Introducing new quality control features for stable isotope laboratories with ArDB software

Mike Seed and Michael Sudnik
Elementar UK Ltd, Cheadle Hulme, United Kingdom (info@elementar.co.uk)

ArDB is an intuitive software tool which has been created to extend the envelope of stable isotope data analysis beyond simple data processing. ArDB stands for Analytical Results Database and it allows users to simply construct, maintain and manage a database of any analytical results including results from IRMS instruments. ArDB allows users to visualize their data with 2D & 3D charts and maps reducing the need to export data to complex additional statistical or GIS software programs. Launched in 2018, the software has since found useful applications in stable isotope ecology, food authenticity and biogeochemistry.

Recently, ArDB has been expanded to offer comprehensive quality control statistics which allows the software to also be used to monitor instrument performance over short and long-time scales. Performance of both internal QC (monitoring gas tuning, stability and linearity) as well as external QC (analysis of certified reference materials, laboratory standards) are recorded and monitored so the base performance can be evaluated of multiple instruments across multiple laboratories.

ArDB performs quality control statistics calculations using the Shewart Tests which can be enabled or disabled and allow consistent testing of all data sets. However, it is not always desirable to apply the same control limits to all results, so it is possible to independently assign different criteria for individual quality controls. Individual quality control criteria can be set at an administrator level so that basic operators can not manipulate results.

It is also possible for ArDB to group records together and to then apply quality control statistics to each group independently which allows for comparison of results across discrete time periods or of one instrument versus another. This makes it easier for the analyst to detect any changes in performance and so ensure that any corrective action is performed before data is compromised.

One significant advantage of utilising ArDB for creating a database of analytical results as well as performing instrument quality control is to be able to validate the results of new/unknown samples in ArDB. By being able to scrutinise internal and external QC results alongside sample data allows the analyst to ensure that only robust data is used for the on-going research themes that they are pursuing.