Tripoli User Guide

June 5, 2024

Contents

Part I

Setup

Chapter 1

Java Download and Installation

Before running Tripoli, you need to download Java and install it on your computer. Tripoli is written in the programming language Java, and it runs on your computer (Windows, Mac, or Linux) using the Java platform. Because it is open source, you can download the latest version of Java for free from several reputable distributors, including Liberica and Azul. You can pick your distribution as long as it includes JavaFX, which has support for rich graphics, and the version is 17 or higher. The following have been tested and work with Tripoli.

1.1 Gather some information about your computer

You've probably needed this information before to install software on your computer. You should know:

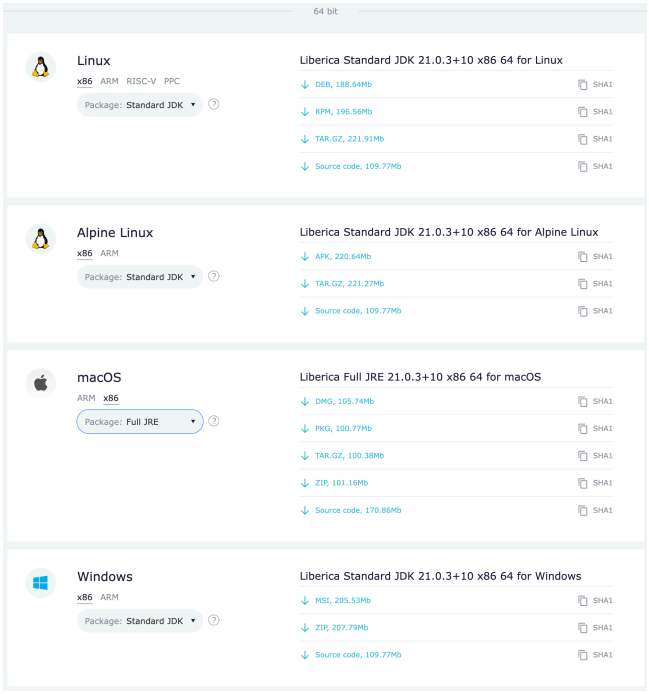
1. Your operating system: Linux, Mac, or Windows,
2. Whether you have a 64-bit (probably) or a 32-bit processor (much older)
3. Does your processor use the x86 or ARM architecture?

Newer Apple products use Apple Silicon (e.g., the M1, M2, etc chips) with an ARM architecture, and older Apple products with Intel chips and Windows machines usually use an x86-compatible architecture. For more information, google how to determine what type of processor is in your computer, then whether it is x86 or ARM.

1.2 Download a Java Distribution

1.2.1 Liberica Distribution (Choice 1, easier install)

1. Go to the bellsoft Liberica page here.
2. Scroll down past the banners the until you the list of 64-bit operating systems and options. If you have a 32-bit operating system, scroll down just a little farther.



3. Underneath the name of your operating system, choose your processor architecture (x86 or ARM), then click on the dropdown menu and choose "Package: Full JRE". For instance, on a Mac with an Intel processor, your choice would look like this, though version numbers are frequently updated:

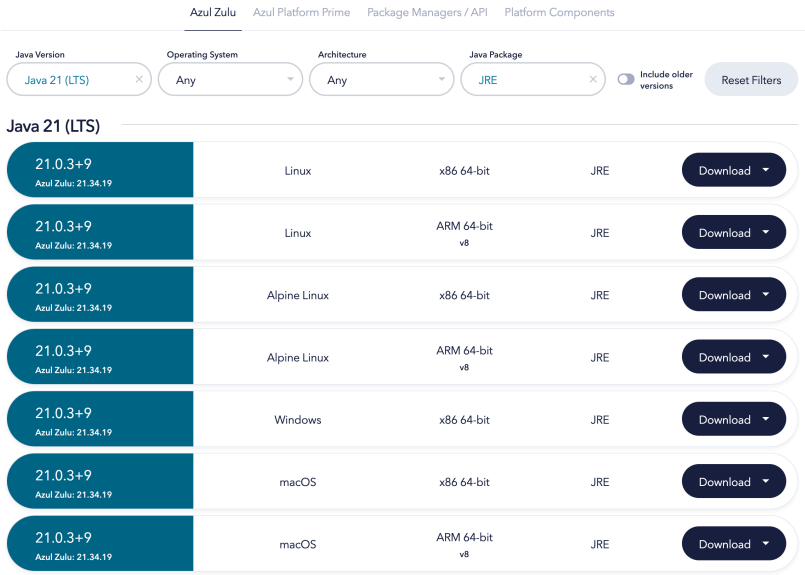
4. Click on the blue text link to the right corresponding to your favorite installer type. For a Mac, DMG and for Windows, MSI are easy to use.

