

Isotopic analysis

How our community analyzes soil and plant water samples for their isotopic composition

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WATSON is a network of researchers and stakeholders interest on the Critical Zone, the dynamic skin of the Earth that extends from vegetation canopy to groundwater.

WATSON collects, integrates, and synthesizes current interdisciplinary scientific knowledge on the partitioning and mixing of water in the critical zone taking advantage of the unique tracing capability of stable water isotopes.

WATSON addresses key environmental problems linked to the sustainable management of water resources.



Isotopic analysis

How our community analyzes soil and plant water samples for their isotopic composition

In 2021, we asked to our fellows in the network WATSON what are the current practices they use for stable isotope analysis of water to study vegetation water use.





This survey fed a meticulous discussion within the network WATSON, which finally brought to the production of a unified/collaborative document.

This document, has been recently published in WIREs WATER [Ceperley et al., 2024].

In this paper, we present the state of the art and review current best practices from potential sample of tree or soil in the field to value ready for interpretation, including a whole section on run arrangement and processes that was contextualized by this survey, whose results we report here.

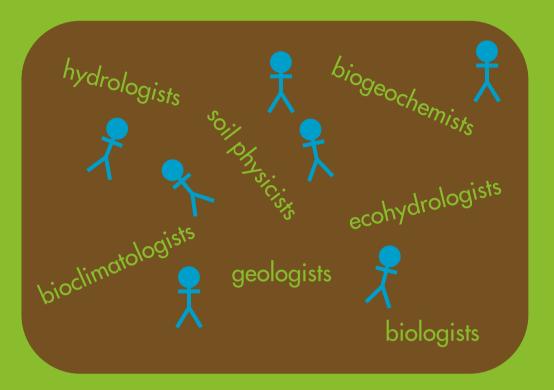
Disclaimer

The results of the survey, published in Zenodo (Ceperley & Barbeta, 2023) and reported in the following pages, are not our recommended best practices but rather an inventory of what people are doing in their laboratories.



Respondents

22 participants9 European Countries

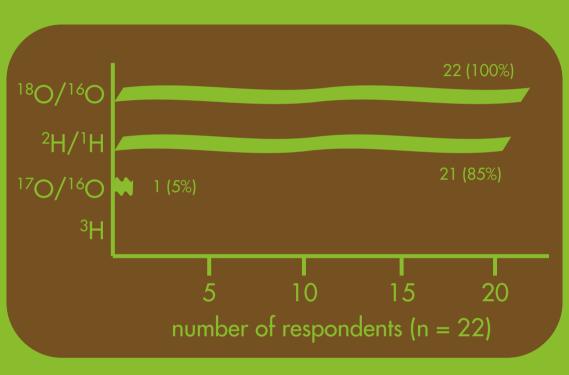






Which elements are analyzed

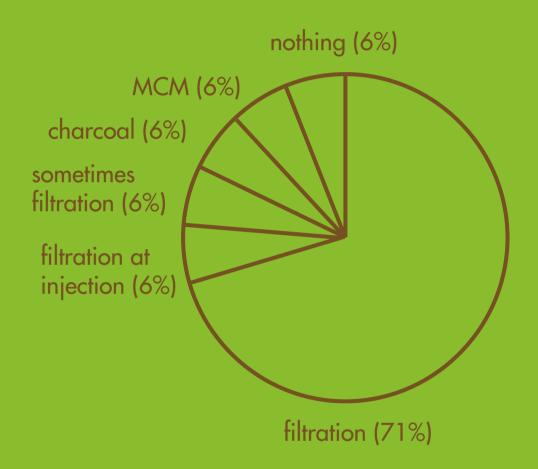
All respondents determine $\delta^{18}O$ and $\delta^{2}H$, except for one who only determines $\delta^{18}O$. One respondent determines ^{17}O .





Preparation of the samples

Filtering water before analysis is common (66%), but some groups also filter at vaporizer injection, using a micro-combustion module or activated charcoal



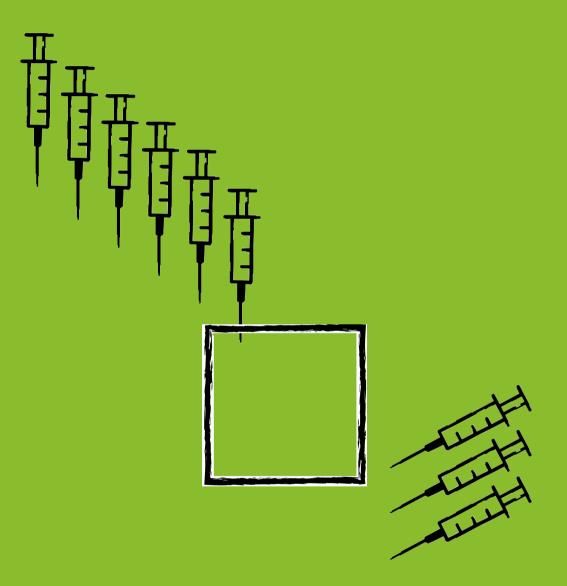
number of respondents (n = 22)



How many injections?

