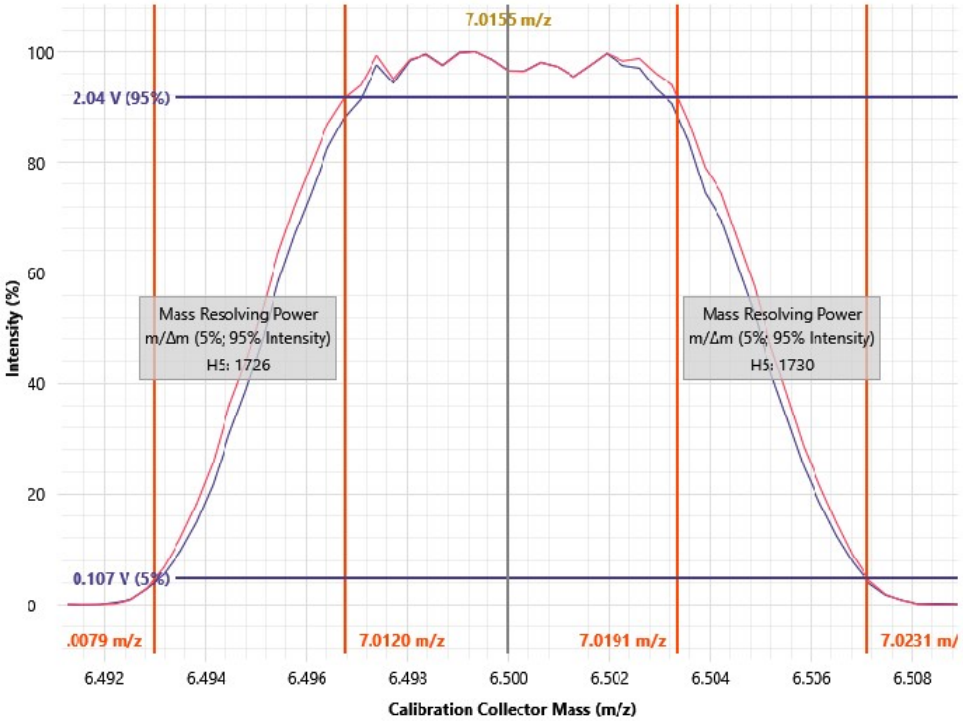
Blank 3 → Loop B

Blank 4 → Loop A

Sample 1 → Loop B

(Repeat alternation for subsequent standards and samples)

II. Peak Shape of ^{7}Li (in red) and of ^{6}Li (in blue), both normalized to 100% for comparison.



III. Table S1: Compilation of recent seawater values reported in the literature and measured by MC-ICP-MS, excluding Neoma* data (over the last 10 years)

Area/Name	δ^7Li (‰) value	2SD**	N	Li (ppb) MC–ICP–MS	References
NASS-5	30.91	0.26	7	N.R.	(1)
Atlantic Ocean	30.97	0.31	7	50	(2)
NASS-6	30.87	0.15	15	112	(3)
N.R.***	31.2	0.4	19	0.5	(4)
Atlantic Ocean	31.1	0.7	14	20	(5)
Atlantic Ocean	31.1	0.3	6	4	(6)
N.R.	31.27	0.4	30	0.2-0.4	(7)
South China Sea	31.4	0.7	18	80	(8)
AEL, EDMM-1-G	31.32	0.83	4	4	(9)
Atlantic Ocean	31.2	0.4	3	20	(10)
Atlantic Ocean	30.88	0.76	4	20	(11)
NASS-6	30.97	0.24	5	1	(12)
N.R.	31.13	0.38	29	0.5	(13)
NASS-7	30.93	0.36	1	5-15	(14)
Average ***31.1 ± 0.09‰ (2SE, N=14)*** ***2SD = 0.4‰***					

**Neoma seawater data published previously are deliberately not included in this table; they are presented in the main text for direct comparison with the Neoma data generated in this study (see Section 6 and Figure 9 main text)*

***External reproducibility*

**** Not reported*

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