

ArDB Introduction

July 2017

IRMS

Langenselbold, Germany



What is ArDB?



ArDB

- ArDB stands for
Analytical Results Database
- It is a piece of software that
 - Allows the creation of a database of results
 - Manages the data
 - Combines the analytical results with the sample meta data
 - Visualizes the data into easily created plots

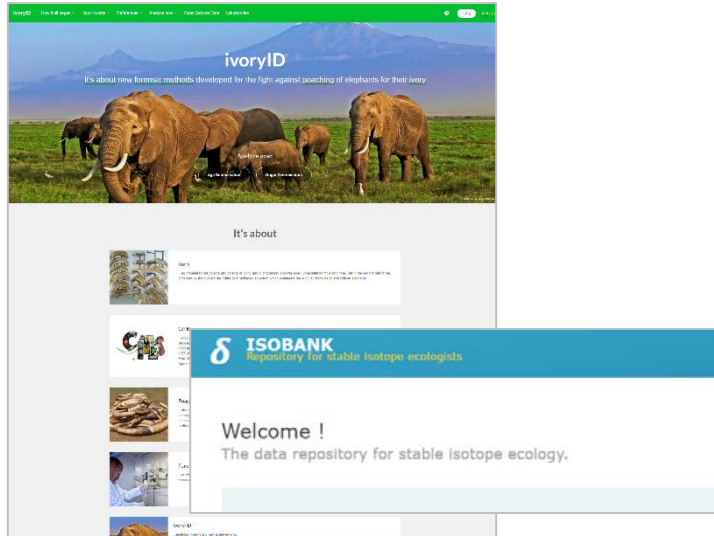
Why do we need ArDB?



ArDB

- ArDB is a completely new offer from an IRMS company
- ArDB allows us to extend our offer to our customers beyond the raw IRMS results.
- We are routinely asked for supplying a database to our customers in certain applications
 - BiovisION – Database of known wines
- **We cannot supply databases of known sample results**
- ArDB is the next best thing – a tool to create the database

Why do we need ArDB?



- There are several examples of groups of people who are trying to create open access databases
- These tend to be generated by academics
- They are commonly designed around a single application
- We want to bring the ability to create databases to private industry
- We want to generate a universal piece of software that can be used for all applications



What is ArDB?



ArDB

- Isotope Ratio Mass Spectrometry is fundamentally about comparing unknowns with knowns
- Therefore, users must build a database of “knowns” to query against
- Is a wine from Bordeaux?
- Is your beef from Korea or Japan?
- Is green tea from India or China?

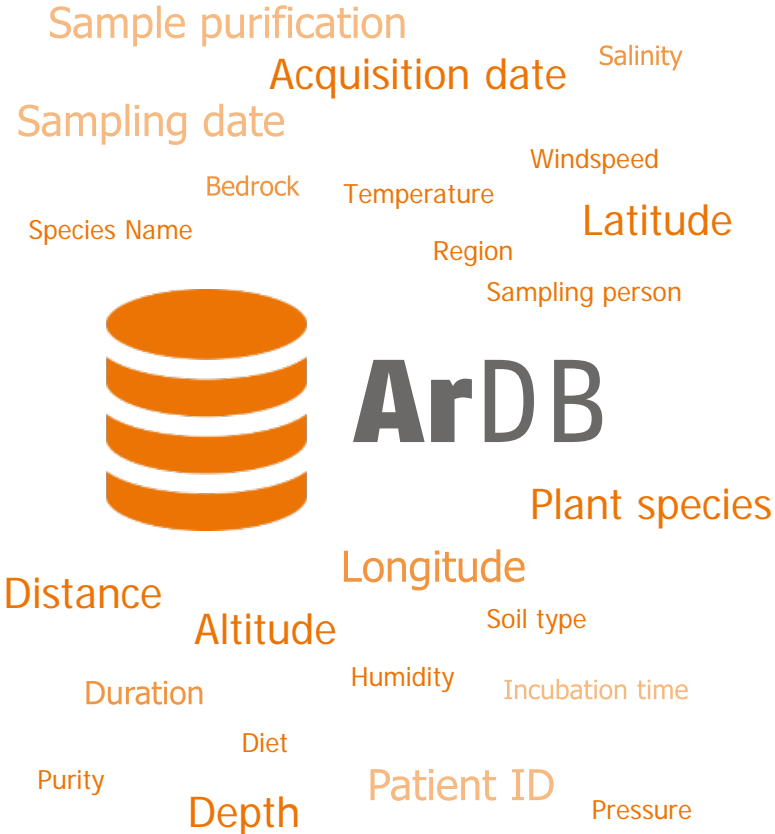
What is ArDB?