5. Once downloaded, run the installer, click through the prompts, and type in your password as needed. Congratulations, you've installed Java!

1.2.2 Azul Distribution (Choice 2, more complicated)

1. Go to the Azul distribution page here. This page should show you only downloads for Java 21 (LTS means long-term stable) and JRE packages (Java Runtime Environment – what you need to run Java on your computer).

2. In the set of dropdown menus at the top, choose your operating system and architecture. Alternately, find your operating system and architecture in the list below the dropdown menus.



3. Hover your cursor over the dark blue Download button next to your OS and architecture, then choose a download file type. For Mac and Windows, a .zip file is good.

4. Your download will start and a bunch of advertisements and some pop-ups will show up. Ignore them and find the .zip file in your browser or computer's Downloads folder.

5. Copy the .zip file to a dedicated folder on your hard drive, then unzip the folder and delete the .zip archive.

6. Add the installation folder to your `PATH` environment variable. Don't know how to do this? Google will help for your system, or just use Liberica (Choice 1).

7. Congratulations, you've installed Java!

Chapter 2

Downloading Tripoli

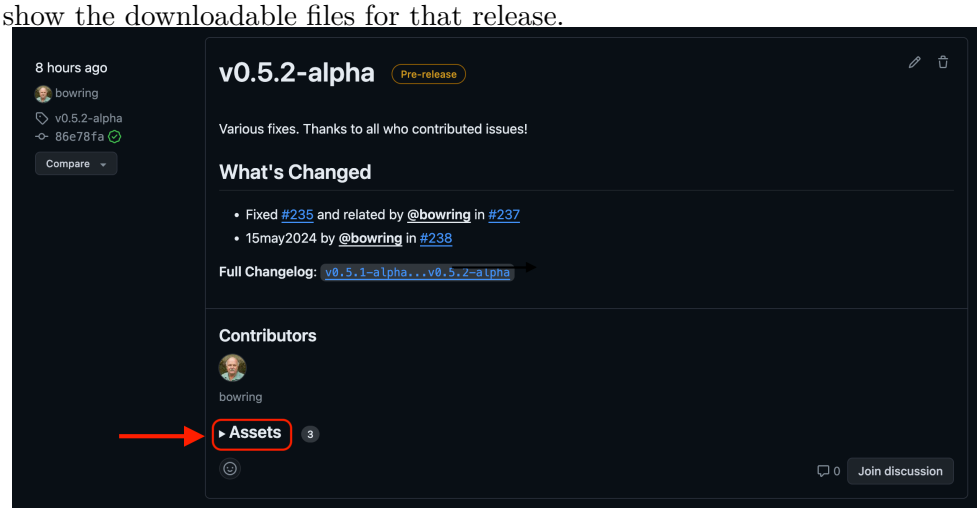
Once you've successfully installed Java, you're ready to download Tripoli from GitHub.

2.1 Go to the Tripoli repository's software releases at GitHub

Go to https://github.com/CIRDLES/Tripoli/releases to find the latest Tripoli release.
We will always release new versions here, along with some release notes that describe what's new in this version. You can scroll down to access all past versions of Redux. Version numbers will get the "-alpha" tag as long as Tripoli is in its initial development stages. Please use Tripoli, find bugs, and make suggestions! We will document how to use Tripoli and how we've tested it here.

