

# Open-source Data Processing in Stable Isotope Ratio Mass Spectrometry

## New Software Packages for Efficient, Transparent and Reproducible IRMS Data Reduction

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For questions/feedback/feature requests, please contact [sebastian.kopf@colorado.edu](mailto:sebastian.kopf@colorado.edu) or create a new issue at <https://github.com/KopfLab/isoreader/issues>

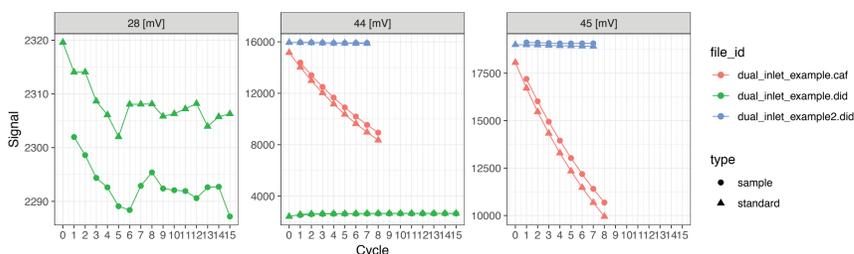
The key to reproducible data reduction and data processing in scientific research is the ability to faithfully record every step of the process in a reproducible format that is transparent and easy to communicate. This is not an easy task. Most of the time in experimental research that is not primarily computational in nature, it falls victim to the enormous effort required to design experiments well, run complex analytical procedures rigorously and efficiently, and interpret the results in the proper geologic, geochemical or biological context, with little time left to invest in documenting and constructing a reproducible data reduction workflow. While this is understandable, it introduces a high risk for error, makes it extremely difficult to share and discuss one's approach or review others', reproduce the calculations at a later point or even just revisit what was done conceptually. One important obstacle that interferes frequently with attempts to remedy this situation in the stable isotope community is the lack of many basic computational and data access tools that enable the kinds of calculations and data processing isotope geochemists need to do on a day to day basis. Here, we introduce a new suite of **open-source** software packages that provide efficient and transparent access to raw stable isotope ratio mass spectrometry (IRMS) data formats and enable reproducible data processing straight from raw analytical output through data reduction, quality control, visualization and data reporting that retains the necessary flexibility required for the enormous breadth of analytical goals in the stable isotope community.

### 2 Aggregate file Information

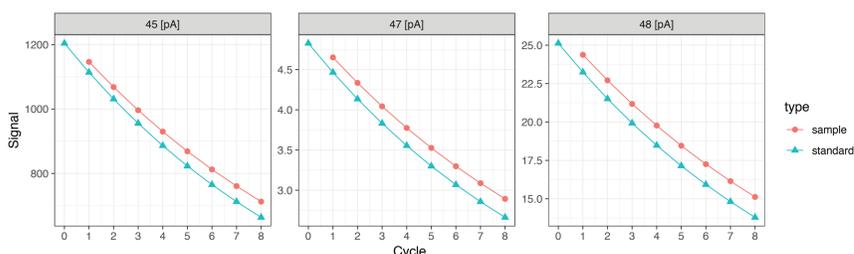
- `iso_get_data_summary()`
- `iso_get_problems()`
- `iso_get_raw_data()`
- `iso_get_file_info()`
- `iso_get_resistors_info()`
- `iso_get_standards_info()`
- `iso_get_vendor_data_table()`

### 4 Visualize Data

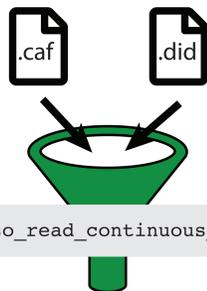
- `iso_plot_dual_inlet()`
- `iso_plot_continuous_flow()`



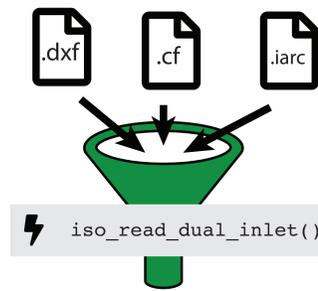
### plot converted signals (voltage to current)



### Dual Inlet Files



### Continuous Flow Files



## Isoreader (isoreader.kopflab.org)

one stop command-line access to raw stable isotope ratio mass spectrometry (IRMS) data

