Goldschmidt 2024 Abstract
https://doi.org/10.46247/gold2024.22947

An R Shiny graphical user interface for analyzing, visualizing, and interpreting high-precision mass spectrometric data

ELIZABETH D LABONE, KYLE M SAMPERTON, SHELBY BOWDEN AND ALEXIS T RICHE

Savannah River National Laboratory

Presenting Author: elizabeth.labone@srnl.doe.gov

We have developed an R package centered on a graphical user interface (GUI) for analyzing high-precision mass spectrometric data. The academic geoscientific community has supported the development of innovative, discipline-specific software suites for mass spectrometry data processing (e.g., Tripoli and ET_Redux [1,2] for U-Pb geochronology) and popular statistical toolboxes (e.g., IsoplotR [3]). However, there is currently a lack of advanced, generalized software for the complete analysis of raw data produced by modern isotope ratio mass spectrometers, including multicollector—inductively coupled plasma—mass spectrometry (MC-ICP-MS) and thermal ionization mass spectrometry (TIMS). This work aims to fill this gap with a GUI accessible to those without programming experience, written in the open source and multi-platform programming language R. The "point-and-click" GUI was written using the Shiny GUI development package and Golem framework for production-grade Shiny applications, the latter of which includes the testing and documentation standards for R packages. The GUI will guide a user with no programming experience through the process of uploading and analyzing their data in a statistically rigorous and standardized method. The software is compatible with raw data file types and structures generated by different MS platforms (TIMS and MC-ICP-MS) and different instrument manufacturers (Nu Instruments, Thermo Scientific, Isotopx). Analyses include calculating isotope ratios; calibrating data based on standard analyses; uncertainty propagation and evaluation; and isotope dilution. A major thrust of the work is accommodating both metrologically-traceable compositional quantities and relative compositions depending on the use case, including both actinide and (non)traditional stable isotope systems. Once the user completes their data analysis, publication-quality graphics and tables can be output and saved from the GUI framework.

[1] Bowring et al., 2011, Geochemistry, Geophysics, Geosystems 12(6). [2] McLean et al., 2011, Geochemistry, Geophysics, Geosystems 12(6). [3] Vermeesch, 2018, Geoscience Frontiers 9(5).