AMS Analysis Software Overview

Squirrel 1.60

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Data Acquisition (DAQ) data files:

Have either a .hdf or .h5 file extension
Have file name format yymmdd_runNumber_*
File name ends with either *_m (**m**ain) or *_p (for **P**ToF unintegrated, or raw) data.
*_p files will be saved in a different directory named PToF and are generally much larger files than the *_m files
*_p files are only necessary if

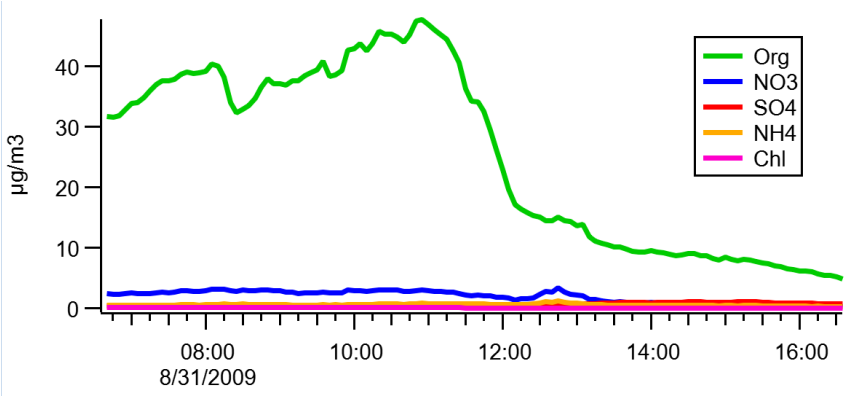
- you want have ePToF data that you want to sum in the PToF dimension OR
- you need to recalculate your PToF sticks OR
- you do high resolution on PToF data (rare)

Name	Date modified	Type	Size
PToF	5/7/2017 8:01 PM	File folder	
090831_044847_m.hdf	6/29/2016 1:31 AM	HDF File	18,769 KB
090831_044887_m.hdf	10/4/2014 9:14 AM	HDF File	18,769 KB
090831_044927_m.hdf	2/10/2010 8:03 AM	HDF File	18,769 KB

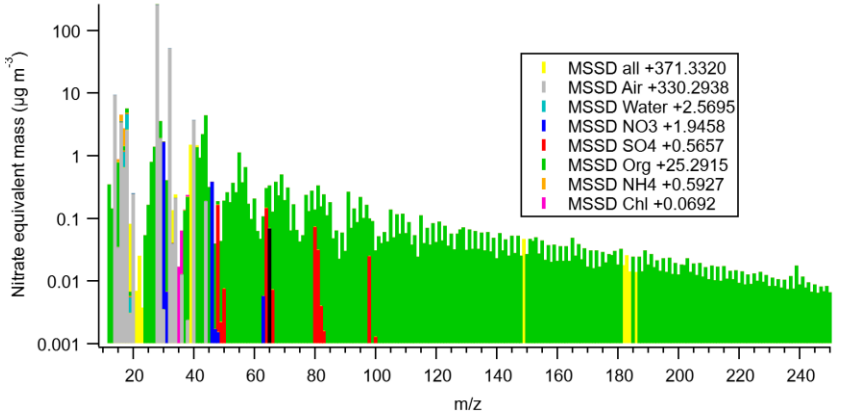
Name	Date modified	Type	Size
090831_044847_p.hdf	2/10/2010 8:03 AM	HDF File	624,179 KB
090831_044887_p.hdf	2/10/2010 8:03 AM	HDF File	624,179 KB
090831_044927_p.hdf	2/28/2015 2:01 AM	HDF File	624,179 KB

Goal for UMR (Unit Mass Resolution) data:

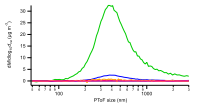
To generate the most precise loadings of:
Organics (Org), Nitrates (NO3), Chloride (Chl), Sulfate (SO4), Ammonium (NH4)
in mainly 3 types of plots:



