water

MDPI

Supplementary Information

Determining Water Isotope Compositions for the IAEA WICO and North West Villages, South Africa

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WICO 2020 $\delta^{18}O$ /$\delta^{2}H$ intercomparison test laboratory report

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Analytical technique: Laser Analyzer
Reporting comments:
Comments for evaluation:

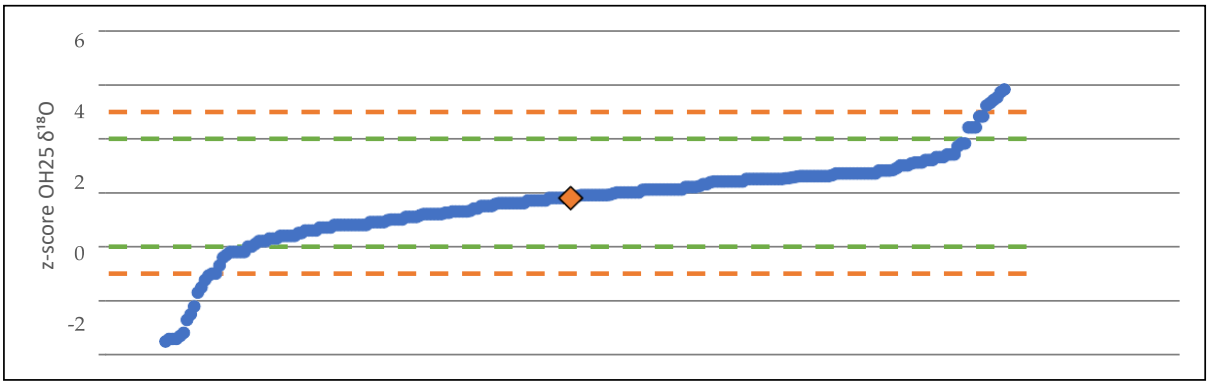
Table S1. Results $\delta^{18}O$.

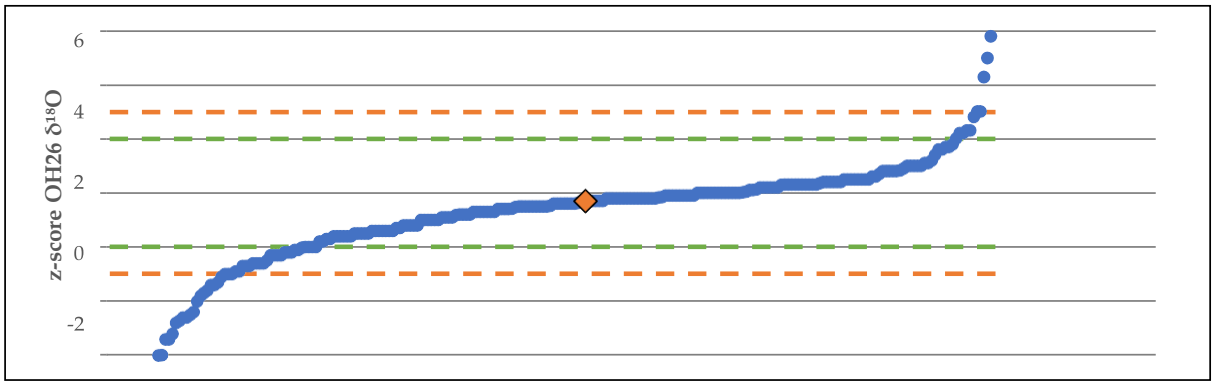
Sample	Reference Value			Submitted Result			Evaluation		Comment
	$\delta^{18}O$	Unc.	σp	$\delta^{18}O$	Unc.	D	z-test	ζ-test	
OH25	−16.98	0.01	0.10	−17.00	0.02	−0.02	−0.20	−0.89	
OH26	−11.20	0.01	0.10	−11.23	0.02	−0.03	−0.30	−1.34	
OH27	−24.89	0.02	0.10	−24.74	0.03	0.15	1.50	4.16	3
OH28	−7.95	0.02	0.10	−8.06	0.04	−0.11	−1.10	−2.46	
OH29	−1.05	0.01	0.10	−1.17	0.02	−0.12	−1.20	−5.37	3
OH30	−11.21	0.01	0.10	−11.18	0.03	0.03	0.30	0.95	

