Tripoli: New Software Tools for Interactive TIMS and MC-ICPMS Data Reduction and Uncertainty Estimation

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High-precision isotope ratio analysis via TIMS and MC-ICPMS provides the foundation for modern geochronology and radiogenic isotope geochemistry. However, the software used to process this critical data often lacks statistical rigor and the interactivity needed for data exploration and discovery. Statistical problems include potentially underestimating uncertainties due to ignoring contributions from baseline measurements and/or beam interpolation. To address these challenges, we have developed Tripoli, a new data reduction platform built on a philosophy of open source design. Tripoli processes raw mass spectrometry data using modern statistical algorithms, provides interactive visualizations for data interrogation, and exports results formatted for established laboratory workflows.

We have focused our software development on two fronts. The first is a complete rebuild of our original Triopoli software (Bowring et al., 2011) with a modernized statistical backend, full cross-platform support, and enhanced graphical capabilities. The second is a novel Markov Chain Monte Carlo algorithm for mass spectrometry data that models static and time-varying mass spectrometer parameters like isotopic fractionation, peak tails, collector relative efficiencies, baselines, and dead times across multiple sequences.

Current development focuses on real-time data ingestion, which improves throughput by helping decide when to stop one analysis and start the next. Exported data, such as isotope ratio means and uncertainties, are available in user-customizable delimited text files and other application-specific formats. Reduced data from multiple analyses can be saved and interpreted together in a “session,” facilitating data compilation and interpretation at a level larger than a single analysis. We encourage community participation in the project through our GitHub and upcoming community workshops.

Bowring, McLean, and Bowring (2011), *Geochem. Geophys. Geosyst.*, 12, doi:10.1029/2010GC003479.