MS Time Series



Average Mass Spectra

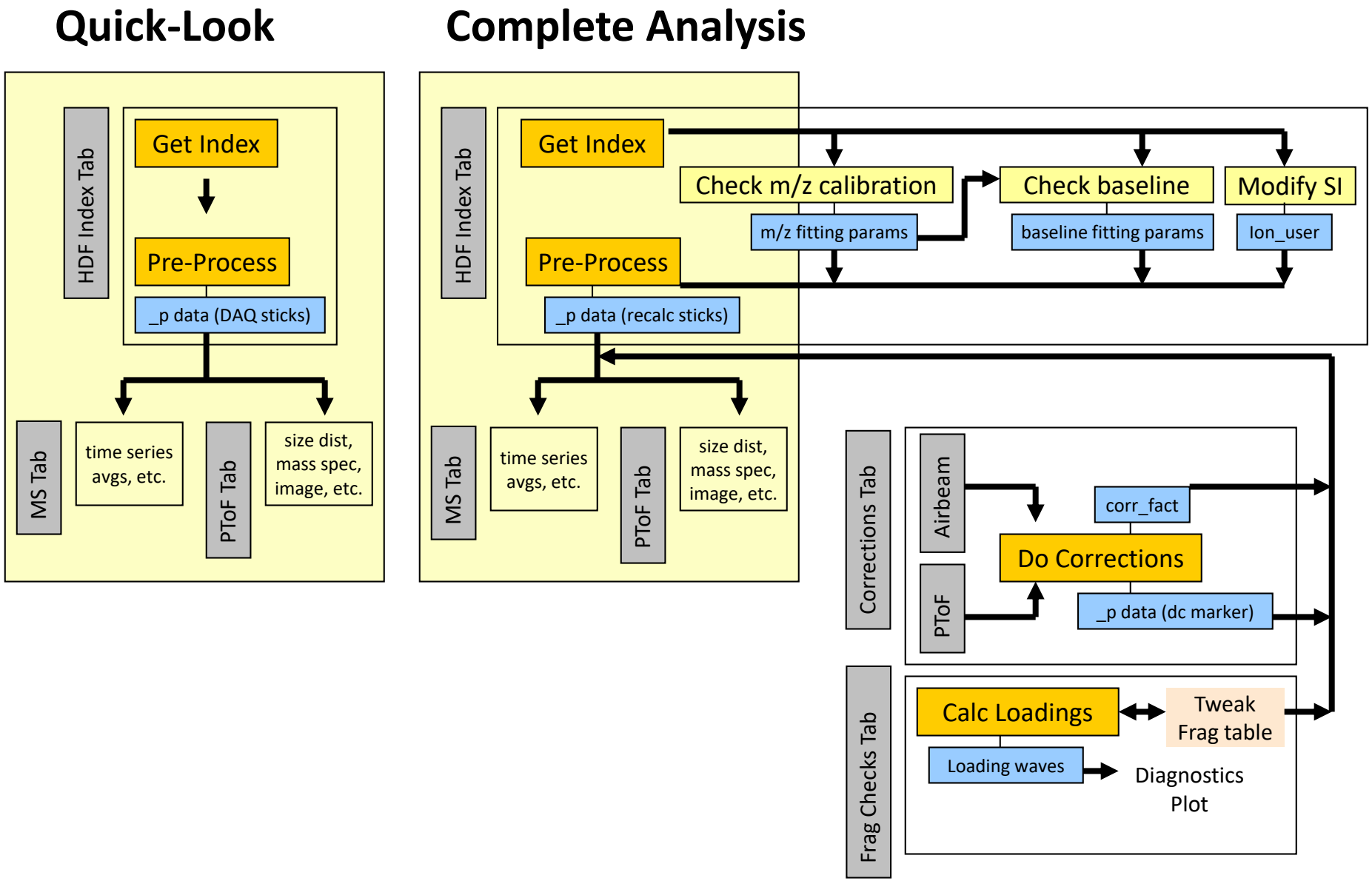


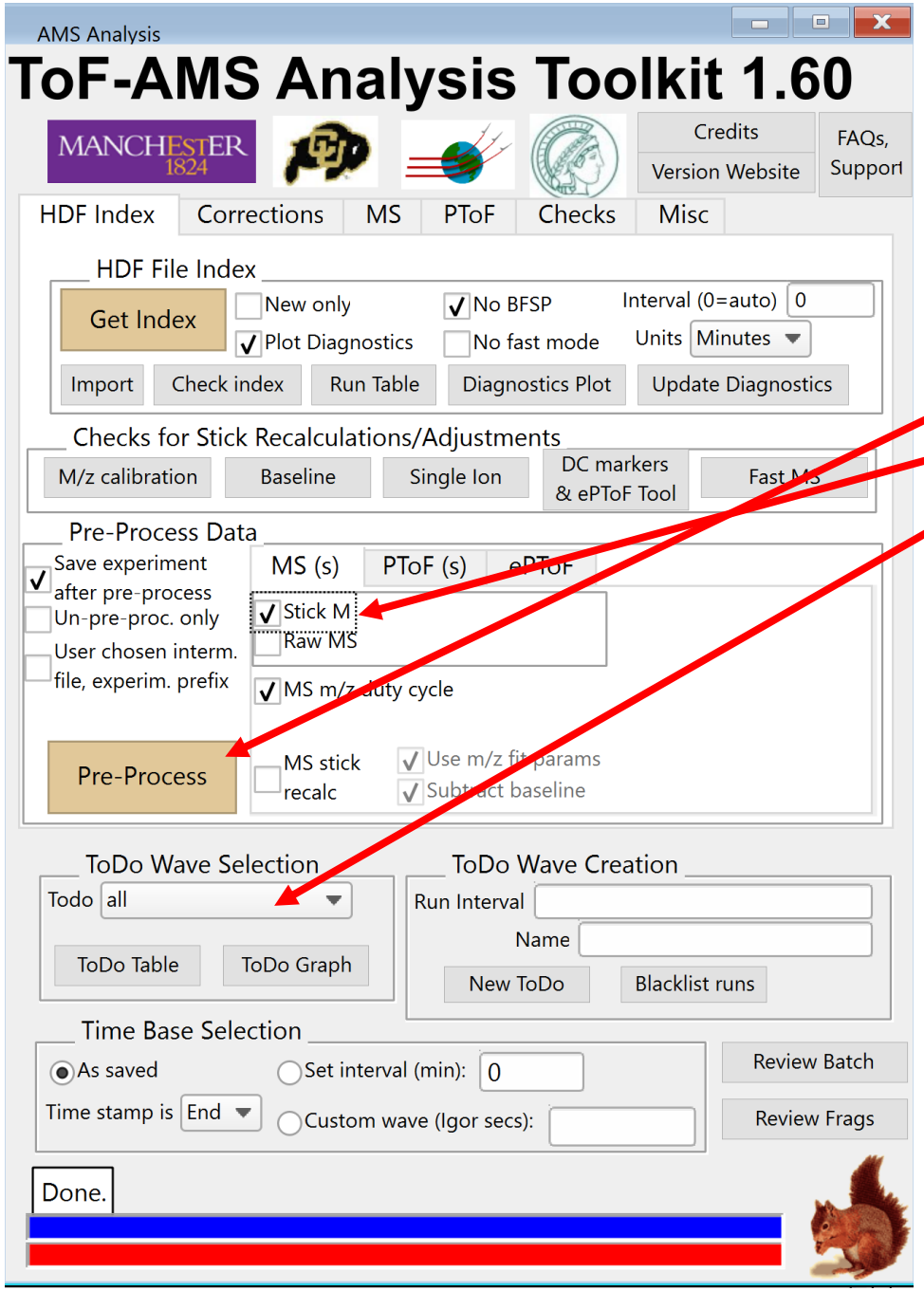
PToF Size Distribution

What is needed to achieve this goal:

- ✓ Accurate UMR integrated spectrum
- ✓ Accurate method for grouping UMR signal to different species
- ✓ Accurate conversion to µg/m^3