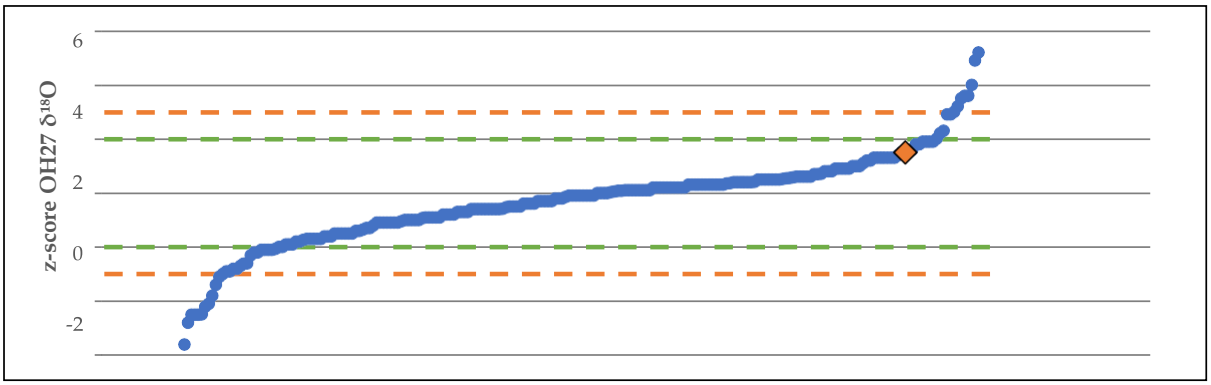
Colour Codes	Overall performance		
Satisfactory	Avg |z| $\delta^{18}O$	0.77	
Questionable	Avg |ζ| $\delta^{18}O$	2.53	6
Unsatisfactory	SD of D $\delta^{18}O$	0.10	

Comments	
3	Good accuracy and poor precision: this result has $\|z\| < 2$ and $\|\zeta\| \geq 3$; the overall performance is satisfactory, but you may have underestimated or overlooked some relevant sources of uncertainty.
6	Over-estimated precision: One or more of the samples present $\|\zeta\| \geq 3$; we suggest that you carefully review the uncertainty estimation of your measurements, especially for samples in the abundance range(s)concerned.

