

# Processing LA-ICP-MS otolith microchemistry data using the Fathom Toolbox for Matlab

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## Introduction

The Fathom Toolbox for Matlab (FTM) is cross-platform collection of custom functions written in the Matlab programming language for processing and analyzing oceanographic and multivariate ecological data sets (Jones, 2012). This open source Toolbox is released under the GNU General Public License (GPL, version 2.0) and is freely available for download from: <http://www.marine.usf.edu/user/djones>. The FTM now includes a suite of functions in the ‘laser’ folder for processing transient signal data generated by Laser Ablation-Inductively Coupled Plasma-Mass Spectrometer (LA-ICP-MS) assays. These functions were primarily written to process microchemistry data from assays of fish otoliths, but are readily adaptable to handle LA-ICP-MS data generated from other types of samples as well.

The FTM takes as input the raw time series of analyte count rates ( $\text{ions}\cdot\text{s}^{-1}$ ) generated by the ICP-MS instrument control software and exported in the Perkin-Elmer Elan ‘XL’ format (\*.xl or \*.csv). The Toolbox provides tools for importing these raw data into the Matlab workspace, parsing the transient signal data into separate signal and background components via a user-friendly graphical user interface (GUI), and reduction of raw count rate ( $\text{ions}\cdot\text{s}^{-1}$ ) data to mean analyte concentrations (ppm) and analyte-to-Ca molar ratios ( $\mu\text{mole}\cdot\text{mole}^{-1}$ ). The GUI allows the user to visually assess the quality of the signal representing each ablation sample and optionally exclude those portions of the signal displaying peaks associated with surface contaminants, etc. The Toolbox also provides support for: (1) user-defined standard reference material (SRM) libraries; (2) calibration via internal and external standards; (3) calculation of limits of detection (LOD); (4) optional mass-specific spike detection and removal from the transient signal data via a standard deviation criterion, Grubb’s Test for outliers, or Rosner’s Test; and (5) optional correction for instrument drift in mass-specific sensitivity via linear interpolation or nearest neighbor methods. The algorithms implemented in this code closely follow established methods of geochemical data reduction (i.e., Halter et al., 2002; Henrich et al., 2003; Jackson, 2008; Longerich et al., 1996; 1997).

## Data Collection

This document provides a worked example using data for otoliths from gag grouper (*Mycteroperca microlepis*) as a tutorial for using the FTM to process raw LA-ICP-MS data. These samples were assayed as part of a larger study using otolith microchemistry to investigate the ontogenetic migration history and habitat connectivity of this species in the Gulf of Mexico. A Photon-Machines Analyte.193 excimer UV laser ablation system,

connected to an Agilent Technologies 7500CX Quadrupole ICP-MS, was employed to characterize the trace elemental composition of sectioned and polished transverse saggital otolith thin sections. Three replicate 83  $\mu\text{m}$  diameter spot samples were ablated near the outermost growth rings of each otolith for 60 s, with the laser set to 86% power at 5 Hz. The ICP-MS was configured in time resolved analysis (TRA) mode with one point per peak and a dwell time of 10 ms. Gas blanks were collected for 60 s before and after each spot scan was performed. NIST-612 silicate glass (Pearce et al., 1997) and MACS-3 micro-analytical carbonate (Koenig and Wilson, 2007) standards were used as external standard reference material (SRM) and ablated in brackets before and after every fifth otolith. Ion count rates ( $\text{ions}\cdot\text{s}^{-1}$ ) were collected for the following 25 target analytes using this instrumentation:  $\text{Li}^7$ ,  $\text{Na}^{23}$ ,  $\text{Mg}^{24}$ ,  $\text{P}^{31}$ ,  $\text{Sc}^{45}$ ,  $\text{V}^{51}$ ,  $\text{Cr}^{53}$ ,  $\text{Mn}^{55}$ ,  $\text{Fe}^{57}$ ,  $\text{Co}^{59}$ ,  $\text{Ni}^{60}$ ,  $\text{Cu}^{63}$ ,  $\text{Zn}^{64}$ ,  $\text{Cu}^{65}$ ,  $\text{Ge}^{72}$ ,  $\text{Rb}^{85}$ ,  $\text{Sr}^{88}$ ,  $\text{Y}^{89}$ ,  $\text{Cd}^{114}$ ,  $\text{Sn}^{118}$ ,  $\text{Ba}^{137}$ ,  $\text{Au}^{197}$ ,  $\text{Pb}^{208}$ ,  $\text{Th}^{232}$ , and  $\text{U}^{238}$ . Since otoliths are aragonitic carbonates,  $\text{Ca}^{43}$  was also quantified and used as the internal standard in subsequent data reduction. These data were exported as comma-separated-values (\*.csv) using the “Tabulate chart CPS data to CSV” menu option in the ‘Data Analysis’ module of the Agilent Technologies instrument control software. This produced an ASCII text file with the data in Perkin-Elmer Elan ‘XL’ format. A summary of the raw transient signal data collected by the Agilent Technologies software is shown as total ion count rates in the time chart depicted in Figure 1. This chart was annotated immediately after the data were collected to allow identification of the signal associated with each ablation sample in subsequent data parsing and processing.

