"Easotope": Software for managing and processing isotope data

D. BOWEN[1]* AND C. M. JOHN[2]

[1]Ziggurat GmbH, Stäfa, Switzerland (*correspondence: devon@easotope.org)
[2]Imperial College London, South Kensington Campus, London SW7 2AZ, UK (cedric.john@imperial.ac.uk)

Recent advances in isotope science, such as clumped isotope geochemistry, have pushed mass spectrometers to the limits of their precision. As a result, the search for new techniques to correct data has become fertile ground for researchers. These techniques often require calculations based on a large number of replicate analysis of standards run over long periods of time by different operators.

To implement correction algorithms, labs have resorted to using a variety of approaches, most often involving Excel spreadsheets or MATLAB routines. But because of the long time-ranges and the large volume of data, these methods can become unwieldy and error-prone, especially when maintained by many researchers of varying experience working on the same mass spectrometer. "Easotope" is a free, multi-platform, client-server application designed to overcome these problems.

Easotope allows users to drag and drop their raw files directly from the computer controlling the mass spectrometer, organize them by project, and archive them on the server. The sample runs remain private, whereas common standard runs are organized automatically by type and are publicly visible to all users. This allows all correction data to be shared.

After entry, data is automatically corrected and processed according to configurable settings and results are immediately presented in user-configurable tables. The user may then choose to look more deeply at the correction steps by viewing graphs and tables that make each step easy to follow and understand.

Although Easotope has been developed to specifically address the problems of the CO_2 clumped isotope community, the software has been designed from the beginning to be flexible and extensible. Adding support for new isotopic systems is relatively easy as is developing new correction algorithms and calculations. We hope that this will allow Easotope to be useful to the isotope community at large and to grow as the science advances.