Squirrel Analysis Flow Charts





Squirrel 1.60 Analysis tool for all AMS data sets

Requires Igor 6.37 or higher

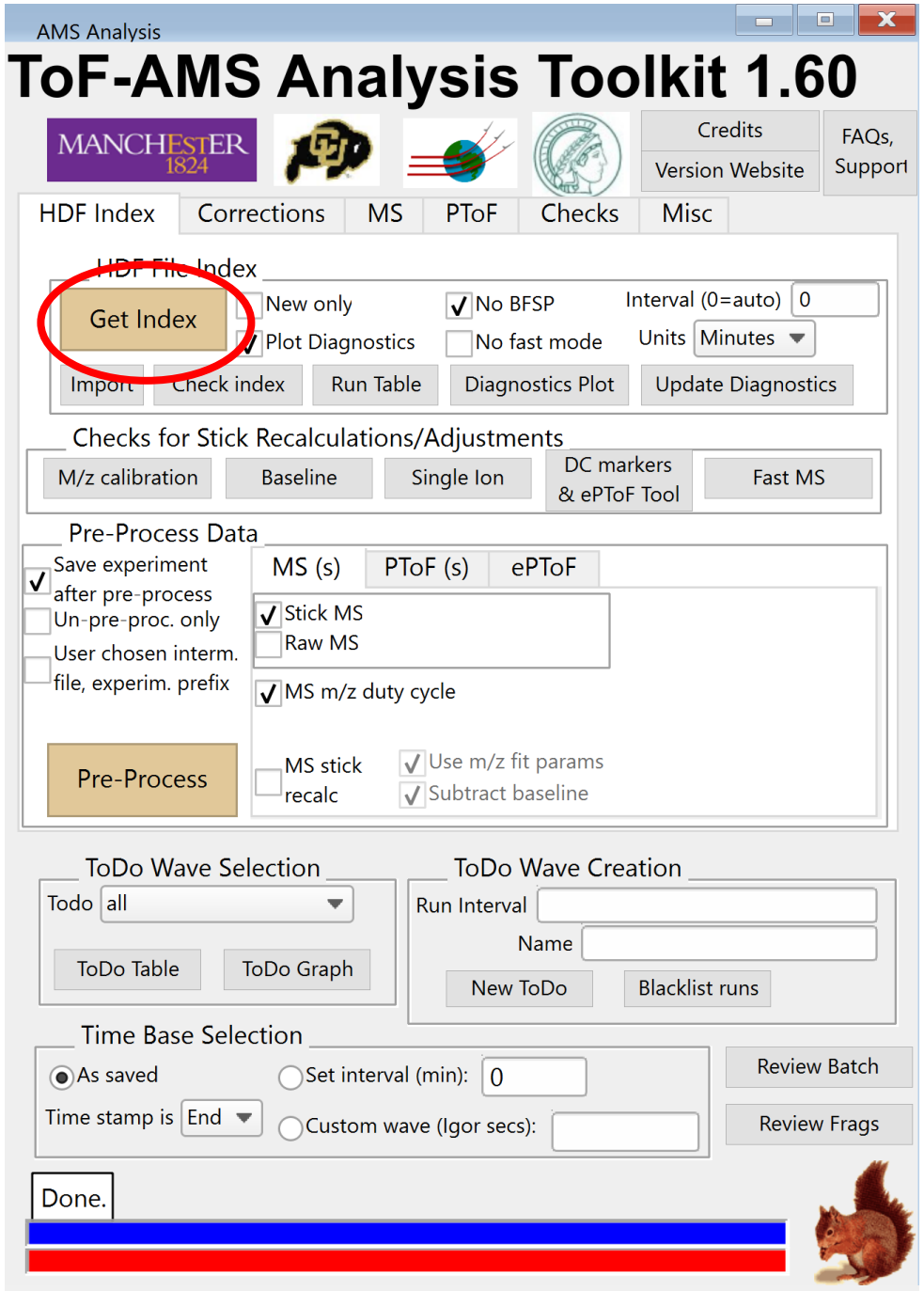
Follow steps in tabs left to right, top to bottom
Gold buttons are either essential or very common

Think of buttons as verbs , i.e. "Do it"
Think of checkboxes as adjectives/adverbs, i.e. "Do it this way"
Think of Todo wave as direct object nouns, i.e. "Do it this way on this"
(A 'Todo" is a grouping of AMS runs)
Think of the history window as a log, i.e. "This is what was done"

Not all data stored in memory; most stored in 'intermediate files"
Intended to be very flexible

Web site that describes software:
http://cires1.colorado.edu/jimenez-group/wiki/index.php/ToF-AMS_Analysis_Software

Web site that describes analysis steps:
http://cires1.colorado.edu/jimenez-group/wiki/index.php/Field_Data_Analysis_Guide



