

Supplementary:

S1. List of materials, instruments, and equipment.

Materials: Dry air bottle (20.5 Vol. % O₂ , Rest N₂ , KW-free), 1l FlexFoil® gas valve bag (263-01, SKC, Dorset, United Kingdom), 500 ml Aluminum-Zip bag (CB400-420siZ, WEBER Packaging, Göglingen, Germany), 250 ml infusion glass bottles ND 32 (VAT 71732100, IVA Analysetechnik, Meerbusch, Germany), 100 ml infusion glass bottles ND20 (IVA70920114, IVA Analysetechnik, Meerbusch, Germany), 1 liter QEC Tedlar® bags, butyl stopper (VAT 71732101, IVA Analysetechnik, Meerbusch, Germany), aluminum cap (VAT 71732800, VAT Analysetechnik, Meerbusch, Germany), PTFE tube with an outer diameter of 1/8 inch (BEMU, Krefeld, Germany), stainless steel connectors (SS-200-1-2, 1/8 inch DE 1/8 inch NPT male tube, Swagelok, Solon, OH, USA), Male Luer Integral Lock Ring adapter (MTLL004-1), syringes (0.80x40 mm and 0.80x80 mm, B.Braun, Melsungen, Germany), syringes (1.20x40 mm and 1.20x80 mm, B.Braun, Melsungen, Germany), silicone (Probau construction and window silicone, transparent, 310 ml) and HDES, ALBI1, BS and KEI standards (known isotopic references).

Instruments and equipment; CRDS isotope analyzer (L2130-i, Picarro Inc., Santa Clara, CA, USA), Electronic Mass Flow Controller (PN 35828, Analyt MTC, Müllheim, Germany), Temperature sensor (Sensirion AG, SHT4X SMART GADGET, Switzerland), Drying oven (memmert, type: ULM 600, Germany), Refrigerator (Samsung, model: RL38T775CS9, Poland) and sealing clip for 32 mm aluminum lid (VAT 70632100, VAT Analysetechnik, Meerbusch, Germany).

Table S1. Observations and evaluation metrics of the decision criteria.

Decision criteria	250 ml infusion bottle (ND 32)	1 L FlexFoil® sample bags	500 mL Aluminum-Zip bags	Verification
Isotopic stability	$\pm 0.5\text{‰}$ for $\delta^{18}\text{O}$ and $\pm 1\text{‰}$ for $\delta^2\text{H}$ within the first 24 hours	$\pm 1\text{‰}$ for $\delta^{18}\text{O}$ and -3 to $+2\text{‰}$ for $\delta^2\text{H}$	-2.5 to -3‰ for $\delta^{18}\text{O}$ and -12 to -25‰ for $\delta^2\text{H}$	See Figure 6
Tightness	Glass, butyl stopper, and aluminum cap	Multilayer with stainless steel gas valve	Aluminum bag with zip closure and silicone septum	Description of container sealing systems (see the Methodology section and Figure 5 in the Results)
Time to analysis	Stable results for up to 24 hours in $\delta^2\text{H}$ and $\delta^{18}\text{O}$.	Greater variations in $\delta^2\text{H}$ and $\delta^{18}\text{O}$ were observed during the first 24 hours.	Significant deviations in $\delta^2\text{H}$ and $\delta^{18}\text{O}$.	See Figure 6

Reusability	Reuse after 24 hours in the oven and flush with dry air	Reuse of the same bag is permitted only after thorough treatment and for sampling within narrow isotopic concentration ranges.	Effectively single-use; reuse is allowed only after thorough dry-air flushing or repeated flushing with a homogeneous water vapor source.	Laboratory practices and experiences of other researchers.
Portability and transport	Considerable weight, but transportable in insulated aluminum cases (over 100 bottles).	Lightweight, but they expand when filled; transport requires strict attention, especially when the number of samples exceeds 100.	Lightweight; expand when filled, prone to punctures, and require careful transport.	Verification through field and laboratory testing
Cost	~2.91€	~32.37 €	~0.67 €	European market

Table S2. Score for the decision criteria.