## Import Data

Use the `f_importXL` function to import a Perkin-Elmer Elan *XL* format (\*.xl or \*.csv) LA-ICP-MS transient signal data file into the Matlab workspace as a structure:

```
% Show help:
>> help f_importXL
- import Perkin-Elmer Elan format (*.xl or *.csv) LA-ICP-MS transient signal data

USAGE: raw = f_importXL('fname');

fname = name of *.xl file to import

raw = structure with the following fields:
.s      = seconds
.cps    = signal intensity in counts per sec
.txt    = cell array of isotope labels for columns of 'cps'
.iso    = corresponding isotope number
.hh     = hour of acquisition
.mm     = minute of acquisition
.gDate  = cell array of Gregorian date of acquisition

% Import raw data:
>> raw_B = f_importXL('101209_B.csv')

raw_B =

    s: [8516x1 double]
   cps: [8516x26 double]
   txt: {1x26 cell}
   iso: [7 23 24 31 43 45 51 53 55 57 59 60 63 64 65 72 85 88 89 114 118 137 197 208 232 238]
   hh: 16
   mm: 51
  gDate: {'09-Dec-2010'}
```

## Parsing Data

The `f_cpsParse` function is used to parse a time series of laser ablation transient signal data into separate components representing the signal and background portions of individual ablation samples. The input data (*raw*) must be a structure created from the `f_importXL` function, which imports data from a Perkin-Elmer Elan *XL* format data file (\*.xl or \*.csv). The GUI created by this function displays a plot of the time series data that allows the user to parse by selecting specific regions. Use the *Pan* or *Zoom* tools to navigate and focus on specific portions of the time series. Use the *Select* tool to highlight a region within the time series that corresponds with the **signal** portion of a sample, add an appropriate name (e.g., o20\_A) within the GUI's *Variable Name* box, then click the *Signal* button to save this portion of the data in a separate variable in the Matlab workspace (Figure 2). Next, use the *Select* tool to highlight the region of the time series that corresponds with the **background** portion of the sample you just exported, and click the *Background* button (Figure 3). This adds a \*.bg field to the signal variable you just created (i.e., to the variable listed in the *Variable Name* dialog box). Repeat this procedure for the remaining spot scans present in the imported data file. Refer to your annotated time chart (see Figure 1) to name each variable accordingly:

```
% Show help:
>> help f_cpsParse
- GUI to parse LA-ICP-MS transient signal data into signal/background subsets

USAGE: f_cpsParse(raw)

INPUT:
raw = structure of raw signal data with the following fields:
.s      = seconds
.cps    = signal intensity (counts per second)
.txt    = cell array of element labels for columns of 'cps'
.iso    = corresponding isotope number
.hh     = hour of acquisition
.mm     = minute of acquisition
.gDate  = date of acquisition

OUTPUT:
Subset of 'raw' input structure with the following fields:
.s      = seconds
.cps    = signal intensity (counts per second)
.txt    = cell array of element labels for columns of 'cps'
.iso    = corresponding isotope number
.hh     = hour of acquisition
.mm     = minute of acquisition
.gDate  = cell array of Gregorian date of acquisition
.idx    = index to corresponding elements of input 'raw' structure
.bg     = structure with the corresponding background data

% Select signal/background regions:
>> f_cpsParse(raw_B); % -> nist_F to nist_GG, macs_F-G, n = 5 otoliths
```

## Data Reduction

```

% Show help:
>> help f_cps2ppm
  - calculate analyte concentration from LA-ICP-MS transient signal data

USAGE: [result,SRM] = f_cps2ppm(UNK,STD,'SRM',IS,dwell,adj,spike,drift,tol,verb);

UNK = structure of measured SAMPLE signal
STD = structure of measured STANDARD signal

...the preceding structures have the following fields:
.s      = time interval (sec)
.cps    = count rate (counts per sec)
.txt    = cell array of text indicating measured elements
.iso    = corresponding isotope number
.hh     = hour of acquisition
.mm     = min of acquisition
.gDate  = date of acquisition
.bg     = structure of corresponding background data (with the same fields)

SRM = name of variable in file SRM.mat to use for Standard Reference Material
      e.g., SRM = 'nist612'

IS = structure of Internal Standard with the following fields:
.txt   = cell array of text indicating element
.ppm   = corresponding concentration in Unknown

dwell = dwell time of the quadrupole (msec); use a scalar for constant
        and a row vector for variable dwell times
adj    = optionally adjust concentrations that fall below LOD to:
        0 (adj=0), LOD (adj=1), or make no adjustment (adj=2, default)
spike  = optional spike removal of background-corrected signal data via Grubbs
        Test (= 'g'), Rosner Test (= 'r'), or STDEV (= 1 to 4)      (default = 0)
drift  = optionally correct for instrument drift using linear interpolation
        (= 1) or nearest neighbor method (= 2)                    (default = 0)
tol    = min value of R2 required to use linear vs. nearest neighbor
        interpolation                                             (default = 0.55)
verb   = optionally send results to display                       (default = 1)

result = structure of results with the following fields:
.txt    = cell array of text for each analyte element
.iso    = corresponding isotope number
.txt_iso = combined element + isotope labels
.ppm    = concentration of unknown                               (ppm)
.LOD    = limits of detection                                   (ppm)
.ratio  = molar ratios to internal standard                     (mMole/Mole)
.SRM    = name of SRM used for external calibration
.adj    = type of adjustment applied to values below LOD       (zero,LOD,none)
.spike  = type of spike removal applied to the time series
.nSpike = total # of spikes removed
.drift  = method of drift correction
.tol    = tolerance for linear interpolation
.R2     = correlation of drift correction line
.bg     = mean background counts of UNK                         (cps)
.gDate  = cell array of Gregorian date of acquisition

SRM = structure of Standard Reference Material values used; provided to
      allow calculation of 'percent relative error', etc.