### 5 Export Data

- `iso_save()`
- `iso_export_to_excel()`
- `iso_export_to_feather()`

### 6 Expand Functionality

- `iso_register_file_reader()`
- `iso_turn_debug_on()`

### 3 Process Data

- `iso_convert_time()`
- `iso_convert_convert_signals()`
- `iso_calculate_ratios()`

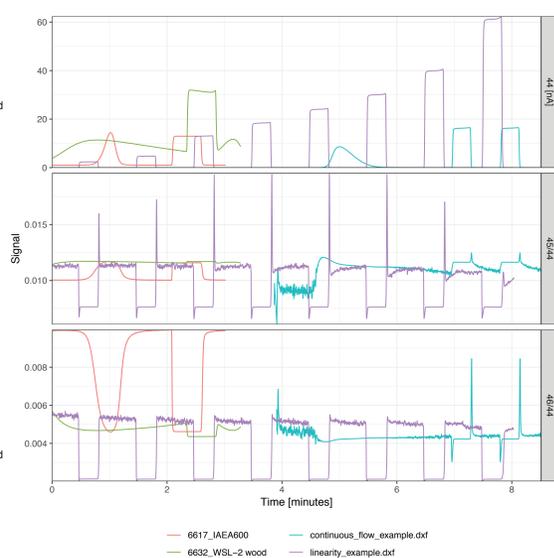
### 7 Future Directions

- peak scan data files
- all main IRMS manufacturer formats

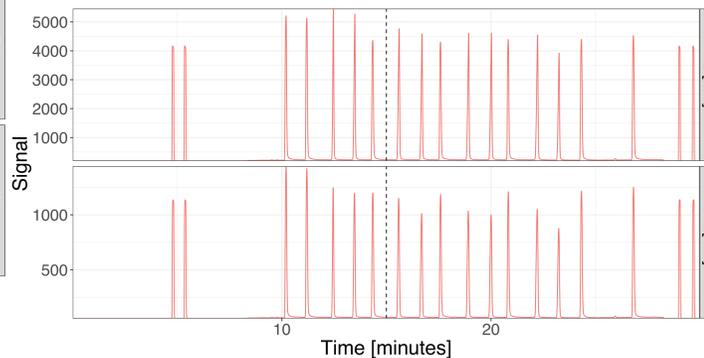


- isoprocessor (isoprocessor.kopflab.org)
- linearity & H3 factor tools
- metadata intergration
- peak detection & mapping
- correction & calibration tools
- error estimation
- what would YOU like to see?

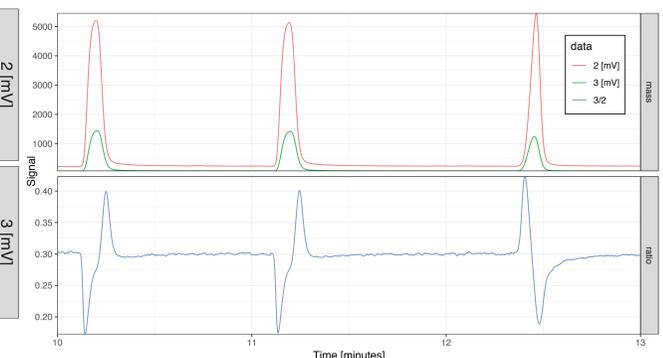
### overplot multiple traces from different instruments



arrange panels, colors, linetype, etc. by plot aesthetics and customize plots with the powerful ggplot2 Grammar of Graphics



### convert time units & plot specific time windows



## Isoviewer (isoviewer.kopflab.org)

- graphical user interface based on isoreader
- platform independent (web-based) visualization of various IRMS data types
- generates executable isoreader code as an RMarkdown report

Try it now at [http://www.kopflab.org/isoviewer\\_demo/](http://www.kopflab.org/isoviewer_demo/)

### Step 1: Load Data Files

assemble collections of data files

switch between one/multiple files in data collections

### Step 2: Explore Data

explore file info, methods and data table

export ALL data to Excel/Feather

visualize raw data

download high quality (PDF) plot

live code preview

scale signals to different units

scale time

select masses & ratios