ArDB

- Users should build their own database of known samples
- Once they have their database, ArDB is able to organise and visualize their data
- ArDB is then able to look for similar samples in the database
- ArDB was conceived as a solution to improve our offer to food forensics labs, but it is applicable to all application areas

Data Construction & Population



We have created **ArDB software** to extend our software offering beyond just generating a delta value



ArDB allows IRMS results to be interrogated alongside the corresponding metadata, and search for comparisons



Metadata is created and planned before sampling



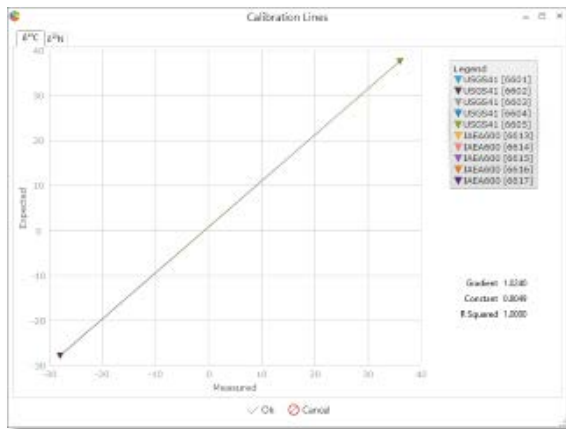
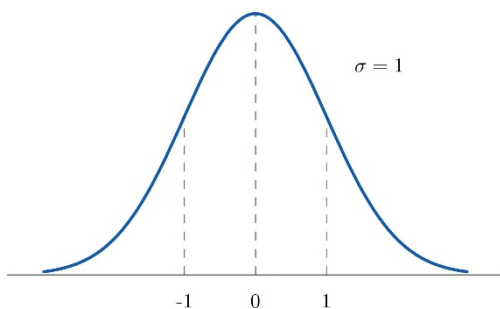
Therefore, ArDB is not just a “post-analysis” tool

IonOS and ArDB



- ArDB is a natural progression from IonOS
- Because IonOS is able to generate multi-point isotope calibration, we are able to pass the calibrated results into ArDB
- Sample data comparisons must only be done on calibrated data
- Therefore, ArDB is a logical conclusion to the work that we have done in IonOS

Data Interrogation



- ArDB demands that all samples are calibrated correctly
i.e. IonOS passes in only calibrated data
- Assumes that results are normally distributed. We are implementing custom distributions
- Is extendable to include other data types, not just stable isotope results
e.g. ICP-MS, Sr isotopes, etc...
- ArDB offers an integration with R statistics – a commonly used, open source stats package (<https://www.r-project.org/>)

GNIP brochure.pdf

Global Network of Isotopes in Precipitation

The Johannesburg Plan of Implementation from the World Summit on Sustainable Development concluded there is an urgent need to expand scientific information to improve understanding of the water cycle. Over the last 50 years, data from the Global Network of Isotopes in Precipitation (GNIP) have become an increasingly important tool to meet these information needs, providing unique insights into hydrological and climatic processes at the local, regional and global scales.



Schematic representation of the water cycle.

While water looks the same everywhere, it carries isotopic 'fingerprints' which can be used to determine its origin and age. Isotopes are atoms of the same element with different weights.