s-Plots δ¹⁸O, OH25-27







s-Plots δ¹⁸O, OH28-30

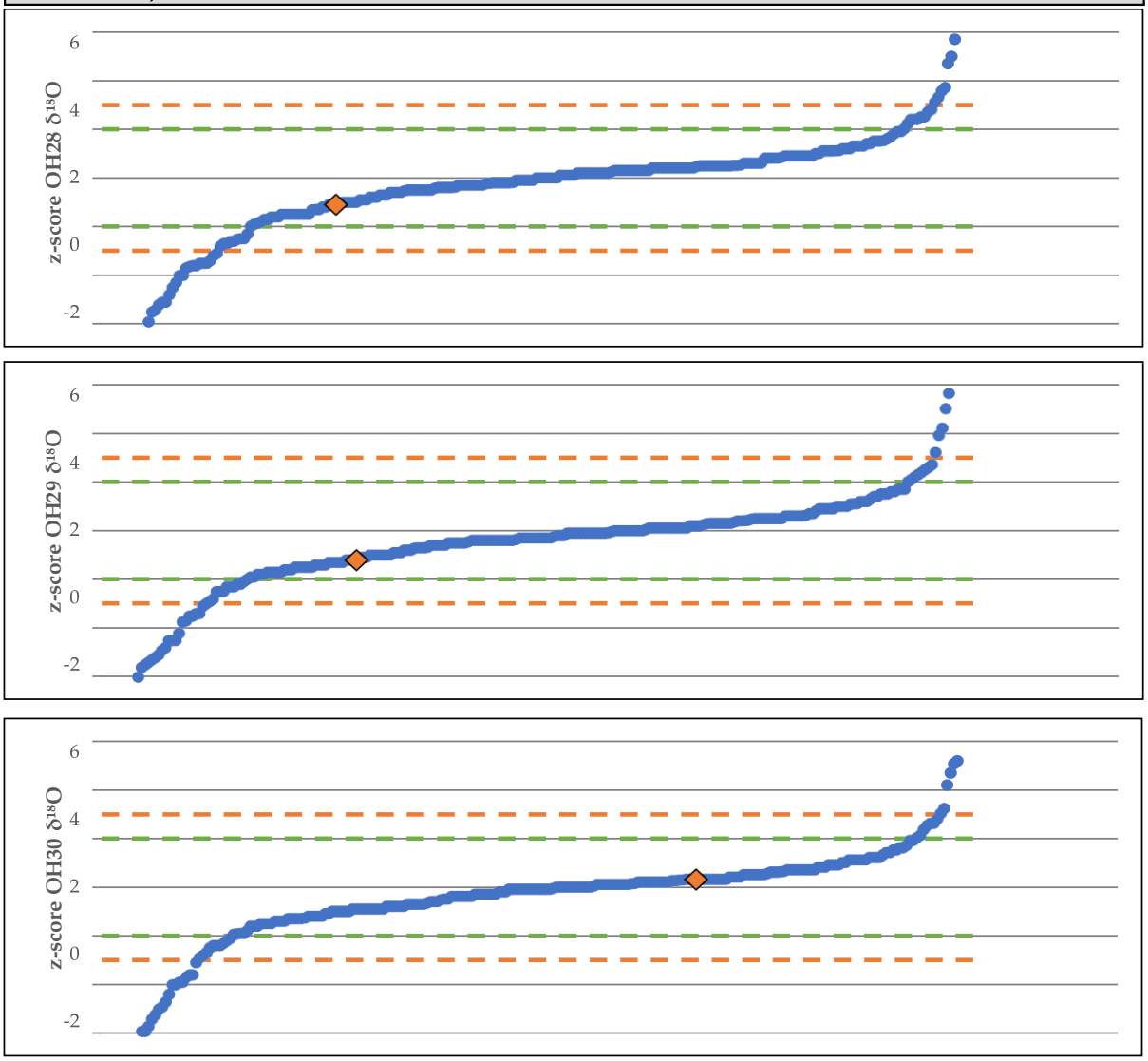


Figure S1. The s-plots vs the mean |z| score for the $\delta^{18}O$ of the IAEA WICO samples OH-28–OH-30.

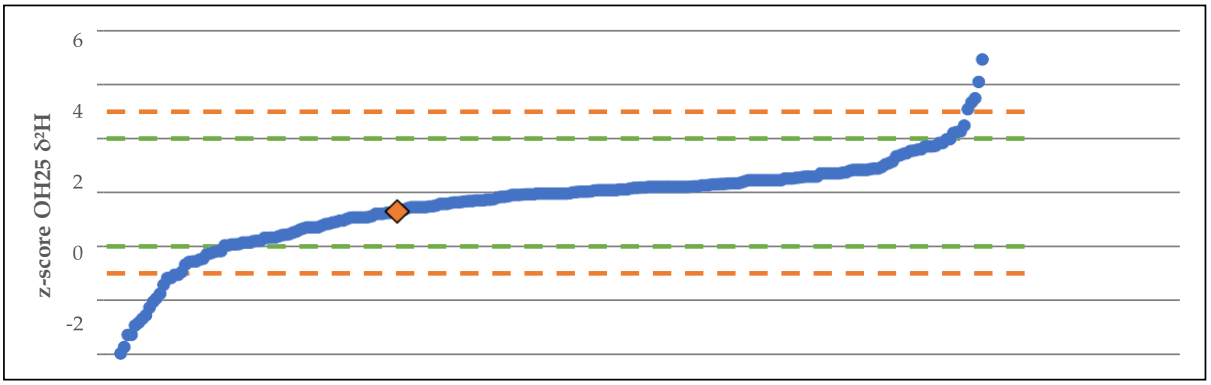
Table S2. Results δ^2H.