2.2 Find the Tripoli .jar file

In the release you want to download (generally the most recent one at the top), click the word "Assets" to show the downloadable files for that release.



2.3 Download Tripoli's .jar file

Click on the blue link text for the top option in Assets, called "Tripoli-X.Y.Z.jar" where X.Y.Z is the version number. This will download the Java ARchive (.jar) file to your browser or OS downloads folder. This file contains all you need to run Tripoli on your computer.

2.4 Move the Tripoli .jar file to a permanent location

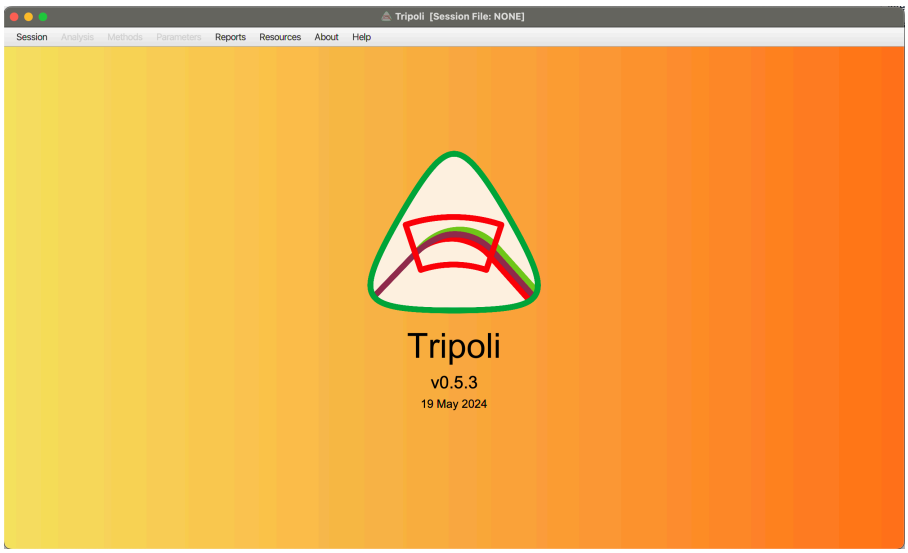
Move the Tripoli .jar file to a folder you've created on your hard drive for Tripoli. Other files that Tripoli creates as part of its data reduction will appear in this folder as well, so leaving it in your very large Downloads folder is not a good idea.

Congratulations, you've downloaded Tripoli! You're ready to fire it up and load in some data!

Are you interested in what all the rest of the information on Tripoli's GitHub page is about? Check out the Tripoli GitHub Page Tour.

Chapter 3

Getting Started in Tripoli

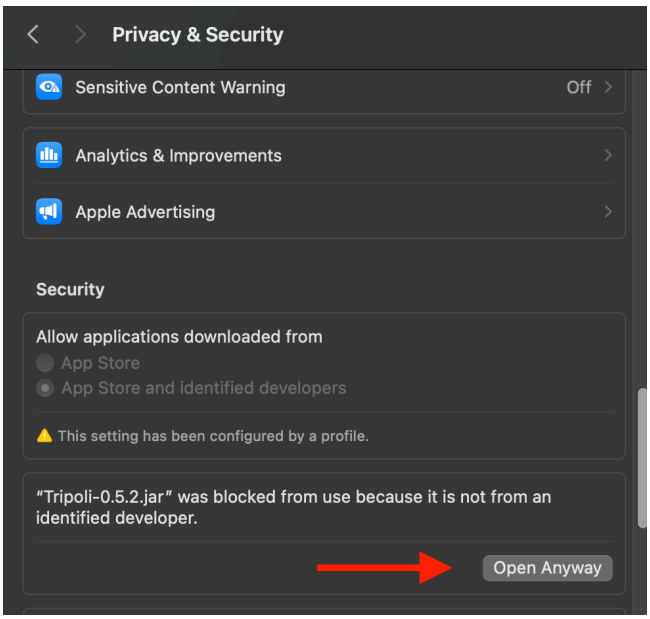


3.1 Start Tripoli

The easiest way to start Tripoli is to double-click on the Tripoli .jar file you downloaded. However, depending on your computer's security settings, you might get hassled by some warnings. Here's what to do:

