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Technical note: On uncertainties in plant water isotopic composition following extraction by cryogenic vacuum distillation

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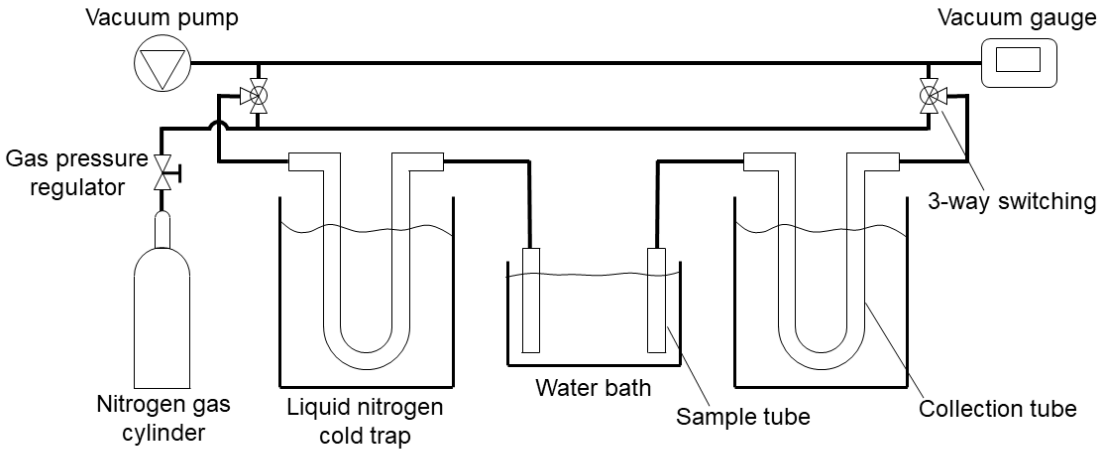

Figure S1. Schematic overview of the cryogenic vacuum distillation extraction setup. The setup is mainly composed of three units, i.e., sample unit, collection unit and pressure control unit. The sample unit includes sample tubes (12 ml Exetainer, Labco Ltd., Lampeter, UK) and a water bath (SBK 25D, Salvis AG, Reussbühl, Switzerland). The collection unit includes U-shaped collection tubes (78 ml, GlasKeller AG, Basel, Switzerland) and liquid nitrogen cold traps (Stainless steel Dewar flask, Cole-Parmer Instrument Company, Vernon Hills, IL, US). The pressure control unit includes a vacuum pump (BS2212, Brook Crompton Ltd, Doncaster, UK), a vacuum gauge (TPG 252, Balzers) and a nitrogen gas cylinder. The setup consists of four independent extraction lines, each comprising five collection units, resulting in a total of 20 extraction slots. The lines are mainly composed of different types of Swagelok fittings (Swagelok Company, Solon, OH, US), flanges, flexible hoses, and steel tubing. An Ultra-Torr vacuum adapter (SS-12-UT-A-16, Swagelok), which was welded to a welding connector (SS-10M0-1-4W, Swagelok), was used for connections between all glassware (i.e., the sample tubes and collection tubes) and the stainless-steel tubing (10 mm diameter). Rubber O-ring was inserted between the Ultra-Torr vacuum adapter and the glassware to ensure a vacuum proof connection.

Table S1. Hydrogen and oxygen isotope compositions (mean ± SD) of the materials used in the experiments

Material	δ^2H (‰)	$\delta^{18}O$ (‰)
Stem pieces	-210.00 ± 3.85*	14.39 ± 0.10
Stem powder	-211.07 ± 2.53*	14.14 ± 0.18
Stem segments	-207.63 ± 3.54*	14.14 ± 0.10
Stem cellulose powder	-177.02 ± 0.74*	17.95 ± 0.25
Twig pieces	-121.53 ± 1.34*	22.44 ± 0.21
Twig segments	-109.40 ± 2.08*	20.63 ± 0.07
Cellulose triacetate	-103.93 ± 3.81	32.66 ± 0.15
Caffeine	-144.06 ± 1.24	11.92 ± 1.79

Note: *represents the calculated δ^2H value of the non-exchangeable carbon-bound hydrogen following Schuler *et al.*, 2022. The stem materials were obtained from the xylem of a trunk disc of a mature *Larix sibirica* grown in Siberia. Twig pieces and twig segments were obtained from young *Larix decidua* trees growing in a forest in Birmensdorf, Switzerland, but not from the same month. Cellulose triacetate ($C_{40}H_{54}O_{27}$) was bought from Sigma-Aldrich (St. Louis, MO, USA, Prod. No. 22199). Caffeine ($C_8H_{10}N_4O_2$) was bought from Fluka Chemie AG (Buchs, Switzerland, Prod. No. 27600).

Table S2. The percentage of moisture that was removed from the sample at different temperatures and for different hours, and the percentage of moisture that was absorbed by the dried sample after cap opening for 5 seconds.

Material	T (°C)	The percentage of moisture removed (%)				Water vapour absorbed in 5s (%)
		12h	24h	36h	48h	
Twig piece	60	5.55±0.06 a	5.60±0.05 b	5.74±0.05 c	5.84±0.06 c	0.72±0.11
	105	8.68±0.21 a	8.89±0.12 a	8.91±0.16 a	8.89±0.08 a	1.80±0.08
Stem powder	60	5.05±0.04 a	5.21±0.04 b	5.31±0.07 c	5.33±0.05 c	0.72±0.06
	105	8.28±0.19 a	8.32±0.25 a	8.28±0.18 a	8.28±0.10 a	1.70±0.13
Caffeine	60	0.44±0.03 a	0.41±0.09 a	0.43±0.04 a	0.43±0.04 a	0.67±0.04
	105	1.50±0.15 a	1.59±0.11 a	1.62±0.09 a	1.58±0.04 a	1.53±0.09

Note: Different letters in each row indicate a statistically significance difference at $p<0.05$ (T-test)

Table S3. Summary of the linear mixed effect models to test the relationships between Δ^2H and $\Delta^{18}O$ as a function of RWC with the AWA as a random factor (AWA had 2 levels: AWA < 400 µl and AWA > 400 µl; Fig. 2) in experiment 2. The model code in R was lmer(Δ^2H (or $\Delta^{18}O$) ~ RWC+(1+RWC|AWA)).

	Δ^2H			**$\Delta^{18}O$**		
Predictors	*Estimates*	*df*	*p*	*Estimates*	*df*	*p*
Intercept	-24.31	14.00	0.386	17.28	14.00	0.254
RWC	0.76	14.00	0.195	-0.23	14.00	0.617
Random Effects						
Intercept	542.62			109.93		
RWC	0.05			0.22		
Residual	21.19			6.89		