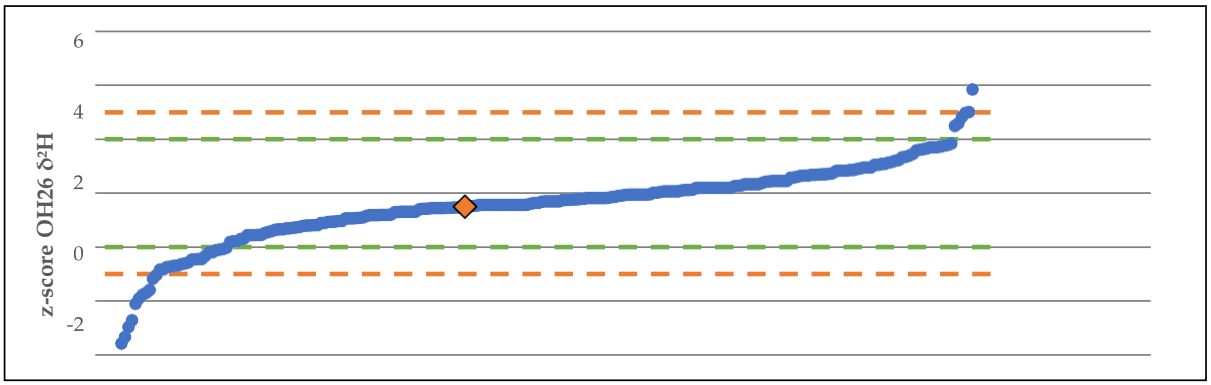
Sample	Reference Value			Submitted Result			Evaluation		Comment
	δ^2H	Unc.	σp	δ^2H	Unc.	D	z-test	ζ-test	
OH25	−129.5	0.2	0.8	−130.0	0.2	−0.6	−0.69	−1.90	
OH26	−78.1	0.2	0.8	−78.5	0.1	−0.4	−0.50	−1.83	
OH27	−190.8	0.2	0.8	−190.5	0.3	0.3	0.37	0.81	
OH28	−49.0	0.3	0.8	−50.4	0.5	−1.4	−1.79	−2.24	
OH29	1.8	0.2	0.8	1.2	0.3	−0.6	−0.78	−1.91	
OH30	−77.9	0.3	0.8	−77.6	0.2	0.3	0.41	0.91	

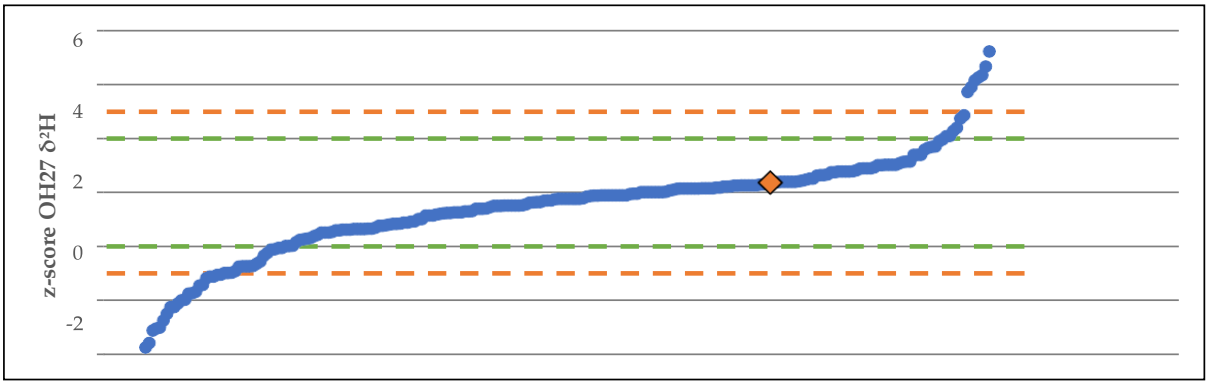
Colour Codes	Overall performance	
Satisfactory	Avg |z| δ^2H	0.76
Questionable	Avg |ζ| δ^2H	1.60
Unsatisfactory	SD of D δ^2H	0.66

Comments:

s-Plots δ²H, OH25-27







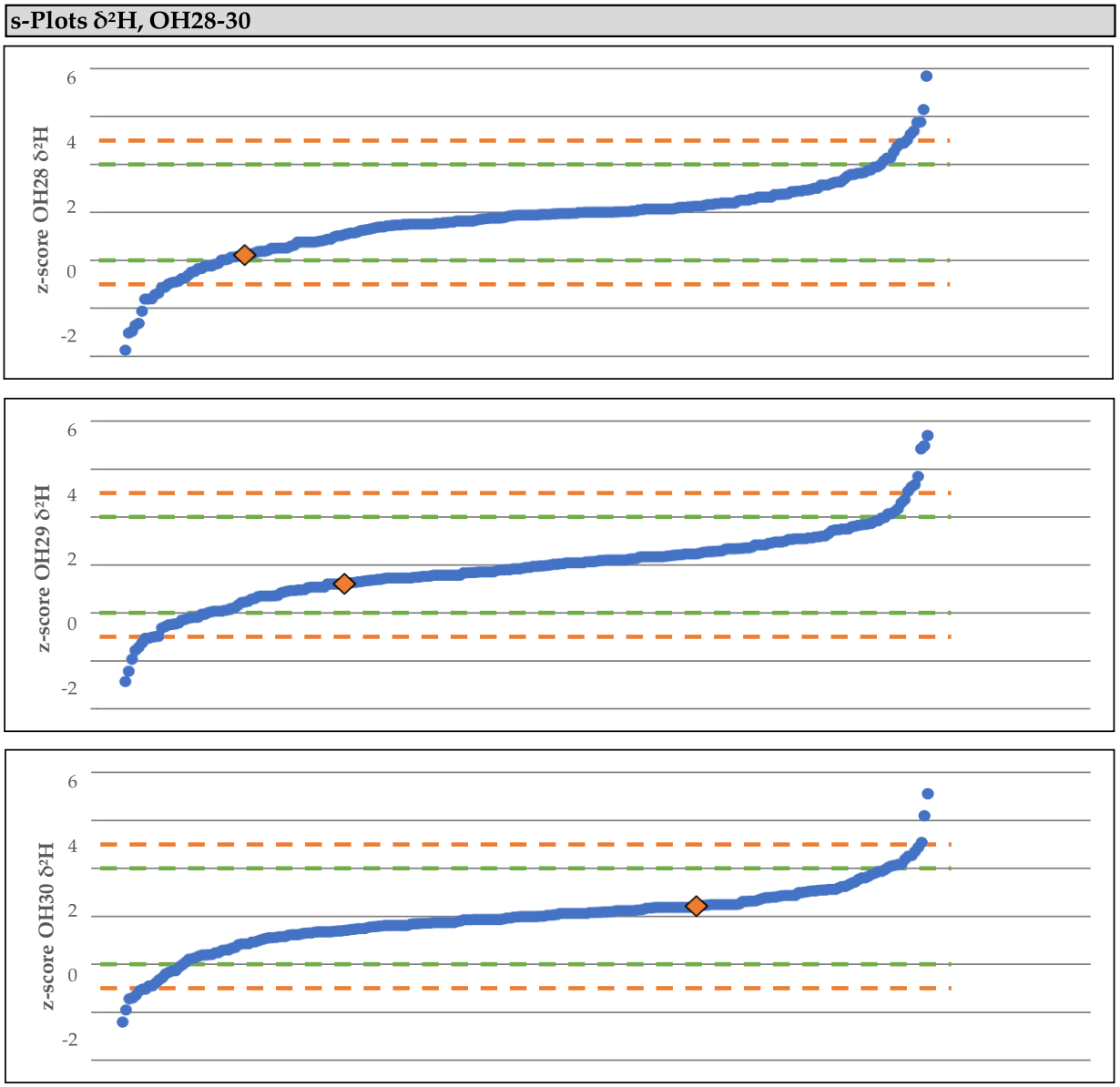


Figure S2. The s-plots vs the mean |z| score for the δ²H of the IAEA WICO samples OH-28–OH-30.

Table S3. Results d-excess.

Sample	Reference Value			Submitted Result			Evaluation		Comment
	δ²H	Unc.	σp	δ²H	Unc.	D	z-test	ζ-test	
OH25	6.4	0.2	1.1	6.0	0.3	−0.4	−0.34	−1.14	-
OH26	11.6	0.2	1.1	11.4	0.2	−0.2	−0.14	−0.57	-
OH27	8.3	0.3	1.1	7.4	0.4	−0.9	−0.80	−1.92	-
OH28	14.6	0.4	1.1	14.1	0.6	−0.5	−0.49	−0.75	-
OH29	10.2	0.2	1.1	10.6	0.3	0.3	0.30	0.92	-
OH30	11.8	0.3	1.1	11.9	0.3	0.1	0.08	0.20	-

Colour Codes	Overall performance		
Satisfactory	Avg |z| δ²H	0.36	-
Questionable	Avg |ζ| δ²H	0.92	-
Unsatisfactory	SD of D δ²H	0.45	-

Table S4. Reference Values vs. Bias - see Annex document.