3.1.1 Mac:

The security settings on your Mac are likely configured so that you get a warning when you try and open an app that you downloaded from the internet. Tripoli is not malware, and we are not secretly downloading your unpublished data – we have enough of our own! To open Tripoli anyway, open System Settings (the gear icon on your dock), then click on "Privacy and Security" in the left-hand menu. Scroll down on the right-hand side of the window until you see a prompt asking if you want to "Open Anyway".



Click the "Open Anyway" button, enter your password if needed, and the Tripoli application will open.

You only need to go to Privacy and Security settings once to open this .jar file. Double-clicking on it in the future will just open Tripoli. However, when you download a new version of Tripoli with a new version number and filename, you'll need to repeat the process. Or, you can open Tripoli from the command line using the instructions in the Starting Tripoli section.

3.1.2 PC:

Double-clicking the Tripoli .jar file should work on a PC right away, as long as you've installed Java. However, if you have an old Java installation, Windows might try and fail to open Tripoli with your older version. To fix this problem, we've created a .bat file, which you can download here:

- Tripoli.bat

Move both the Tripoli .jar file you want to run and the .bat file to a new folder, then double-click on the .bat file to open Tripoli.

3.1.3 Linux:

If you're running Linux, you probably have the expertise to use the command line interface to open Tripoli.

3.2 Loading data files into Tripoli

The easiest way to open a mass spectrometer data file in Tripoli is to drag and drop it into the Tripoli window. Other methods are detailed in Loading Data.

3.2.1 Find your data file

Open Windows Explorer, Mac Finder, or your Linux file manager. If you don't have a data file handy, try a file from the KU TIMS:

- Pb data file
- U data file

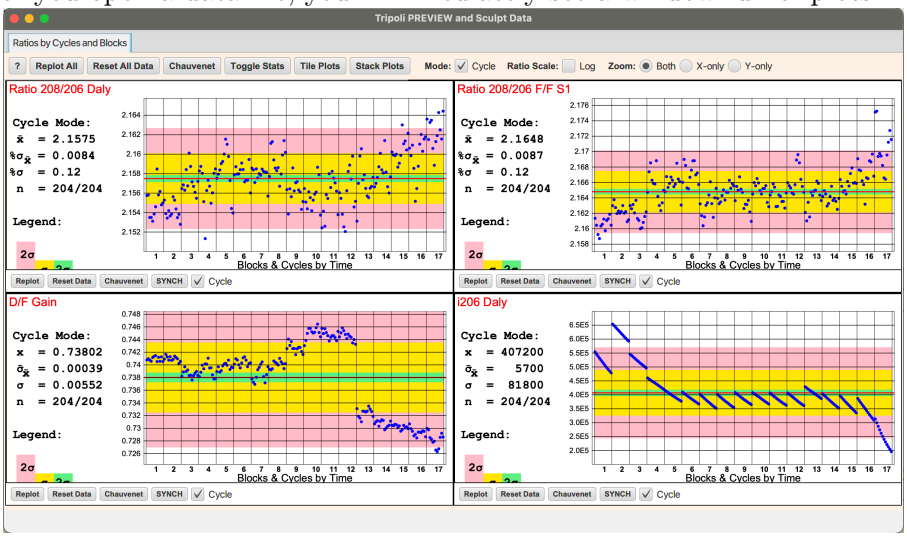
3.2.2 Drag and Drop

Drag and drop the data file out of your file manager and into Tripoli. If there's already a data file open in Tripoli, that's ok! Tripoli will add the new file to your session. Read more about sessions at

Loading Data.