Across the globe, proportions of isotopes in water molecules in precipitation vary as a result of natural processes of evaporation and condensation, and because of the effects of temperature and altitude. Consequently, precipitation in each location has its own isotopic 'signature' or 'fingerprint'. These isotopic 'fingerprints' are carried into groundwater and can be used to determine the age, recharge rates, and flow velocities of groundwater.

Through study of water isotopes 'naturally archived' in polar ice caps, lake sediments, and groundwater, past hydrological conditions can be reconstructed. Understanding how past hydrological and climate systems have changed over time holds the key to predicting future change — looking 'back to the future' — to develop options for minimizing the adverse effects of the world's changing climate.

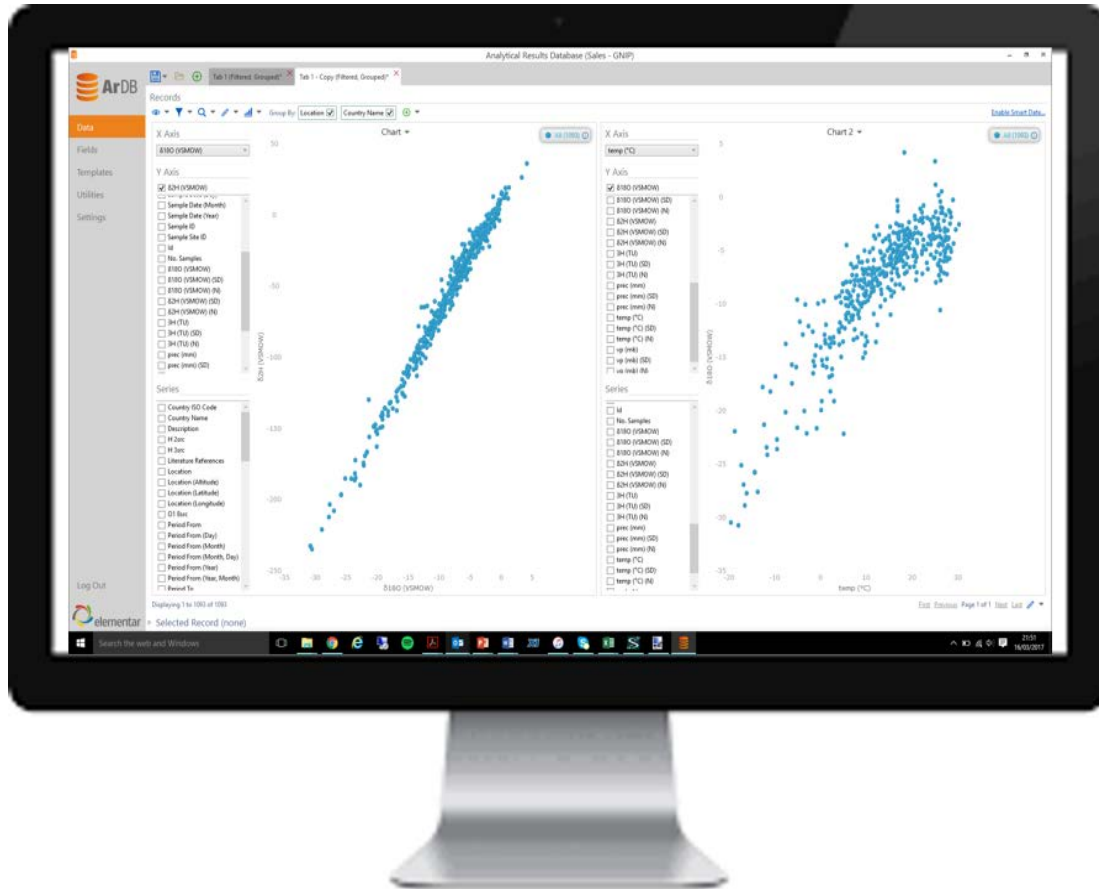
IAEA Water Resources Programme

"Human survival and the quality of life... will always be inextricably tied to the availability of fresh water"