Decision criteria (level of importance)	250 ml infusion bottle (ND 32)		1 L FlexFoil® sample bag		500 mL Aluminum-Zip bag	
Isotopic stability (50%)	4.5	2.25	4	2	1	0.5
Tightness (20%)	3	0.6	4	0.8	4	0.8
Time to analysis (10%)	5	0.5	4	0.4	1.5	0.15
Reusability (10%)	5	0.5	3	0.3	1	0.1
Portability and transport (5%)	4	0.2	3	0.15	3	0.15
Cost (5%)	4	0.2	1	0.05	5	0.25
Weighted total (Σ)		4.25		3.7		1.95
Score (%)		85		74		39

Water vapor sampling: During sampling at four flow rates (35, 75, 100, and 125 ml/min), the H₂O concentration (ppm) reached a stable plateau after 25 minutes at 100 and 125 ml/min. At 75 ml/min, a plateau was reached only around minute 31, while at 35 ml/min it was not fully attained within 35 minutes. After 5 minutes of sampling, a stable plateau for $\delta^{18}\text{O}$ and $\delta^2\text{H}$ was evident at 100 and 125 ml/min, whereas at 35 and 75 ml/min the isotopic plateau developed more gradually. In all cases, the reported values correspond to the mean of the last 5 minutes (stable plateau).

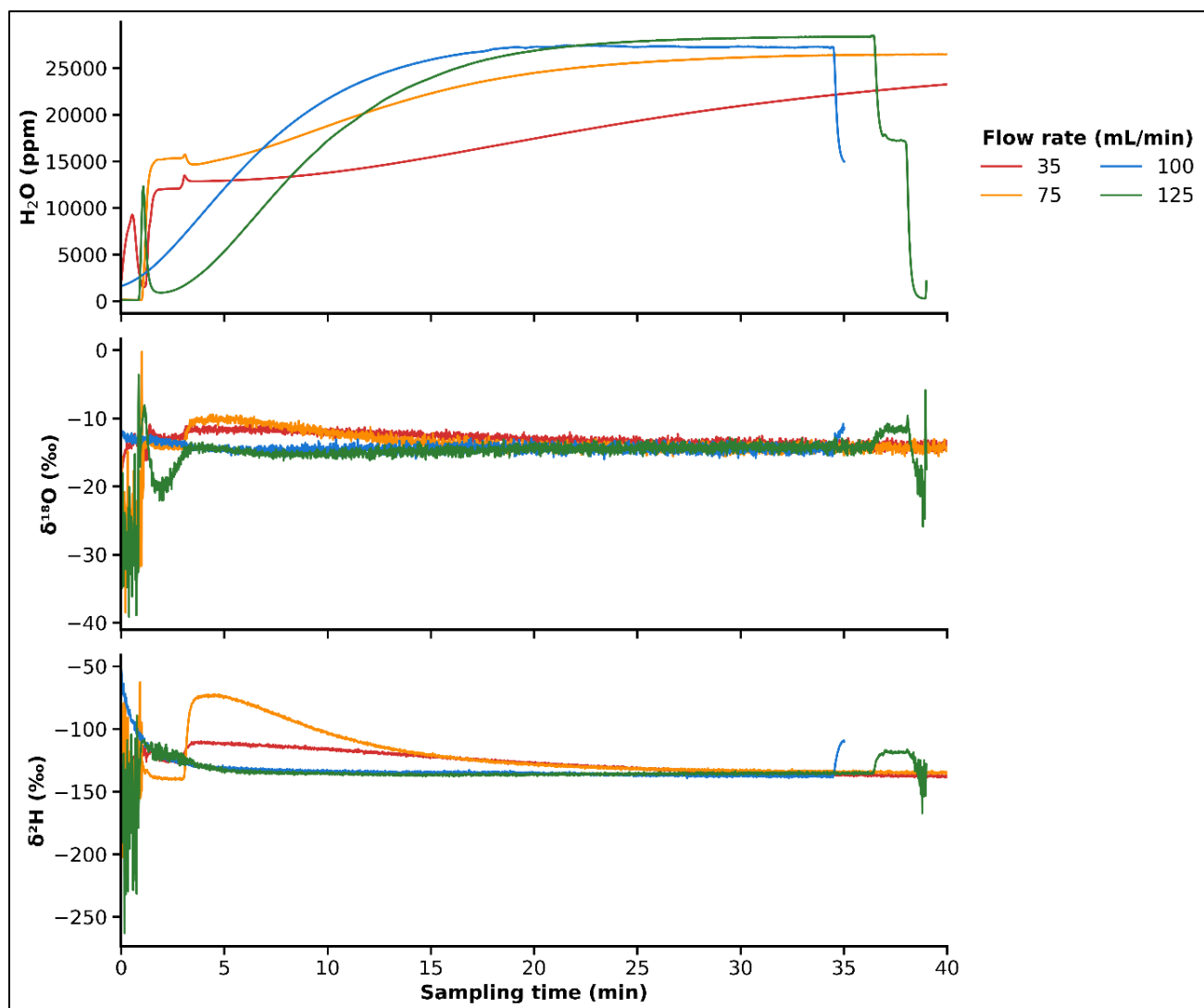


Figure S1. Water vapor behavior during sampling in 250 mL glass bottles at four flow rates.

