Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.20476

A web-based open tool for boron isotope reduction from mass spectrometry

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In recent years, the technique for measuring boron isotopes has undergone significant development and has gained lots of attention. Despite this progress, there is currently no specific tool available for boron isotope data reduction.

We have established a boron isotope measuring method for low B contents in the FIERCE laboratories (Frankfurt Isotope and Element Research Center), in which laser ablation is combined with a Neptune mass spectrometer for boron isotope analysis. The data processing currently works through an adapted excel spreadsheet otherwise used for U-Pb dating. Such adaptations are routinely done, but have many shortcomings, such as only being compatible with Windows systems, no documentation, only one or few persons who knows how this works, no real manual, insufficient and no scalable visualizations.

We translated and expanded the existing excel boron data reduction tool into a Python program. The code has been implemented into a web-based Streamlit app, which can be accessed at https://boron-reduction.streamlit.app/ or at geoplatform.de (go to Mass Spectrometry, and on the sidebar select Boron). The entire codebase has been made available on GitHub, along with a comprehensive Quarto documentation on how to use the program, and how the program works. With this online tool, users can easily upload their own data and perform boron isotope data reduction, as it is easily accessible by the global isotope community through only a browser. We hope that this case study will help the transition from isolated local data processing solutions towards open and reproducible research software following FAIR (Findable, Accessible, Interoperable, Reproducable) principles for mass spectrometer laboratories.