	Slope	Intercept	R^2	Plot
$\delta^{18}O$	−0.011	−0.151	0.804	◎
$\delta^{2}H$	−0.005	−0.862	0.294	◎

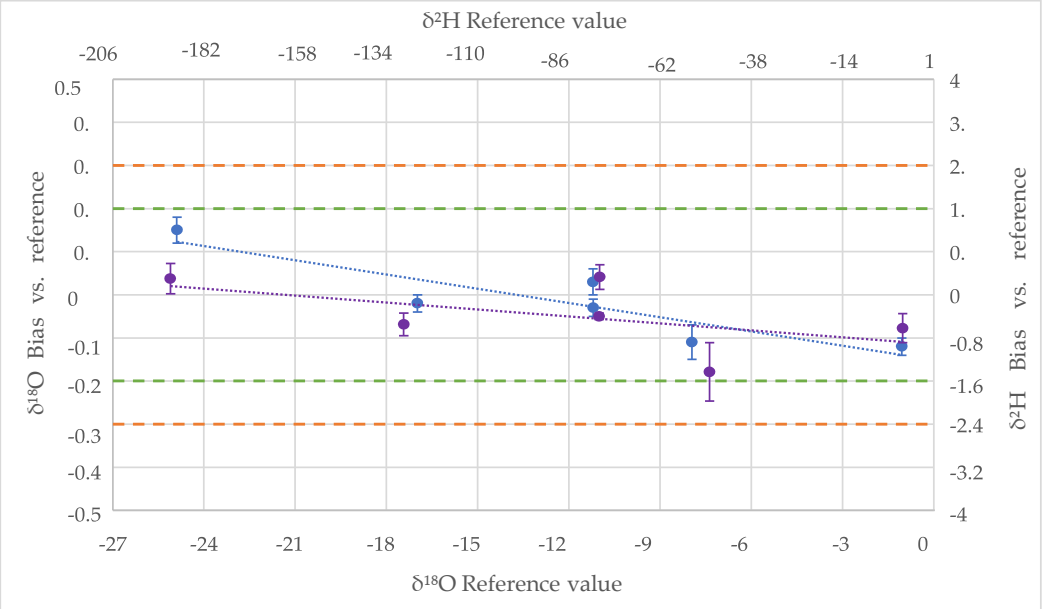


Figure S3. A plot of $\delta^{18}O$ Bias vs. reference value.

Table S5. Internal Reproducibility OH-26 vs. OH-30 - see Annex document.

Submitted Results				Submitted Results			
Sample	**Plot**	**$\delta^{18}O$**	**Unc.**	**Sample**	**Plot**	**$\delta^{2}H$**	**Unc.**
OH26	●	−11.23	0.02	OH26	●	−78.5	0.1
OH30	●	−11.18	0.03	OH30	●	−77.6	0.2
|ζ|			**1.39**	|ζ|			**3.79**

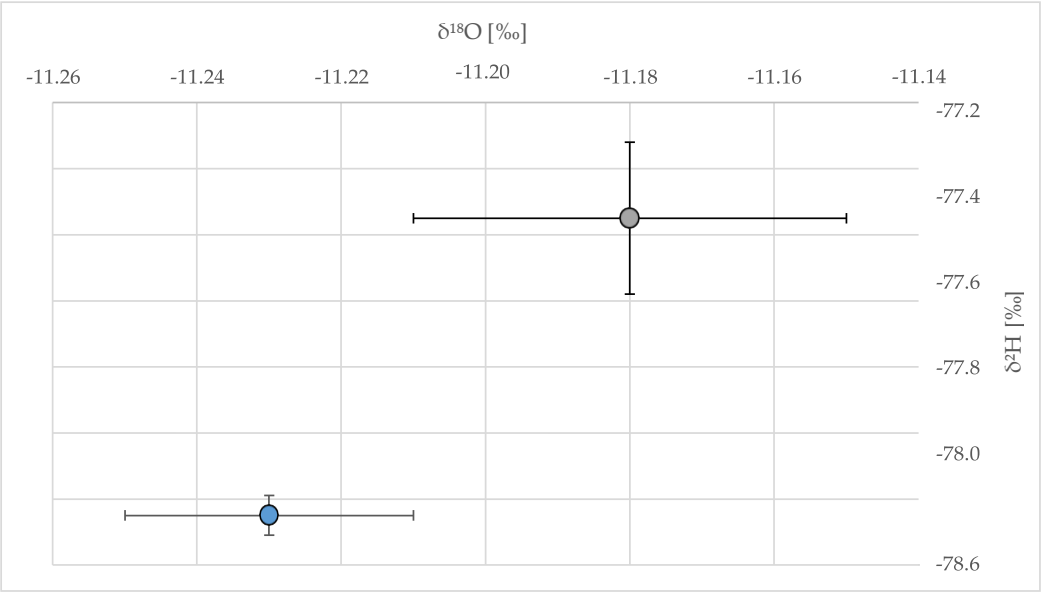


Figure S4. Plot of ^{2}H [‰] vs $\delta^{18}O$ [‰].