Get Index

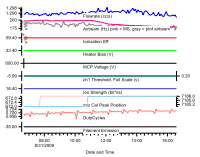
Always step #0

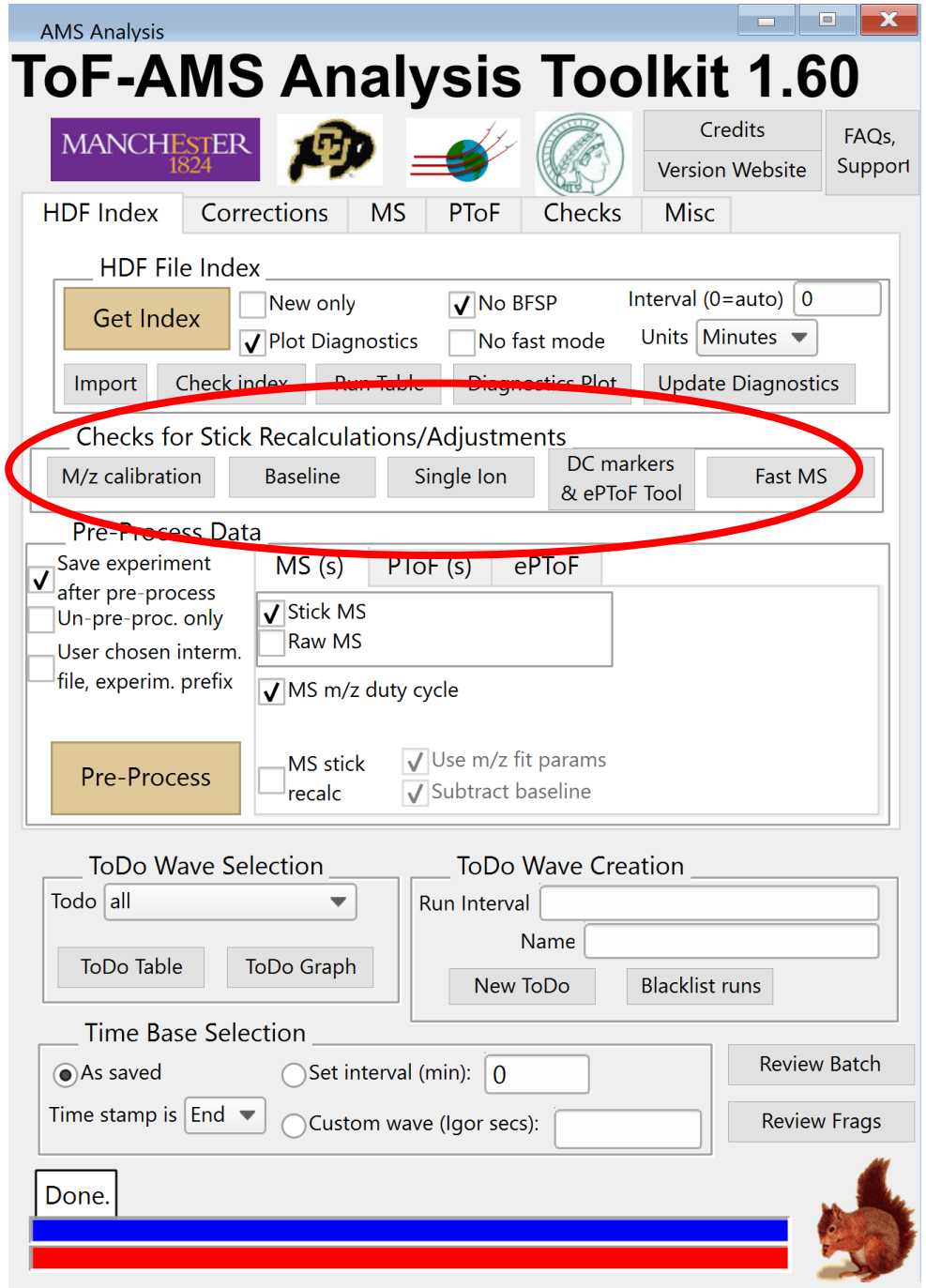
Asks where to find the DAQ files

Maintains a system of saving and retrieving all data sets (only parts of DAQ files are loaded and saved into memory)

Does not load in any spectra

Generate a diagnostics plot which indicates general instrument conditions





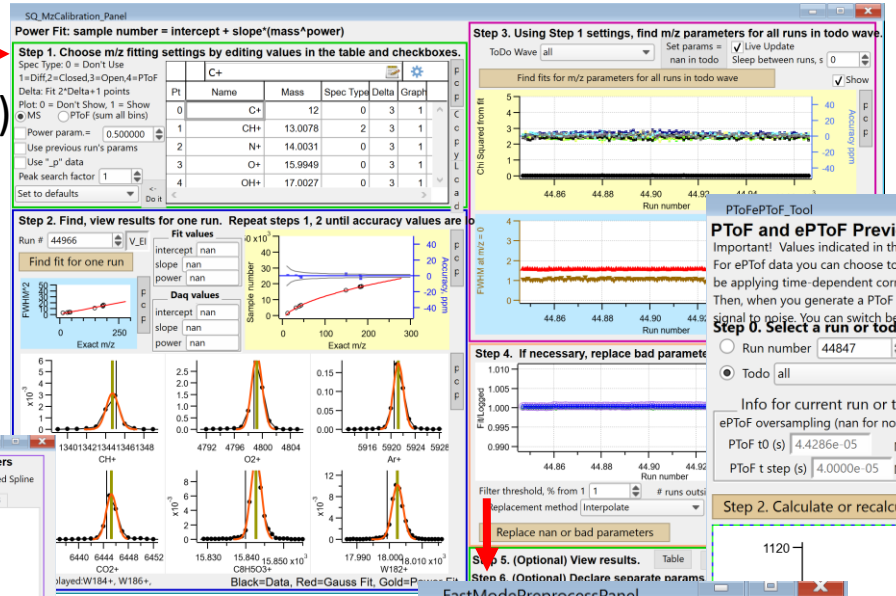
✓ **Accurate UMR integrated spectrum**

Requires:

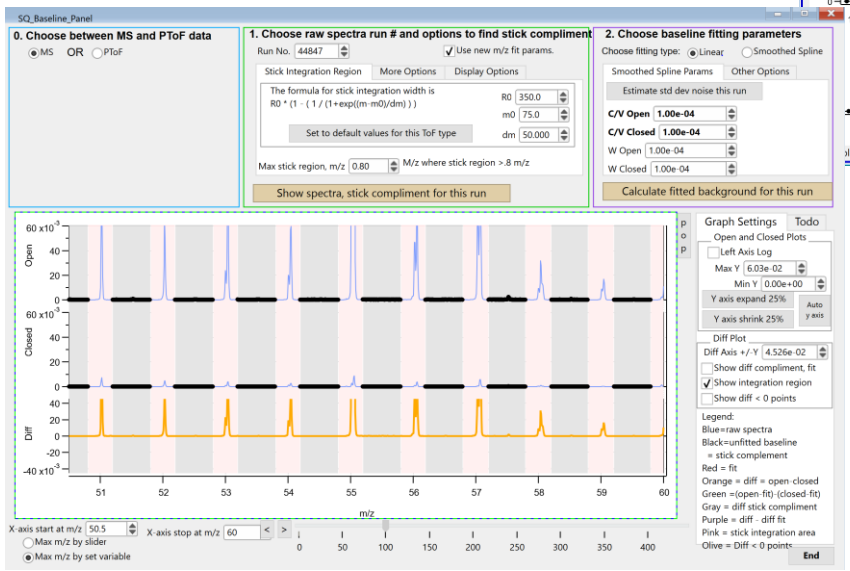
- Good m/z calibration
- Good designation of integration region and spectral baseline subtraction
- Conversion from bits to ion counts (result in Hz)
- For PToF, DC marker settings, which subtract an estimated background (similar to MS Closed)
- For Fast Mode data interpolated Fast MS Closed (rare)