```

The `f_cps2ppm` function is used to process the transient signal data of a single ablation sample parsed into separate signal and background components by the `f_cpsParse` function. Both `UNK` and `STD` inputs must have been previously created by the `f_cpsParse` function. `SRM` identifies the reference material represented by the `STD`. `IS` identifies the analyte that serves as the internal standard and its concentration in the `UNK` (e.g., for an otolith `IS.txt = {'Ca'}`; `IS.ppm = 40*10000`).

The `adj` parameter specifies optional adjustment of values that fall below the limits of detection. Values that fall below LOD can be set to 0 (`adj=0`) if you consider these values cannot be distinguished from 0. On the other hand, setting these values to LOD (`adj=1`) provides a “maximum likely concentration” (Heinrich et al., 2003). No adjustments are made by default (`adj=2`).

The `spike` parameter is used to optionally remove outliers from the transient signal of each analyte separately in both the `UNK` and `STD` portions of the signal. The Grubbs Test (`spike = 'g'`) does this by estimating a critical value using  $\alpha = 0.05$ . The Rosner Test (`spike = 'r'`) examines the residuals between the original times series and one that has been smoothed via a Butterworth filter. Spikes can also be removed by identifying values that fall beyond a specific number of standard deviations from the overall mean (e.g., `spike = 2.5`). Spikes identified by the Grubbs Test are replaced with values from a running mean, while those identified by the Rosner Test are replaced with values from the filtered time series.

The `drift` parameter allows optional correction for mass-specific changes in the instrument's sensitivity coefficient ( $m$ ) with time. The linear interpolation method (`drift=1`) corrects for drift by interpolating values of  $m$  along a correction line created by regressing the time of acquisition ( $t$ ) of multiple `STD`'s vs. the calculated value of  $m$  for each `STD`, given the time of acquisition of the `UNK`. Use of a linearly interpolated drift correction line assumes there is a strong linear relationship between  $m$  and  $t$ , which may not be the case. Therefore, if the correlation ( $R^2$ ) of  $t$  vs.  $m$  is not above a specific tolerance (`tol`) for a particular analyte, nearest neighbor interpolation is used instead for that analyte. This function outputs the value of  $R^2$  for the linearly interpolated drift correction line of each analyte, though returns a value of 0 when the tolerance (`tol`) value of  $R^2$  was not reached and the nearest neighbor method was used instead. The nearest neighbor method (`drift=2`) uses the value of  $m$  associated with the `STD` acquired closest in time with that of the `UNK`. Correction for drift using either method requires that data from more than one `STD` is input to the function, which can be achieved by packing multiple `STD`'s into a cell array (e.g., `cSTD = {STD_01 STD_02 STD_03}`).

Create two new variables in the Matlab workspace, one specifying the internal standard and another that stacks multiple external standards into a cell array:

```
% Setup Internal Standard (IS):
>> IS.txt = {'Ca'};
>> IS.ppm = 40*10000; % Otolith

% Stack multiple STD's:
>> cSTD = {nist612_F nist612_FF nist612_G nist612_GG};
```