1/3 of participants injects the same sample 6 times 1/5 of participants injects the same sample 8 times 1 participant injects 10 times

Over half of the respondents retain the last three injections, and three keep as many as six



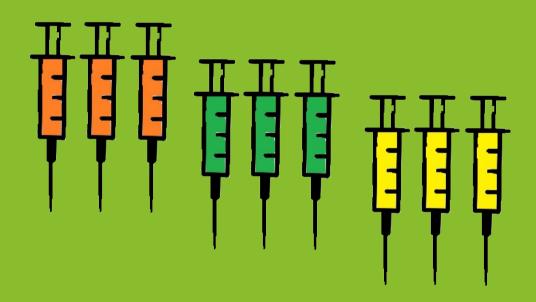


Reference materials (standards) 1

2/3 of participants use three standards Some participants use two standards One participant use six standards

All participants analyze standards in replicates distributed throughout the analytical sequence

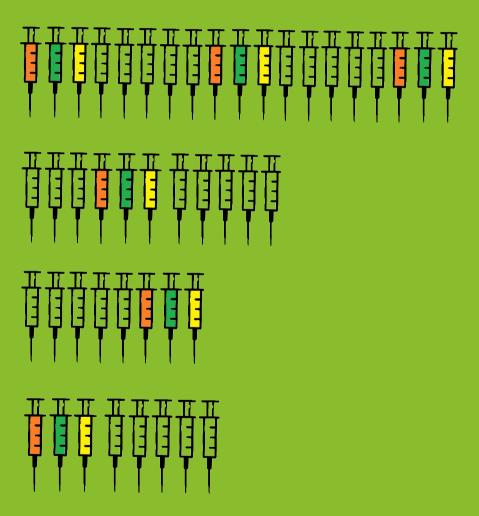
Injections of standards vary from three to ten, but between six (38%) and eight (24%) are most common.





Reference materials (standards) 2

The standards are generally distributed as a block throughout the samples (62%), but some respondents use a block of standards in the middle, the end, or more often at the beginning (43%).





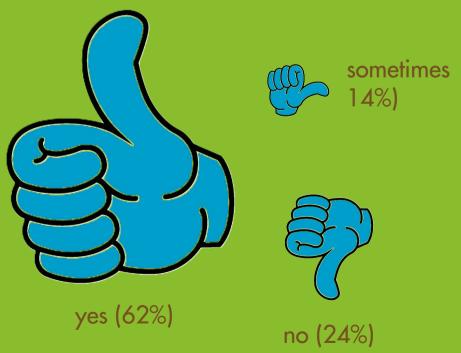
Using quality controls

Some respondents use an additional quality standard, e.g., two standards every ten samples, or another arrangement.

Half of the respondents use a drift quality control, such as deionized water; 18% do not, and 14% do sometimes.

Drift control standards are run every four to ten samples.

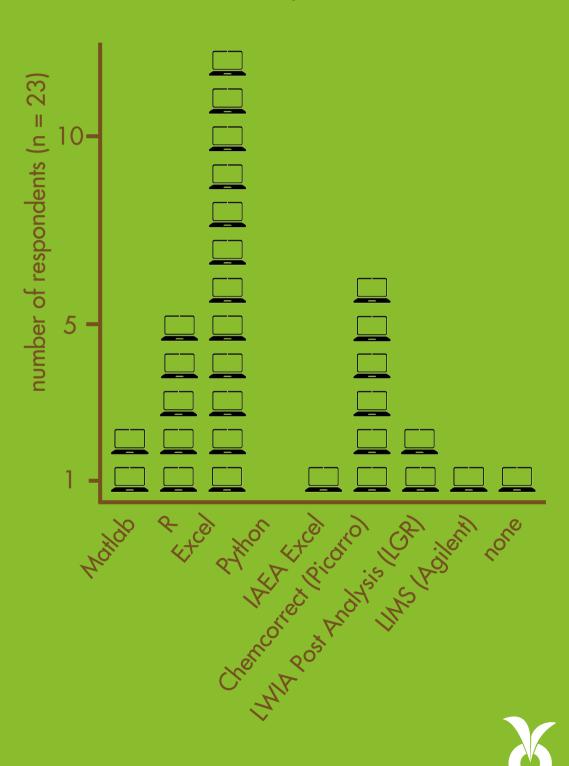
We did not survey whether respondents use a quality control standard to look at long-term changes and laboratory performance over time, as recommended by van Geldern and Barth (2012).