✓ **Accurate UMR integrated spectrum 'finalize sticks'**

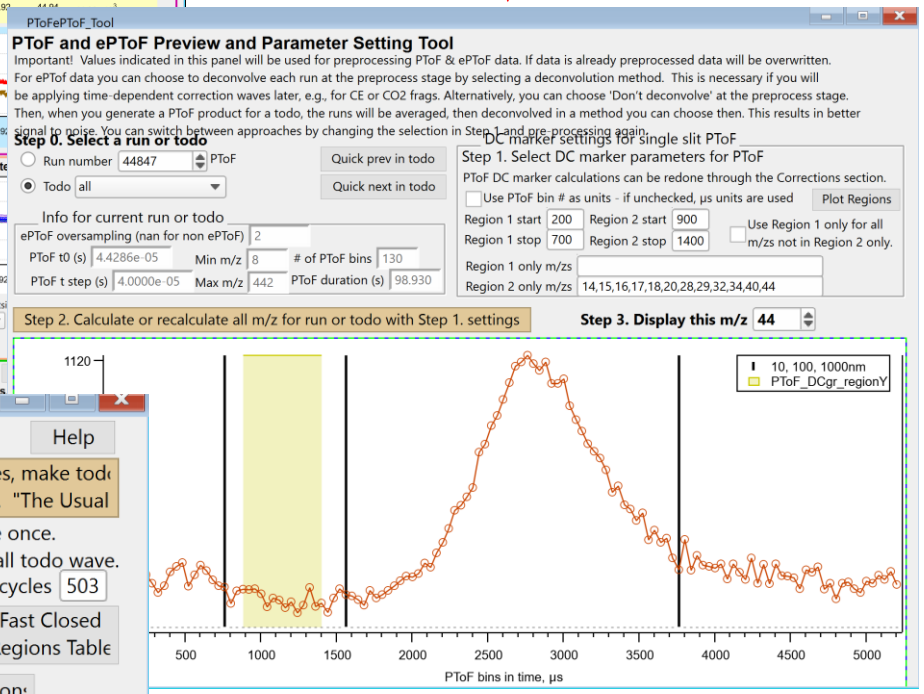
Good m/z calibration panel
(Each run has m/z calibration parameters)

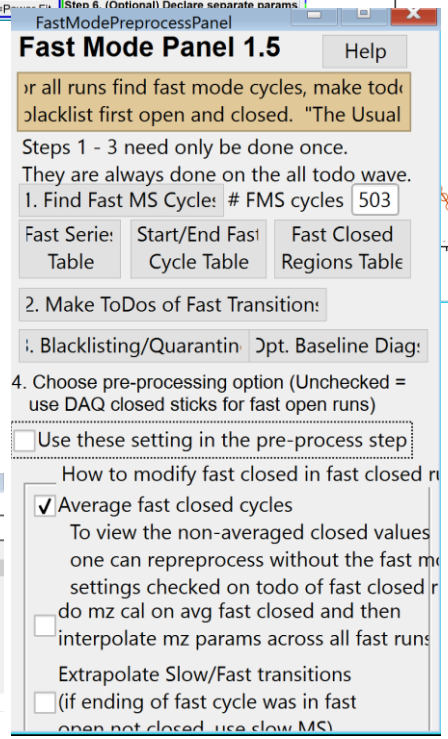


Baseline, UMR integration panel
(One set of settings for each tuning)



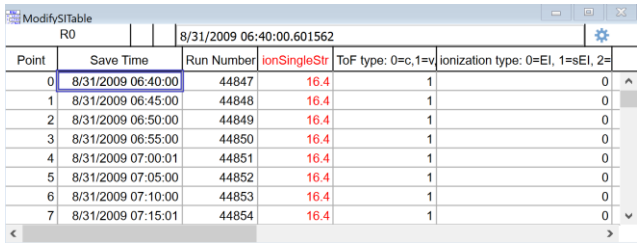
PToF DC Marker settings
(Optional ePToF settings)