Water vapor measurement: Samples were measured for 6 minutes after conditioning. Although H₂O concentration decreased during analysis, isotopic ratios remained stable, showing a clearly defined plateau similar across the three replicates. The reported values correspond to the 2-minute average within that plateau.

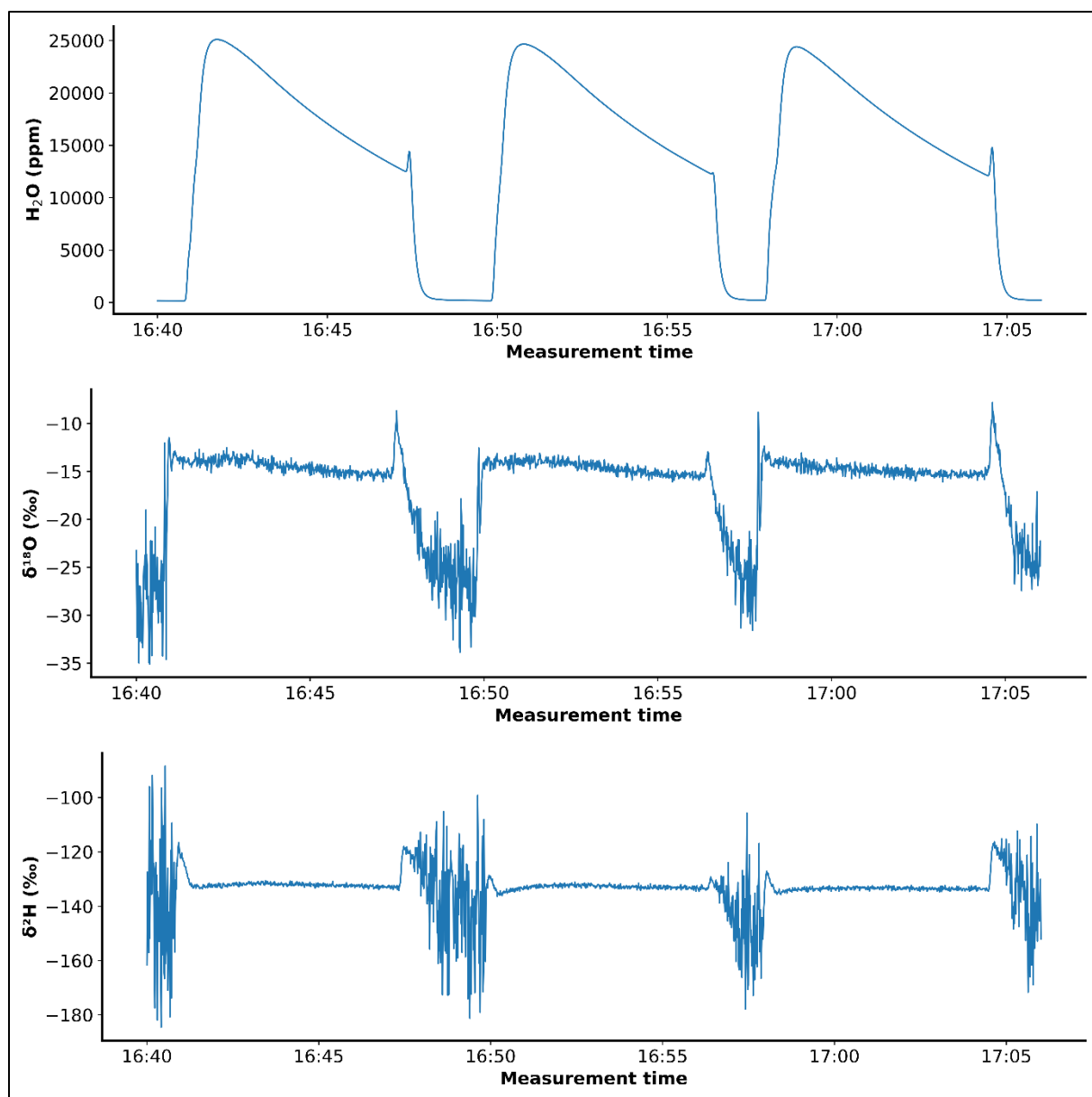


Figure S2. Water vapor measurements for the three replicates after the storage time.