Mohammed ElBaradei
IAEA Director General

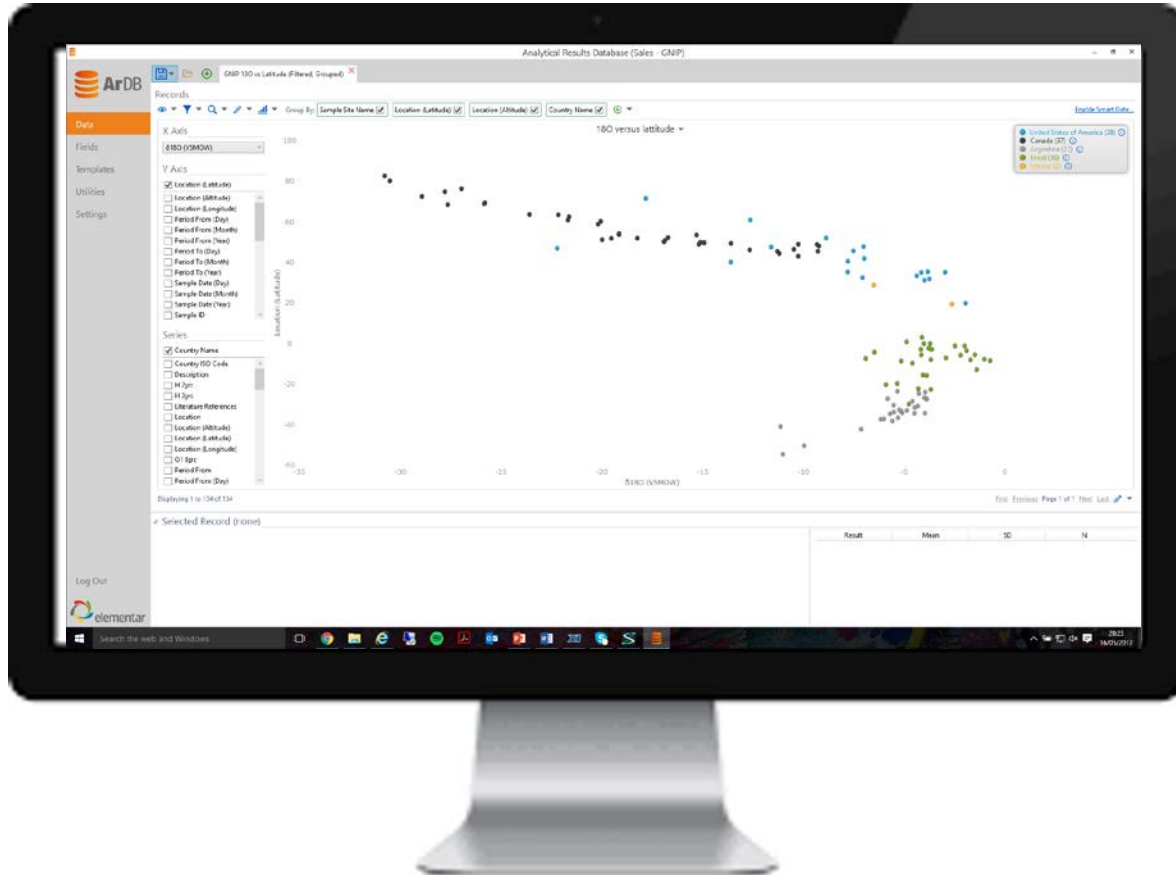
- ArDB will be supplied with a snapshot of the Global Network of Isotopes in Precipitation database
- IAEA/WMO (2016). Global Network of Isotopes in Precipitation. The GNIP Database. Accessible at: <http://www.iaea.org/water>
- Over 125,000 data points in the database
- ArDB is able to process, filter and render the data extremely quickly
- GNIP database is used by many customers to relate samples to local precipitation isotope values

What does it look like?