Perform standard data reduction of the transient signal data to generate mean analyte concentrations and molar ratios:

```

% Process data:
% dwell = 10 ms : dwell time of the quadrupole
% adj = 0 : adjust all values < LOD to 0
% spike = 'r' : remove spikes using the Rosner Test
% drift = 1 : correct for instrument drift using linear interp.
% tol = 0.55 : R2 must be at least 0.55 to use linear interp.
% verb = 1 : show results in display

>> f_cps2ppm(o20_A,cSTD,'nist612',IS,10,0,'r',1,0.55,1);

=====
'Analyte'  'ppm'      'LOD'      'mMole/Mole'  '# spikes'  'Drift R2'
'Li7'      [ 0.29579] [ 0.028704] [ 0.0042698] [ 0]         [ 0.91308]
'Na23'     [ 2648.6]  [ 5.2702]   [ 11.543]    [ 0]         [ 0.84286]
'Mg24'     [ 18.849]  [ 0.062083] [ 0.077704] [ 0]         [ 0.97218]
'P31'      [ 125.39]  [ 4.5297]   [ 0.4056]    [ 0]         [ 0]
'Ca43'     [ 400000]  [ 35.904]   [ 1000]      [ 1]         [ 0]
'Sc45'     [ 0.11601] [ 0.0908]   [0.00025855] [ 4]         [ 0]
'V51'      [ 0.047926] [ 0.036853] [9.4264e-05] [ 0]         [ 0]
'Cr53'     [ 0]        [ 0.27981]  [0.00048098] [ 3]         [ 0]
'Mn55'     [ 0.099284] [ 0.073516] [0.00018107] [ 1]         [ 0]
'Fe57'     [ 219.95]  [ 0.91298]  [ 0.39462]   [ 0]         [ 0.84816]
'Co59'     [ 0.22105] [ 0.014159] [0.00037582] [ 0]         [ 0.96357]
'Ni60'     [ 0.3063]  [ 0.089473] [0.00052288] [ 4]         [ 0]
'Cu63'     [ 0.70591] [ 0.13112]  [ 0.001113]  [ 0]         [ 0.75547]
'Zn64'     [ 1.9096]  [ 0.10614]  [ 0.002926]  [ 0]         [ 0.59565]
'Cu65'     [ 0.86246] [ 0.14063]  [ 0.0013599] [ 0]         [ 0.59897]
'Ge72'     [ 0.15059] [ 0.12002]  [0.00020772] [ 0]         [ 0]
'Rb85'     [ 0.082167] [ 0.017693] [9.6325e-05] [ 2]         [ 0.80606]
'Sr88'     [ 1880.6]  [ 0.12195]  [ 2.1505]    [ 1]         [ 0.86216]
'Y89'      [ 0]        [0.0045579] [3.7911e-06] [ 0]         [ 0.99101]
'Cd114'    [ 0.082234] [ 0.042774] [7.3297e-05] [ 1]         [ 0]
'Sn118'    [ 0.50128] [ 0.041494] [ 0.0004231] [ 0]         [ 0]
'Ba137'    [ 6.3626]  [ 0.018038] [ 0.0046422] [ 0]         [ 0.66995]
'Au197'    [ 0]        [0.0093391] [ 2.638e-06] [ 4]         [ 0]
'Pb208'    [ 0.34798] [ 0.042558] [0.00016827] [ 0]         [ 0]
'Th232'    [ 0]        [0.0029745] [6.9857e-07] [ 1]         [ 0.84554]
'U238'     [0.0025237] [0.0022237] [1.0623e-06] [ 0]         [ 0]

-----
SRM          = nist612
LOD adjustment = zero
Spike removal = Rosner Test
Drift correction = linear
NaN          = analyte not present in SRM

Drift R2 is the correlation of the linearly interpolated drift correction line:
0 = indicates Nearest Neighbor interpolation was used instead
- = indicates NO interpolation was performed
-----

```

Table 1. (A) The variables created in the Matlab workspace when clicking the *signal* button in the GUI created by the *f\_cpsParse* command are structures, as shown here for the data collected by the *nist\_FF* spot scan. (B) The *background* button appends an additional structure to this variable under the field name *.bg*.

```
>> nist612_FF
nist612_FF =
    s: [157x1 double]
   cps: [157x26 double]
   txt: {1x26 cell}
   iso: [7 23 24 31 43 45 51 53 55 57 59 60 63 64 65 72 85 88 89 114 118 137 197
208 232 238]
   hh: 16
   mm: 51
  gDate: {'09-Dec-2010'}
   idx: [716 872]
   bg: [1x1 struct]

>> nist612_FF.bg
ans =
    s: [97x1 double]
   cps: [97x26 double]
   txt: {1x26 cell}
   iso: [7 23 24 31 43 45 51 53 55 57 59 60 63 64 65 72 85 88 89 114 118 137 197
208 232 238]
   hh: 16
   mm: 51
  gDate: {'09-Dec-2010'}
   idx: [587 683]
```