3.3 Interactively Visualize Your Data

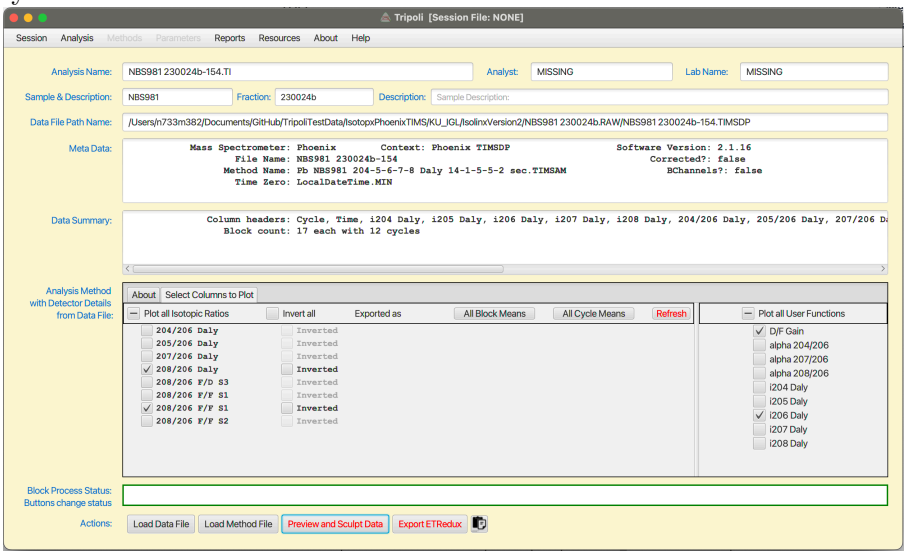
After you open a data file, you'll immediately see a window full of plots.



Buttons along the top of the window and inside each time series plot control the display of your data. Hover your cursor over a plot to see a tooltip with mouse button actions to zoom in/out, enter "sculpt" mode to perform data rejection, and more. The summary statistics beside each plot update as you reject or restore data, as do the graphical summaries shown as shaded regions behind the data points.

3.4 Manage Your Analysis

The Tripoli "Analysis Manager" window behind your plots now shows details about your loaded analysis.

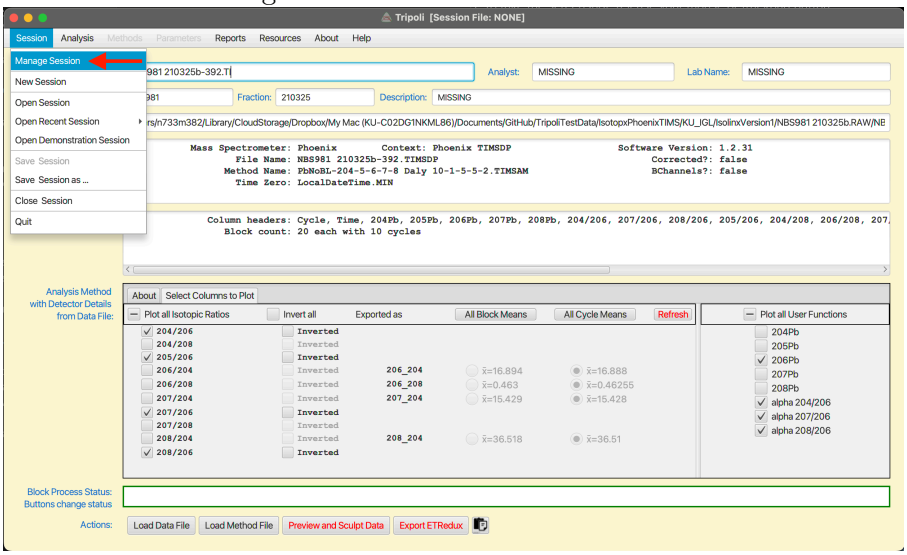


An interactive panel at the bottom of the window contains checkboxes for showing or hiding different measured isotope ratios or intensities. At the bottom of the Analysis Manager, there are buttons to launch the plot window as well as to export the (U-Pb) data to ET_Redux and to the clipboard.