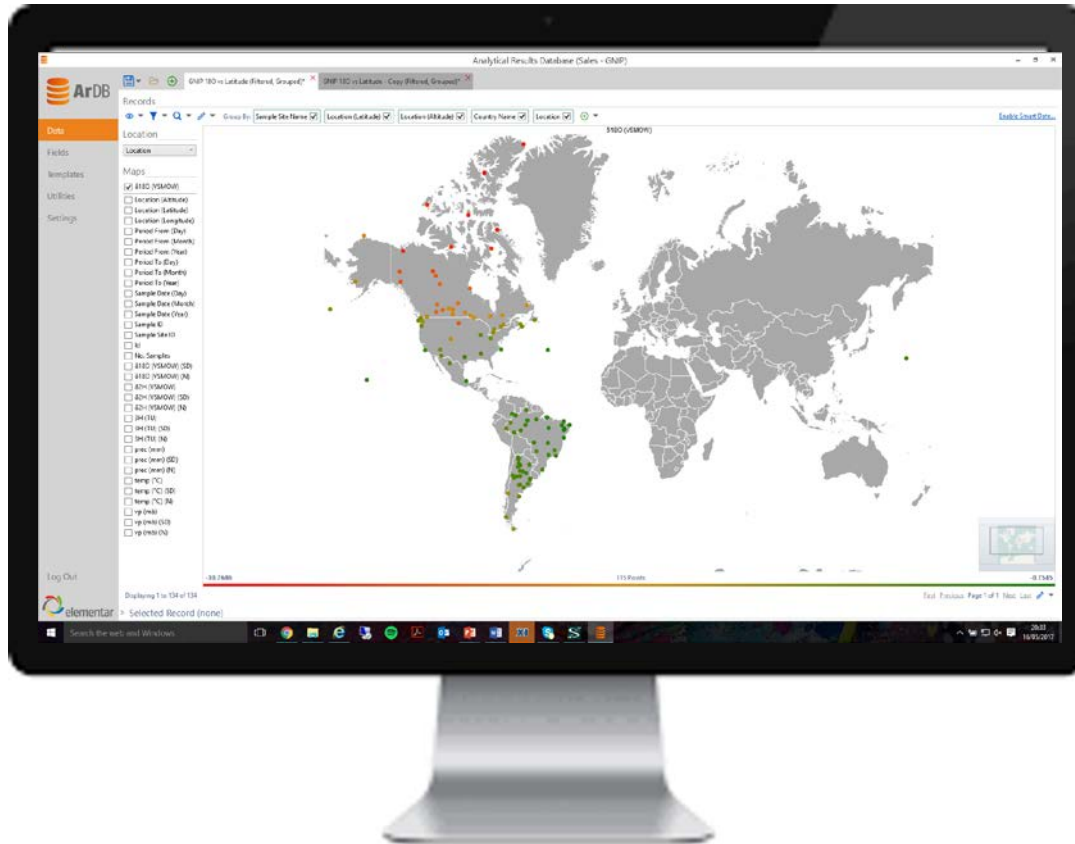
- Plot of hydrogen versus oxygen isotopes of global rainwater samples (left)
- Plot of oxygen isotopes with temperature (right)

What does it look like?