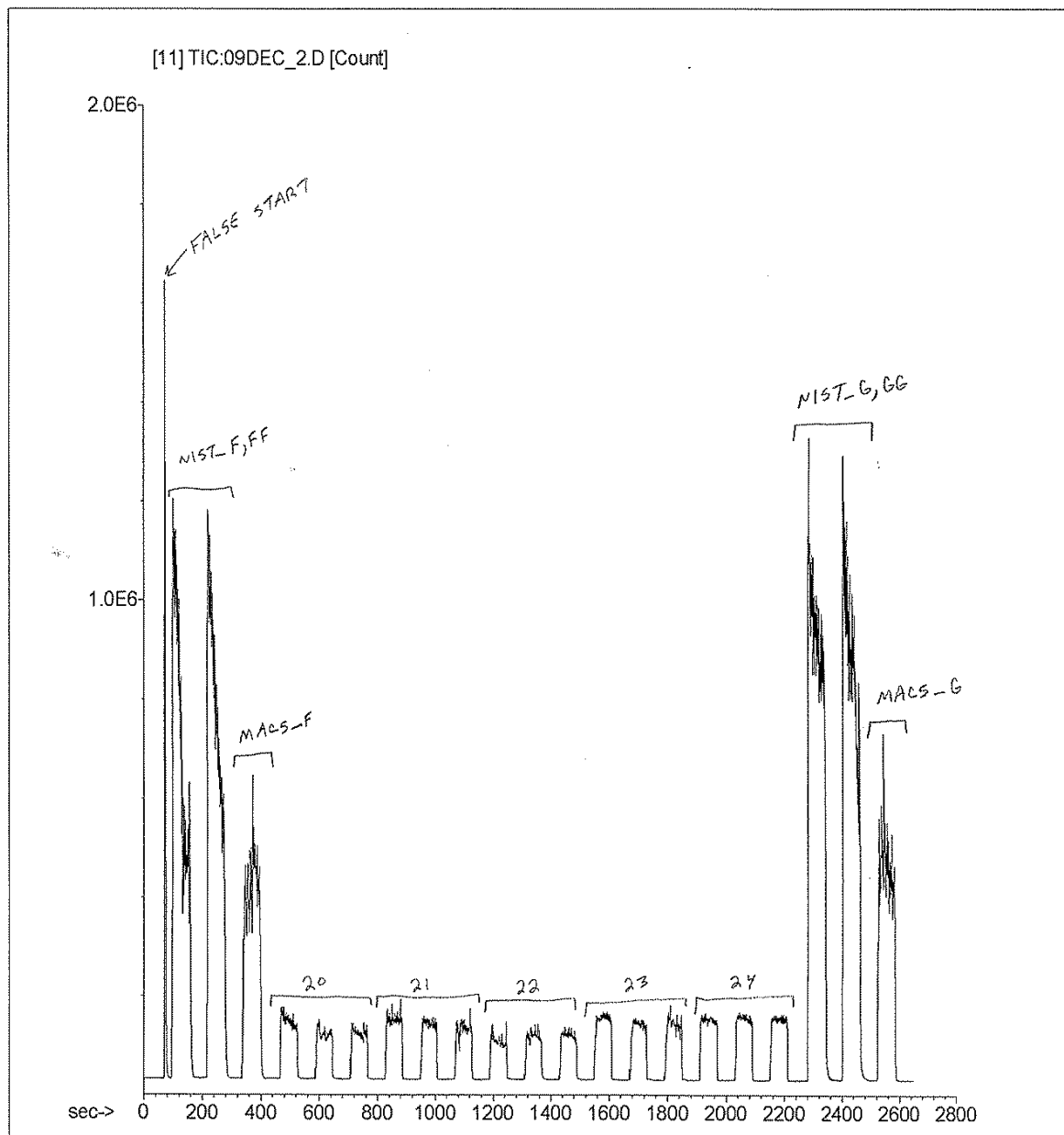


Figure 1. Annotated time chart printed from the Agilent Technologies 'Data Analysis' module depicting total ion count rates (cps) for the transient signal data exported to the file 101209\_B.csv. The first peak represents a false start when the scan sequence set in the laser ablation control software (i.e., Chromium) was paused in order to change the laser sampling parameters. All other scan sequences are bracketed by 60 s gas blanks and labelled as either spot scans of external reference material (NIST or MACS) or otolith thin sections (samples 20–24, with  $n = 3$  replicates).