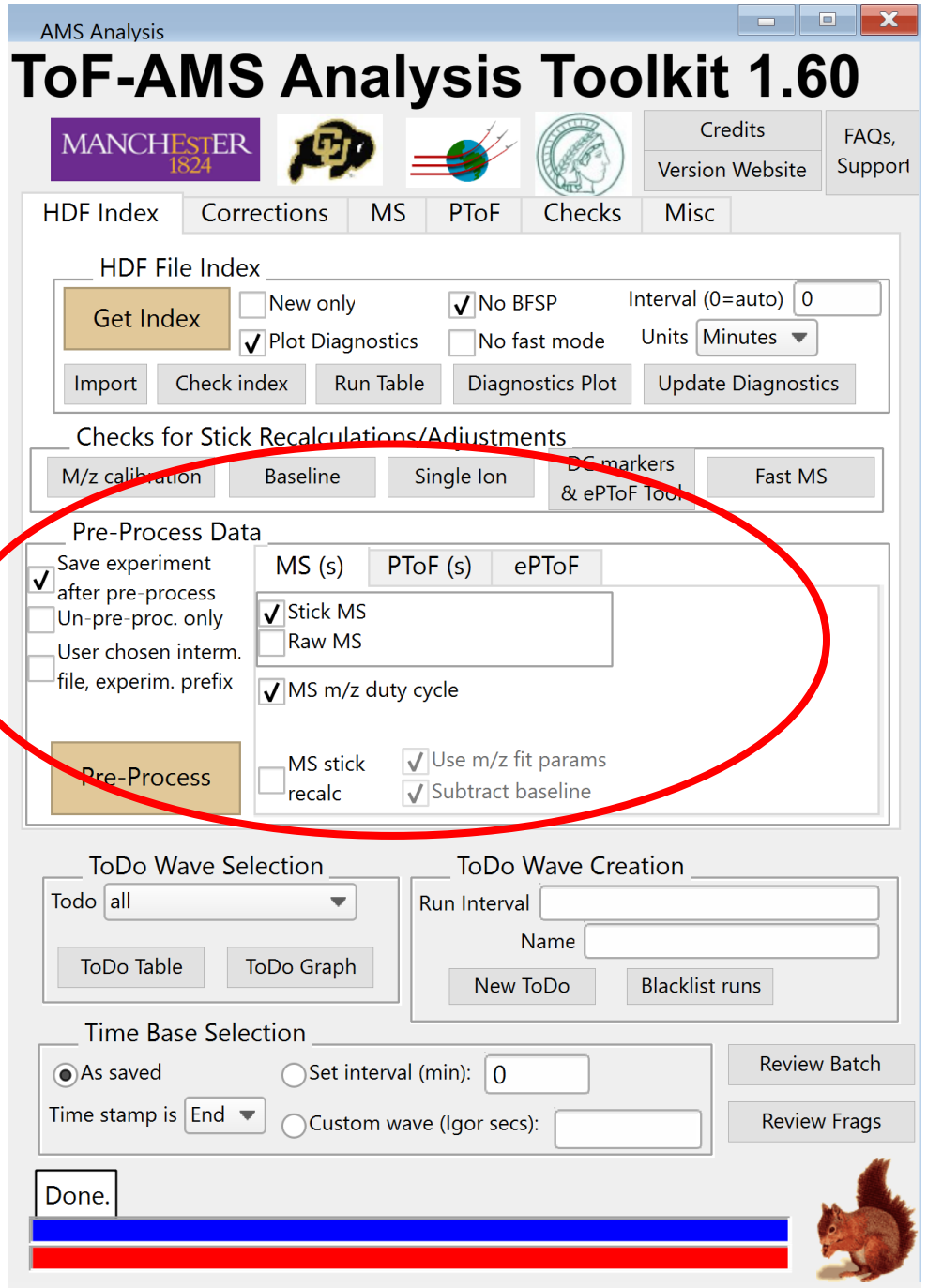


Fast Mode Settings
(Describe how to interpolate fast MS Closed spectra. Rare, except for aircraft platforms)

Single ion Table
Single ion unit is ions/bits



Point	Save Time	Run Number	ionSingleStr	ToF type: 0=c,1=v	ionization type: 0=EI, 1=sEI, 2=
0	8/31/2009 06:40:00	44847	16.4	1	0
1	8/31/2009 06:45:00	44848	16.4	1	0
2	8/31/2009 06:50:00	44849	16.4	1	0
3	8/31/2009 06:55:00	44850	16.4	1	0
4	8/31/2009 07:00:01	44851	16.4	1	0
5	8/31/2009 07:05:00	44852	16.4	1	0
6	8/31/2009 07:10:00	44853	16.4	1	0
7	8/31/2009 07:15:01	44854	16.4	1	0