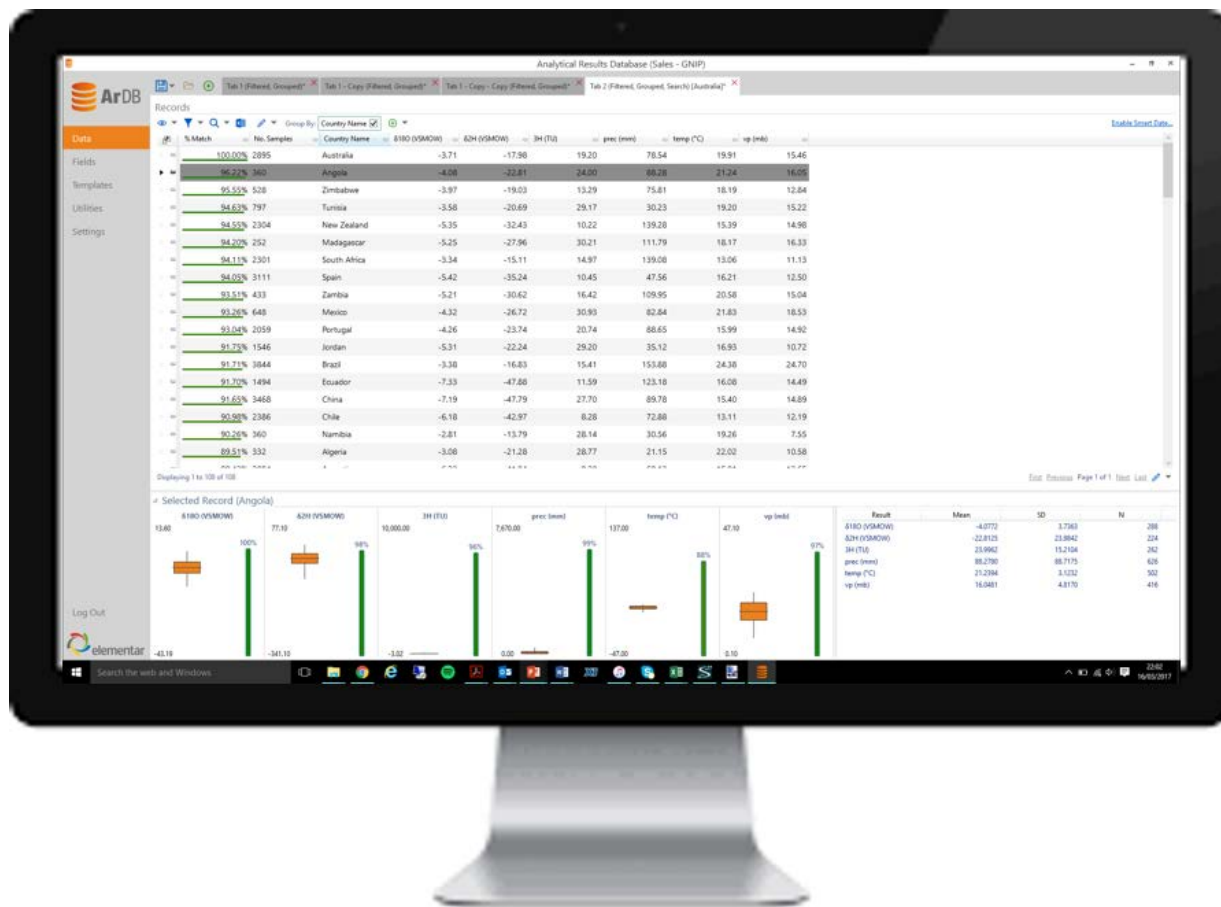
- Here is a plot of oxygen isotopes of global rainwater samples versus latitude
- Shows the variation in ^{18}O across the Americas

What does it look like?