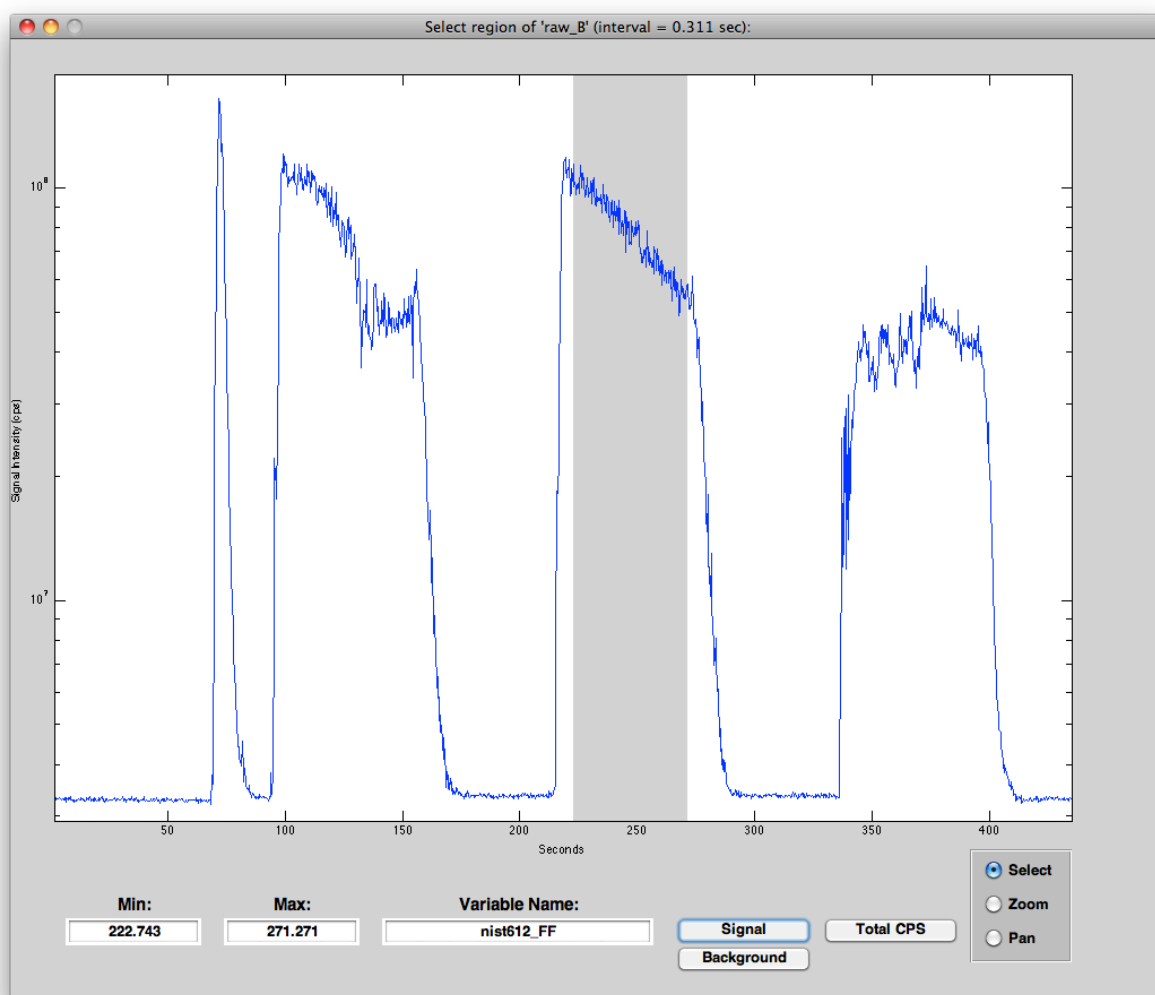


Figure 2. Graphical user interface (GUI) created by the `f_cpsParse` function to select and extract the region of the raw ion count time series corresponding to the **signal data** collected while ablating standard reference material *nist612\_FF*. See Table 4A for the corresponding variable created in the Matlab workspace.