How do we handle data

Self-made templates in spreadsheets or scripts in R or Matlab are the most popular post-run processing tool, followed by manufacturer's tools (ChemCorrectTM by Picarro or Spectral Contamination Identifier by LGR Inc.).



Post run corrections

There seems to be no consensus about the corrections that need to be performed by post-run processing tools. Post-run processing almost always includes a standard curve adjustment according to international standards (86%), and a check for drift (67%), which is only sometimes corrected (48%, Figure 1g). Although almost half (48%) of the respondents used post-run processing to flag samples containing organic compounds, only half of them (24% of the respondents) corrected the flagged samples with post-processing algorithms.

Standard curve adjustment
Calculate uncertainty
Organic contaminant flag
Correct organic contamination
Drift Check
Drift correct
Injected volume correct

Injected volume correct

Injected volume correct

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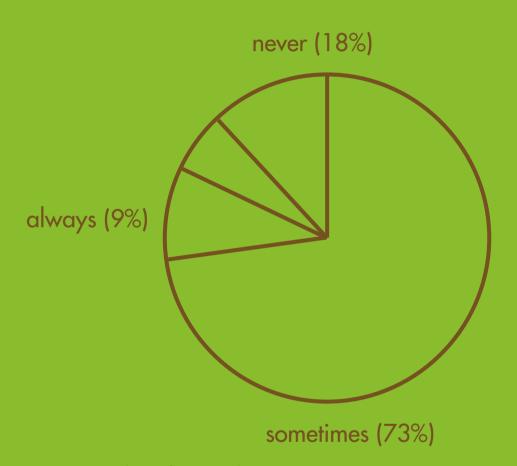
Injected volume correct

Injected volume c



Comparison among instruments

Most respondents (73%) analyzed a subset of the samples analyzed with IRIS suspected of organic contamination with IRMS.

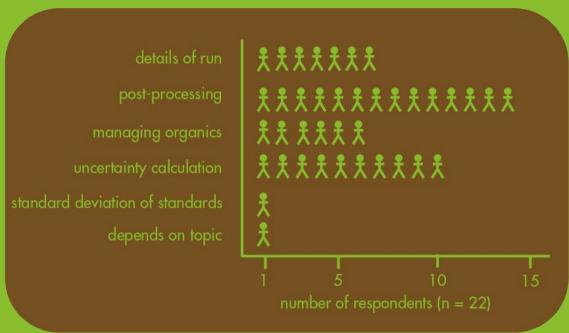


number of respondents (n = 22)



What procedure is reported in publications

Most respondents reports the details regarding post processing (71%) and uncertainty calculations (52%) in their scientific publications.





The uncertainty reported in figures

Most respondents use the standard deviation of sample injections as error bar in figures.

76%

standard deviation of kept injections

10 %

error reported by the instrument

difference between analytical and sample uncertainty

5 %standard deviation of standard injections

5 %standard deviationof replicates





WATER ISOTOPES IN THE CRITICAL ZONE

How to cite the survey

Ceperley, N., & Barbeta, A. (2023). Isotopic analysis: How our community analyzes soil and plant water samples for their isotopic composition [Data set]. Zenodo. https://doi.org/10.5281/zenodo.10125128

How to cite the paper

Ceperley, N., Gimeno, T.E., Jacobs, S.R., Beyer, M., Dubbert, M., Fischer, B., Geris, J., Holko, L., Kübert, A., Le Gall, S., Lehmann, M.M., Llorens, P., Millar, C., Penna, D., Prieto, I., Radolinski, J., Scandellari, F., Stockinger, M., Stumpp, C., Tetzlaff, D., Van Meerveld, I., Werner, C., Yildiz, O., Zuecco, G., Barbeta, A., Orlowski, N., Rothfuss, Y., 2024. Toward a common methodological framework for the sampling, extraction, and isotopic analysis of water in the Critical Zone to study vegetation water use. WIREs Water e1727. https://doi.org/10.1002/wat2.1727





To participate in the survey https://forms.gle/usjRzsVr2cyLaCZo6





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