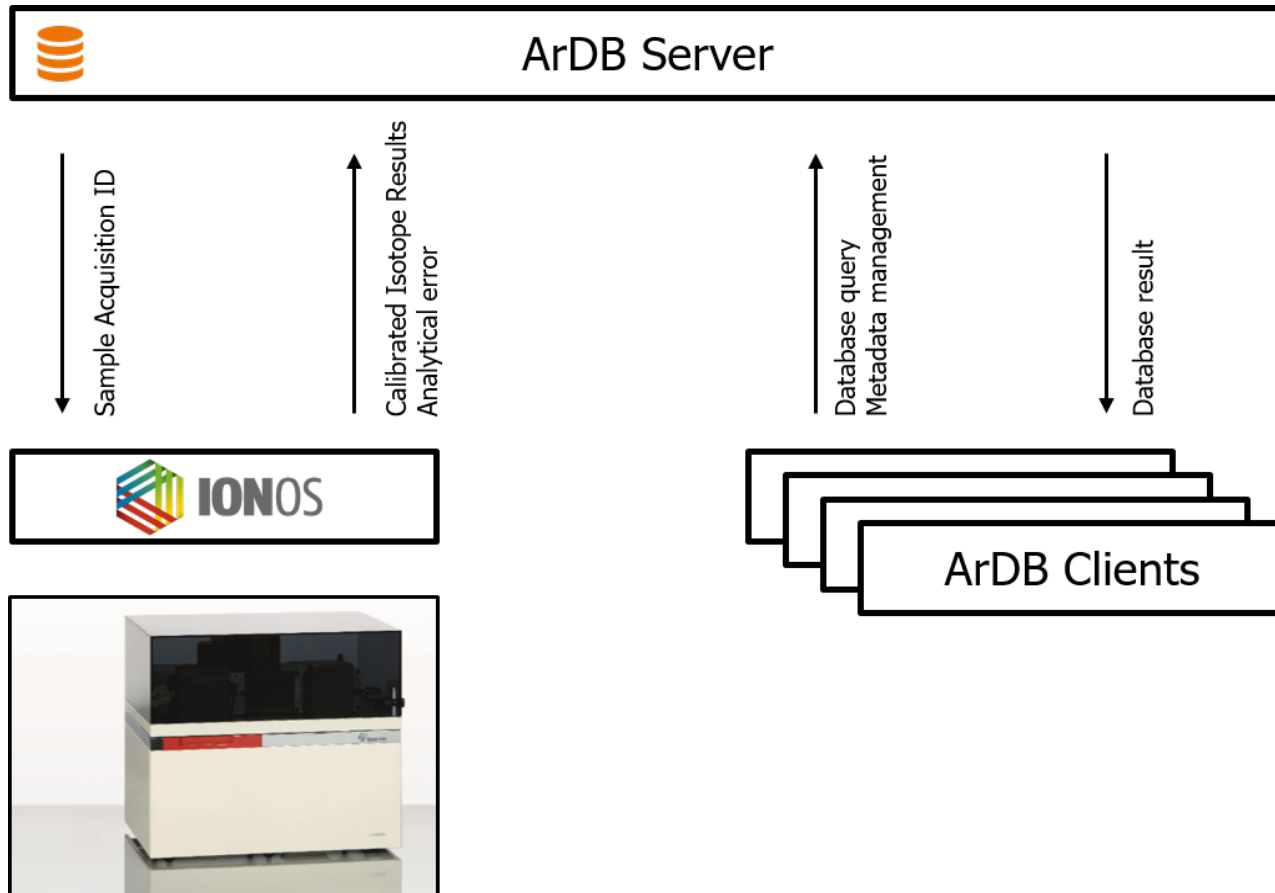
- This is the same data from the chart but plotted on the map
- Color scale demonstrates the 180 value

What does it look like?



- Here is a comparison of a unknown sample to a data base
- % Similarity is Hellinger distance assuming a normal distribution

ArDB Interfaces



ArDB License options

Fully private instance

- Run on a private network
- All clients must have access to that network
- Unlimited database size
- 5 client licenses
- ArDB installed on a local server
- Client licenses installed as required on other workstations

Cloud based private instance

- Cloud based ArDB server
- Database hosted in the cloud running on Elementar server
- Clients need access to the internet to query the database
- Costs dependent on database size and number of clients

Phase 2

ArDB License options – customer dependent

Fully private instance

- Preferred by private companies
- Want to be in control and to protect their data
- This is the version that has had most interest so far

Cloud based private instance

- Preferred by academia
- Should be possible for people to collaborate across the globe on a single research project
- Provide a shared environment to plan, organise and implement sample analysis and interpretation



www.elementar.co.uk