## Mass Spec Data from RSES

### Background

PRN File comes from the Mass specrometer.

A despiked file is also created

### Processing

Open Macro and enable

Choose the despiked prn file from the mass spec.

Then select the appropriate parameters

reference mass (43)

Ranges for background,

standards at start and finish

sample (run) start and finish

Smooth using value =1 (no smoothing).

400000 for Ca reference mass (43)

Standard used.

Despike the rest using the macro tool.

### File management

Save the file. …Data/Slide/filename.xlsx [filename = “slide””run” eg: B2.xlsx]

Save data sheet (Data-NIST610\_Calibration) (as) .csv - …Data/filename.csv [eg B2.csv]

Use simple template file and create a Table of Otolith Number(=LarvalID) with start, core, end and ranges for samples for edge1, core and edge2. This is the metadata file which will be named starting with lowercase m.

Save this file as: slide run DB connect. …/data/mfilename [eg:mB2.xlsx]

Save as csv with same name (mfilename.csv)

In this way all .xlsx file end up in their slide sub folders but all .csv files are in together. This makes it easier for the r work to follow.

## Then in R

### Munge:

For each data file:

Remove smoothed data block in middle of data frame

Delete empty variables.

Import mass spec data from the .csv file called “*Slide””Run”.csv*

Merge this file with metafile add numbers edge positions etc.

Delete between end and next start (background mass detection)

Save and append to single data file for analysis

### Analysis

Create variable Sr:Sr and Ba:Ba ratios

For each element , Ca ratio and Sr and Ba Isotope ratios

Compare edge1 and edge 2. If not different combine?

Create means and SD and export file for import to database

Plots

Report

Summary Report