INTRODUCING ANALYTICAL RESULT DATABASE (ArDB): INTUITIVE DATABASE MANAGEMENT, DATA VISUALISATION AND QUALITY CONTROL

M. Sudnik¹, K. W. R. Taylor¹, M. Seed¹

¹Elementar UK Ltd, United Kingdom

Analytical Results Database (ArDB) is an intuitive software tool developed by Elementar UK which has been created to extend the envelope of analytical data analysis beyond simple data processing. Ultimately, ArDB simplifies and centralises the management of data, a particularly critical issue when generating large quantities of data associated with high-resolution and/or high-throughput analysis.

ArDB allows users to simply construct or import, maintain and manage their databases of any analytical results, including (but not limited to) results from stable isotope, elemental, and total organic carbon analysis 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. Statistical transformations such as linear discriminant analysis (LDA) and principle component analysis (PCA) are available to generate predictive models against which unknown samples can be tested, whilst compatibility with R ensures further extended statistical analysis is also possible. Launched in 2018, the software has since been utilised by analysts with applications in ecology, food authenticity and biogeochemistry.

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

ArDB performs QC statistics calculations using the Shewart Tests, which can be enabled or disabled, allowing consistent testing of all data sets. However, it is not always desirable to apply the same control limits to all results, so it is also possible to independently assign different criteria for individual quality controls. Individual QC criteria can be set at an administrator level so that basic operators cannot make unauthorised alterations, ensuring a secure controlled data management environment. It is also possible for ArDB to group records together and to then apply QC statistics to each group independently, allowing for comparison of results e.g. across discrete time periods, or between individual instruments. This makes it easier for the analyst to detect any changes in instrument performance, or issues with the quality of the materials/standards being measured, and thus to 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 QC evaluation is to be able to validate the results of new/unknown samples in ArDB, and to demonstrate quantifiable confidence in the database data. By being able to scrutinise internal and external QC results alongside sample data allows the analyst to ensure that only robust qualified data is accepted for population of their databases, and ultimately that the data used for the ongoing research themes they are pursuing is demonstrably robust and reliable.