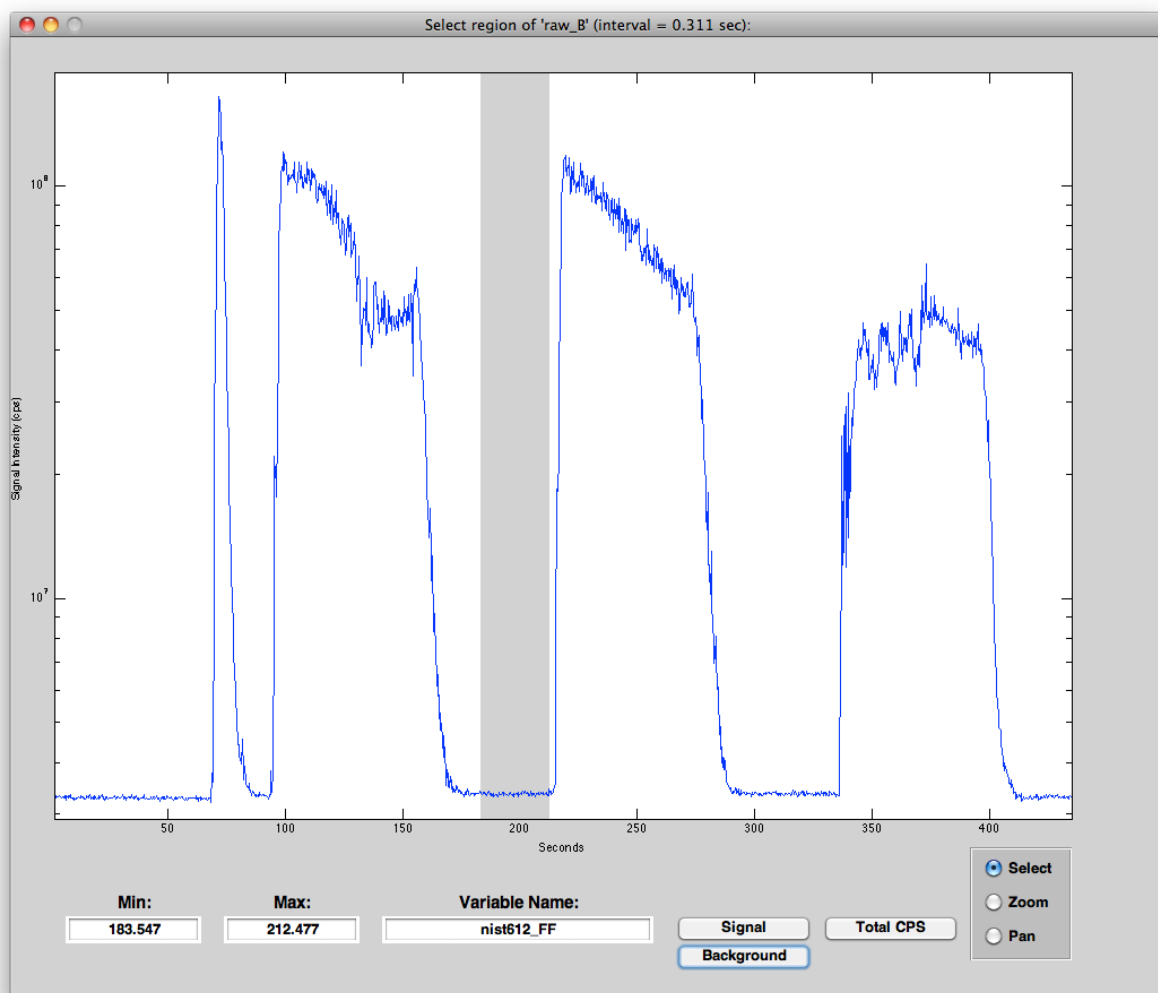


Figure 3. Graphical user interface (GUI) created by the  $f\_cpsParse$  function to select and extract the region of the raw ion count time series corresponding to the **background data** collected prior to ablating standard reference material *nist612\_FF*. See Table 4B for the corresponding variable created in the Matlab workspace.

Name ▲	Value	Min	Max
IS	<1x1 struct>		
cSTD	<1x4 cell>		
fname	'exampleDataRed...'		
macs_F	<1x1 struct>		
macs_G	<1x1 struct>		
nist612_F	<1x1 struct>		
nist612_FF	<1x1 struct>		
nist612_G	<1x1 struct>		
nist612_GG	<1x1 struct>		
o20_A	<1x1 struct>		
o20_B	<1x1 struct>		
o20_C	<1x1 struct>		
o21_A	<1x1 struct>		
o21_B	<1x1 struct>		
o21_C	<1x1 struct>		
o22_A	<1x1 struct>		
o22_B	<1x1 struct>		
o22_C	<1x1 struct>		
o23_A	<1x1 struct>		
o23_B	<1x1 struct>		
o23_C	<1x1 struct>		
o24_A	<1x1 struct>		
o24_B	<1x1 struct>		
o24_C	<1x1 struct>		
raw_B	<1x1 struct>		

Figure 4. Matlab workspace showing the list of variables created by parsing the raw transient signal data (*raw\_B*) into separate signal/background components for the standard reference material (e.g., *nist612\_F*, *macs\_G*) and otolith samples (e.g., *o20\_A*). Note that “\_A” through “\_C” represent replicate spot scans taken within the same otolith thin section. The NIST-612 SRM was used as a calibration standard and the MACS was used to evaluate subsequent experiment-wise percent relative standard deviations (%RDS).

## Batch Processing Data from Spot Scans

The *f\_cps2ppm\_SPOT* function is used to batch process all the LA-ICP-MS spot sample data within the file(s) specified by a filename parameter (*fname*). Each file must contain spot data that have already been imported into the Matlab workspace using the *f\_importXL* function, parsed into signal/background components using the *f\_cpsParse* function, and saved as a \*.mat Matlab file. Each file must contain the following variables:

External Standards: a cell array containing one or more external standards, each a variable of type structure created by the *f\_cpsParse* function, following the naming convention of either *cSTD*, *fSTD*, and/or *sSTD*. A cell array of multiple standards can be created using a command such as: *cSTD = {STD\_A STD\_B STD\_C}*.

Sample Unknowns: ablation samples must consist of variables (formatted as Matlab structures) created by the *f\_cpsParse* function that strictly conform to one of the following strict naming convention:

*o#####\_A*: 1) begins with the letter “o” (= otolith); 2) followed by a variable length numeric tag unique to each fish; and 3) followed by an underscore (“\_”) and letter (“A”) indicating replicate spot samples taken from the otolith of this fish. Example: “*o1120\_B*” refers to the variable containing the second replicate of otolith spot sample data taken from fish # 1120

*oto#####A1*: 1) begins with the letters “oto” (= otolith); 2) followed by a variable length numeric tag unique to each fish; 3) followed a letter indicating right vs. left otolith (A or B); and 4) followed by a number indicating the replicate spot sample taken from the otolith of this fish Example: “*oto10B2*” refers to the variable containing the second replicate of otolith spot sample data taken from fish # 10

*f#####\_A*: similar to “*o#####\_A*”, but used to match fin rays rather than otoliths; requires the corresponding external standards to be named “*fCTD*” and an appropriate internal standard (*IS*)

*s#####\_A*: similar to “*o#####\_A*”, but used to match fin spines rather than otoliths; requires the corresponding external standards to be named “*sCTD*” and an appropriate internal standard (*IS*)

By default, the date of acquisition (*gDate*) is determined from the *UNK* structure passed to the *f\_cps2ppm* function, which may have originated from the original \*.csv file imported by the *f\_importXL* function. However, if the acquisition date is missing (e.g., *gDate = {'NaN'}*), it can be determined from the filename, if they are named according to the *yymmdd.mat* format, by setting *DAY=1*.

Setting *VERB=1* assists in tracking down which files and/or variables produce errors in *f\_cps2ppm* when, say, no background is provided or the background and signal portions overlap, etc.