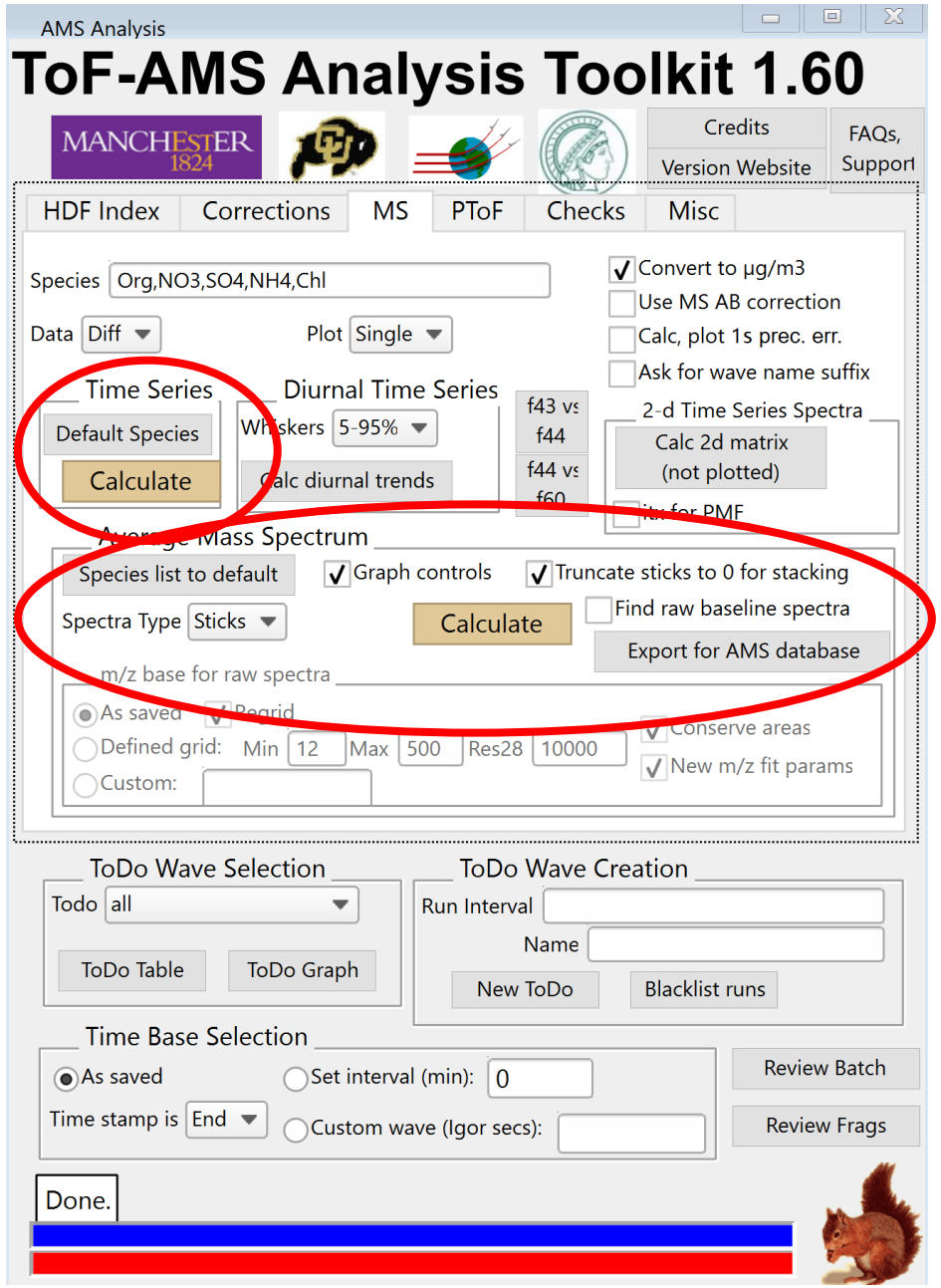


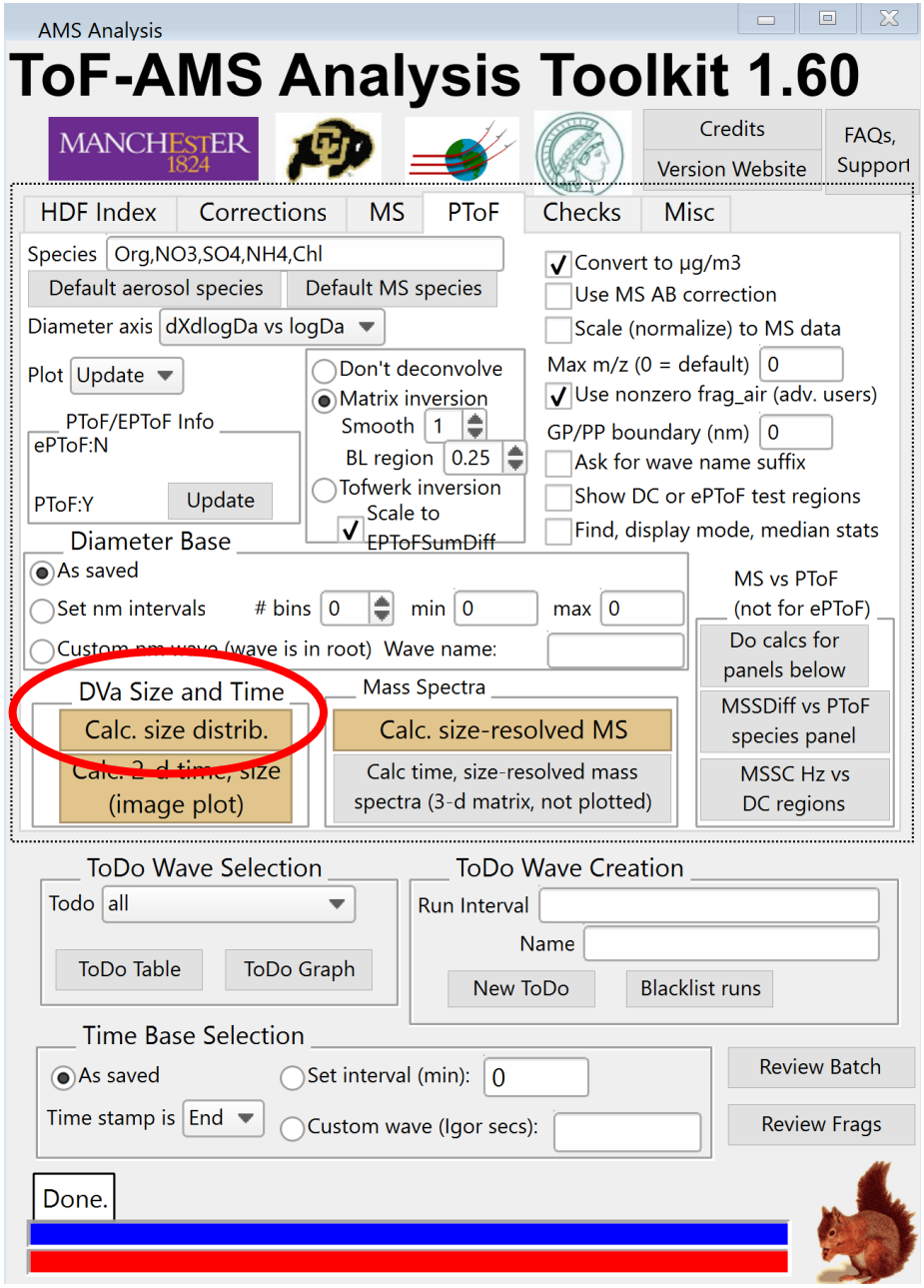
✓ **Accurate UMR integrated spectrum 'finalize sticks'**

After all the settings have been investigated, we finalize UMR sticks.
Typically one recalculates UMR sticks using all the settings that have just been investigated.
"Raw" MS = unintegrated
"Stick" MS = integrated
There is a section for each type of data:
MS, PToF, ePToF, and one can do each data set independently or all together.