3.5 Manage Your Session

You can load more than one mass spectrometer file into Tripoli at a time. Close the plot window if it's open, and then drag another mass spectrometer data file onto the main Tripoli window. The new file and plots should open immediately.

To see both analyses in your new session, go to the menu at the top of the Tripoli window and choose Session → Manage Session.



You can name your session, see a list of the analyses included in this session, and add notes. To save the entire session, including the data, data rejection, and data visualization choices for all analyses, go to Session → Save Session as... The resulting session file will have the .tripoli extension.

3.6 Recap

Now you're ready to load more mass spectrometry data files, examine the results, and export your data interpretations. Tripoli is still under active development. If you find issues or bugs, go to the main Tripoli menu and find Help → Contribute an Issue on GitHub. If you have a question or want to start a discussion about new features to add, go to the main Tripoli menu and find Help → Visit Tripoli Discussions on GitHub. Note that both require a GitHub username and password (these are very handy!).

For more detailed information on starting Tripoli, loading data, and making plots, please see the next section of the manual, Using Tripoli.

3.7 Read More:

Part II

Using Tripoli

Chapter 4

Running the Tripoli Application

4.1 Before you start

Before you start Tripoli, make sure that you have:

- Downloaded and installed the correct Java application,
- Downloaded the latest Tripoli .jar file from the GitHub repository, and
- Moved the Tripoli.jar file to a dedicated folder on your hard drive, for instance a folder named "Tripoli" inside your "Documents" folder.

4.2 The easy way: double-click a .jar file

In most cases, the simplest way to start the Tripoli application is to double-click on the .jar file you downloaded from the GitHub repository. The .jar file contains everything you need to open the application and start reviewing data. This approach is likely the best when setting up Tripoli on a shared lab computer, where users with a variety of software comfort levels will be opening Tripoli. If you just double-clicked the Tripoli .jar file and nothing happened, or you got a warning, see OS-specific troubleshooting below.

4.2.1 Mac

Include text from QuickStart.

4.3 The better way:

Command Line

Chapter 5

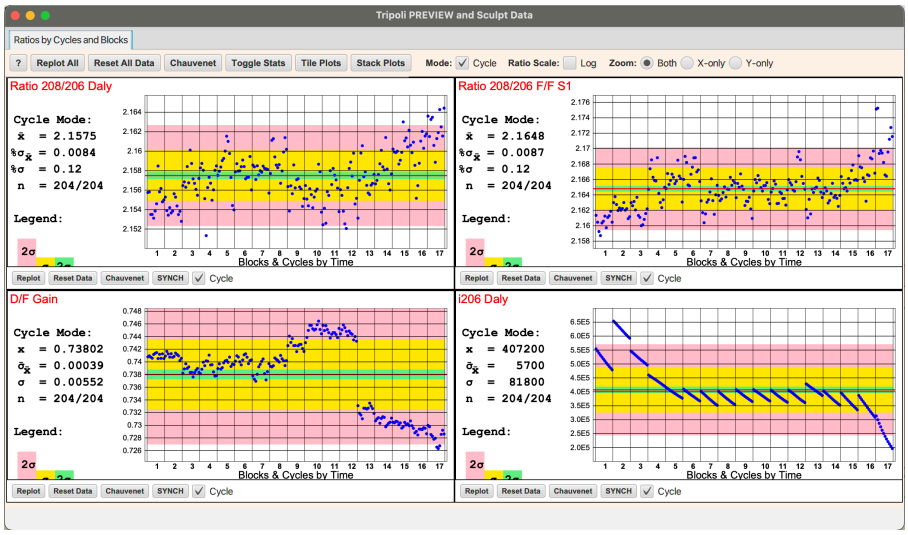
Loading Data Into Tripoli

5.1 Locate a data file to load into Tripoli.

Chapter 6

Plotting Mass Spec Data

6.1 Making Plots in Tripoli



Part III

How It Works

Chapter 7

Basic Statistics for Mass Spectrometry

Software for all major mass spectrometer manufacturers provides some out-of-the-box statistics to summarize measured data. Mass spectrometry