Replicate spot scans from each sample are first checked for the presence of outliers (based on PPM), then within-sample averages of PPM, LOD, and RATIO are calculated for those replicates not identified as outliers.

```

>> help f_cps2ppm_SPOT
- batch process parsed LA-ICP-MS spot data

USAGE: [result,all] = f_cps2ppm_SPOT(fname, 'SRM', IS, dwell, adj, spike, drift, tol, verb, match, day);

fname = cell array of file(s) to process
SRM    = name of variable in file SRM.mat to use for Standard Reference Material
        e.g., SRM = 'nist612'
IS     = structure of Internal Standard with the following fields:
        .txt = cell array of text indicating element
        .ppm = corresponding concentration in Unknown
dwell  = dwell time of the quadrupole (msec); use a scalar for constant
        and a row vector for variable dwell times
adj    = optionally adjust concentrations that fall below LOD to:
        0 (adj=0), LOD (adj=1), or make no adjustment (adj=2, default)
spike  = optional spike removal of background-corrected signal data via Grubbs
        Test (= 'g'), Rosner Test (= 'r'), or STDEV (= 1 to 4) (default = 0)
drift  = optionally correct for instrument drift using linear interpolation
        (= 1) or nearest neighbor method (= 2) (default = 0)
tol    = min value of R2 required to use linear vs. nearest neighbor
        interpolation (default = 0.55)
verb   = verbose output of progress (default = 1)
match  = regular expression pattern to match names of otolith spot scans
        1: matches o1140_A (replicates A-C) (default = 1)
        2: matches o1140_A (all replicates)
        3: matches oto10A1
        4: matches f1140_A (replicates A-C)
        5: matches s1140_A (replicates A-C)
day    = determine date of acquisition from file name

result = structure of results with the following fields:
.oto    = numeric tag identifying individual otoliths
.txt    = cell array of text for each analyte element
.iso    = corresponding isotope number
.txt_iso = combined element + isotope labels
.nRep   = # within-otolith replicate spot samples used to calculate averages
.ppm    = concentration of unknown, averaged across replicates (ppm)
.LOD    = limits of detection, averaged across replicates (ppm)
.ratio  = molar ratios to internal standard, averaged across replicates (mMole/Mole)
.SRM    = name of SRM used for external calibration
.adj    = type of adjustment applied to values below LOD (zero, LOD, none)
.spike  = type of spike removal applied to the time series
.drift  = method of drift correction
.tol    = tolerance for linear interpolation
.SRM    = name of SRM used for external calibration
.gDate  = cell array of Gregorian date of acquisition

all = structure of results (NOT averaged across otoliths):
.oto    = numeric tag identifying individual otoliths
.txt    = cell array of text for each analyte element
.iso    = corresponding isotope number
.txt_iso = combined element + isotope labels
.ppm    = concentration of unknown (ppm)
.LOD    = limits of detection (ppm)
.ratio  = molar ratios to internal standard (mMole/Mole)
.bg     = mean background counts of UNK (cps)
.gDate  = cell array of Gregorian date of acquisition

```

Workspace

Stack: Select data to plot

Name	Value	Min	Max
IS	<1x1 struct>		
cSTD	<1x14 cell>		
fname	'101209'		
macs_A	<1x1 struct>		
macs_B	<1x1 struct>		
macs_C	<1x1 struct>		
macs_D	<1x1 struct>		
macs_E	<1x1 struct>		
macs_F	<1x1 struct>		
macs_G	<1x1 struct>		
nist_A	<1x1 struct>		
nist_AA	<1x1 struct>		
nist_B	<1x1 struct>		
nist_BB	<1x1 struct>		
nist_C	<1x1 struct>		
nist_CC	<1x1 struct>		
nist_D	<1x1 struct>		
nist_DD	<1x1 struct>		
nist_E	<1x1 struct>		
nist_EE	<1x1 struct>		
nist_FF	<1x1 struct>		
nist_G	<1x1 struct>		
nist_GG	<1x1 struct>		
o1003_A	<1x1 struct>		
o1003_B	<1x1 struct>		
o1003_C	<1x1 struct>		
o1004_A	<1x1 struct>		
o1004_B	<1x1 struct>		
o1004_C	<1x1 struct>		
o1006_A	<1x1 struct>		

Workspace

Stack: Select data to plot

Name	Value	Min	Max
IS	<1x1 struct>		
cSTD	<1x12 cell>		
fname	'101216'		
macs_A	<1x1 struct>		
macs_B	<1x1 struct>		
macs_C	<1x1 struct>		
macs_D	<1x1 struct>		
macs_E	<1x1 struct>		
macs_F	<1x1 struct>		
nist_A	<1x1 struct>		
nist_AA	<1x1 struct>		
nist_B	<1x1 struct>		
nist_BB	<1x1 struct>		
nist_C	<1x1 struct>		
nist_CC	<1x1 struct>		
nist_D	<1x1 struct>		
nist_DD	<1x1 struct>		
nist_E	<1x1 struct>		
nist_EE	<1x1 struct>		
nist_FF	<1x1 struct>		
o1062_A	<1x1 struct>		
o1062_B	<1x1 struct>		
o1062_C	<1x1 struct>		
o1063_A	<1x1 struct>		
o1063_B	<1x1 struct>		
o1063_C	<1x1 struct>		
o1070_A	<1x1 struct>		
o1070_B	<1x1 struct>		
o1070_C	<1x1 struct>		
o1073_A	<1x1 struct>		

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