7.1 The arithmetic mean and its uncertainty

7.1.1 The arithmetic mean

The arithmetic mean $\bar{x}$ for n measurements indexed $i = 1 \dots n$ is

$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \tag{7.1}$$

7.1.2 The variance

The variance σ^2 measures the scatter of the data points around the mean value.

$$\sigma^2 = \frac{1}{n-1} \sum_{i=1}^{n} \left(x_i - \bar{x}\right)^2 \tag{7.2}$$

where $\bar{x}$ is the mean defined in equation (7.1) and n is the number of data points. The variance is tricky because it has the same units as your measurements, squared.

7.1.3 The standard deviation

The standard deviation also measures how your data points scatter around the mean, but this time in units that you actually understand.

$$\sigma = \sqrt{\sigma^2} \tag{7.3}$$

where σ^2 is the variance defined in equation (7.2).

7.1.4 The standard error

The standard error tells you how well you know the mean. It gets smaller as n gets bigger, reflecting your improved knowledge of the mean as you make more measurements.

$$\sigma_{\bar{x}} = \frac{\sigma}{\sqrt{n}} \tag{7.4}$$

7.1.5 Standard deviation vs. standard error

Both the standard deviation and the standard error are used to represent uncertainties in measurements. So which should you use?

Use the **standard deviation** when you're looking to describe the scatter among your measured data points. The standard deviation doesn't change as you measure more data and increase n. For instance, you might use the standard deviation to measure the reproducibility of your reference material measurements. You could use the standard deviation of your past reference material measurements to predict the range of values where your next reference material measurement is likely to be.

Use the **standard error** when you're describing the uncertainty in a mean value. According to equation (7.4), the standard error gets smaller as n increases, reflecting your increased confidence in the mean as you take more measurements. If you've just measured 100 isotope ratios, then the standard error best reflects your uncertainty in the mean of those 100 ratios. If you want to improve the uncertainty in the mean by a factor of two, then equation (7.4) says that you need to collect four times as much data with the same standard deviation.

7.1.6 Relative uncertainties

A relative uncertainty an absolute uncertainty (a standard deviation or a standard error) divided by the mean value. Relative uncertainties are often expressed in percent (e.g., $100\,\sigma/\bar{x}$), but could also be expressed for instance in per mille or ppm.

7.2 Confidence Intervals

You can calculate a mean, standard deviation, and standard error for any dataset with more than one measurement. These three statistics are just the numbers that are calculated by the formulas given above. However, we usually want to make some more quantitative estimates about our data. For instance, a 95% confidence interval for the mean would be expected to contain the true value of the mean about 95% of the time. This idea helps you make the leap from an uncertainty (just a number) to a mental picture of what range of values might reasonably be attributed to the parameter (e.g., isotope ratio) you're measuring.

Isotope ratio data are often presented as a mean value and a $\pm 2\sigma$ confidence interval, interpreted as a 95% confidence interval. To construct a 95% confidence interval in this way, the σ that you want is the standard error, since it tells you about the uncertainty in the mean value. For instance, if you measure 100 isotope ratios with a mean of 1.234 and a standard deviation of 0.0120, then the standard error of the ratios is

$$\sigma_{\bar{x}} \;=\; \frac{\sigma}{\sqrt{n}} \;=\; \frac{0.0120}{\sqrt{100}} \;=\; 0.0012, \tag{7.5}$$

and a 95% confidence interval for the mean ratio would be

$$\bar{x} \pm 2\sigma_{\bar{x}} \;=\; 1.234 \pm 0.0024. \tag{7.6}$$

To make a 95% confidence interval in this way, though, requires that you make a number of assumptions that are not always met by mass spectrometer data. For datasets that do not meet these assumptions, you can calculate a $\pm 2\sigma$ confidence interval (these are just numbers that come from formulas), but it will not be a 95% confidence interval.

7.2.1 Assumptions

The following assumptions are baked into the way we report and think about

Chapter 8

Glossary