Pressing the "Preprocess" button pushes generates "intermediate" files, which contains spectra processed according to the new settings previously found in the m/z calilbration, baseline, etc. steps

At this point, one is able to generate all thedata products identified: MS time series, Average mass spectra, PToF size distribution

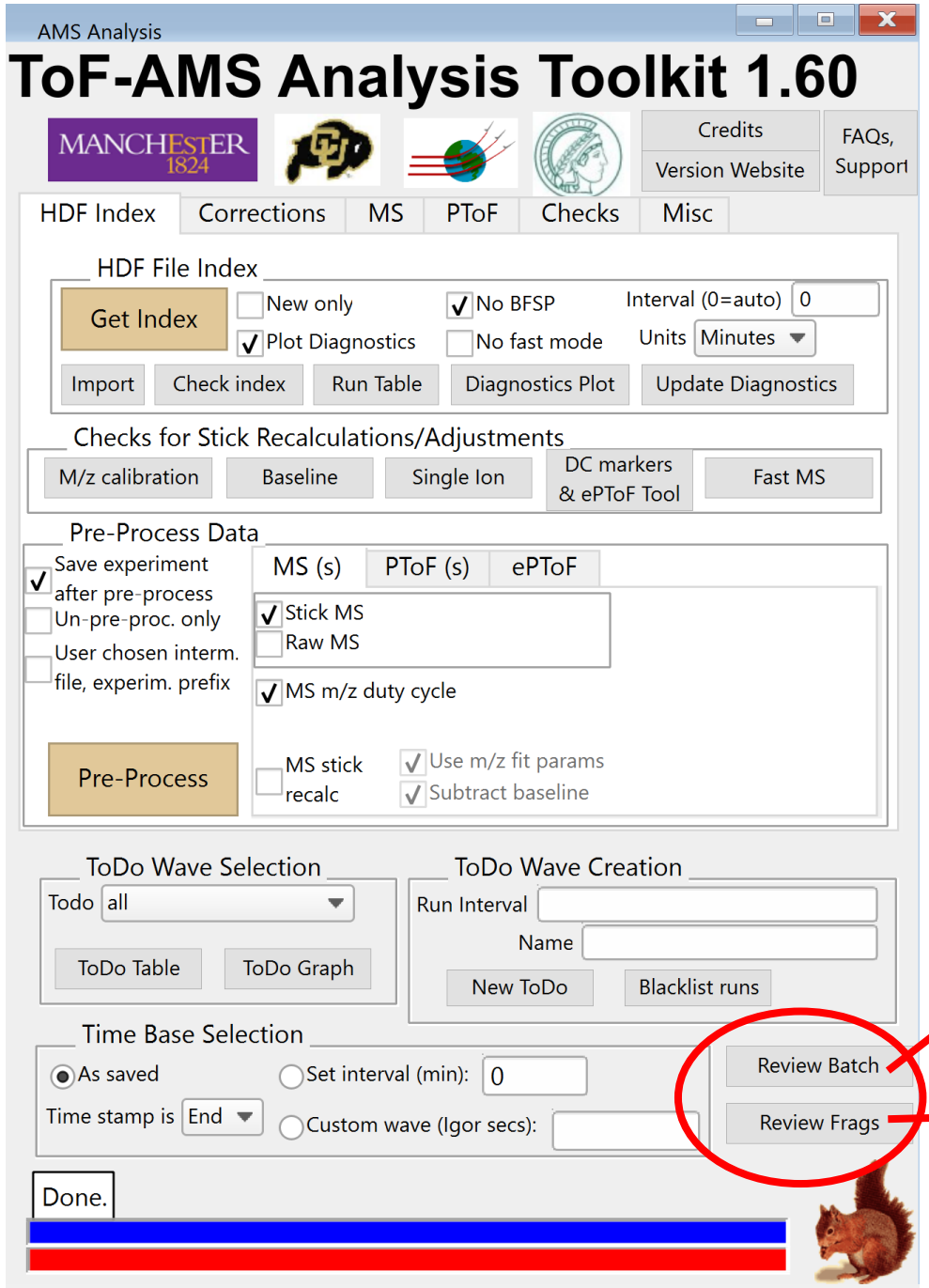




✓ **Accurate method for grouping UMR signal to different species**

Batch table defines species

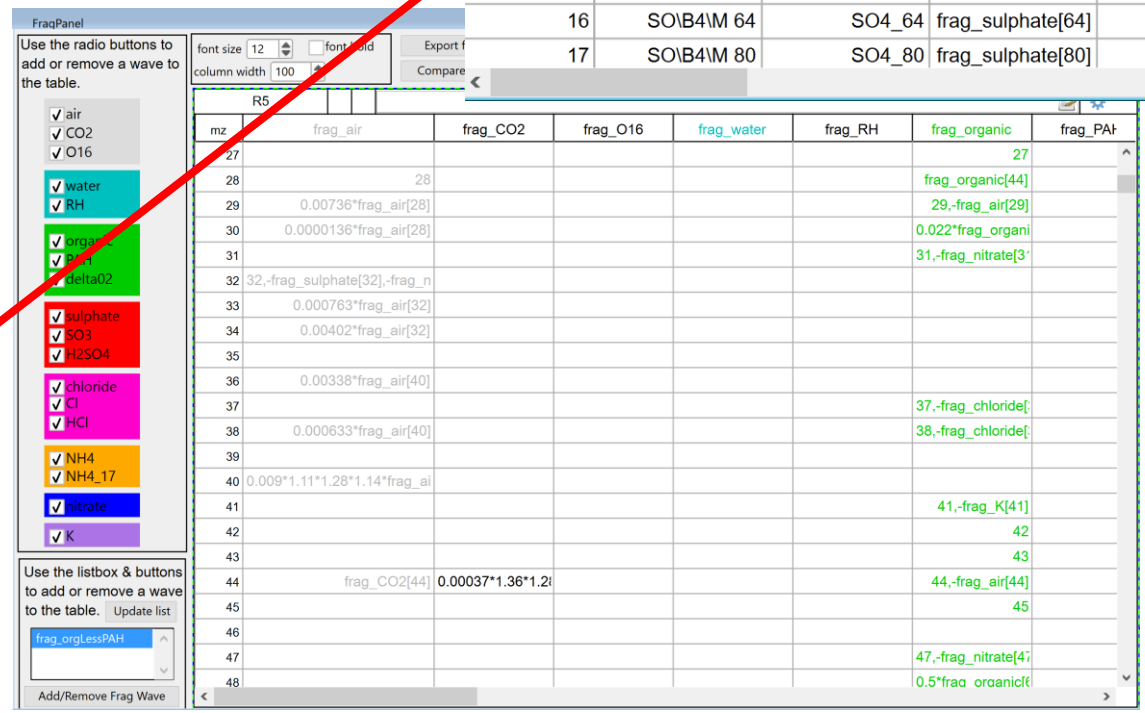
Frag ('fragment') table apportions UMR signals to species

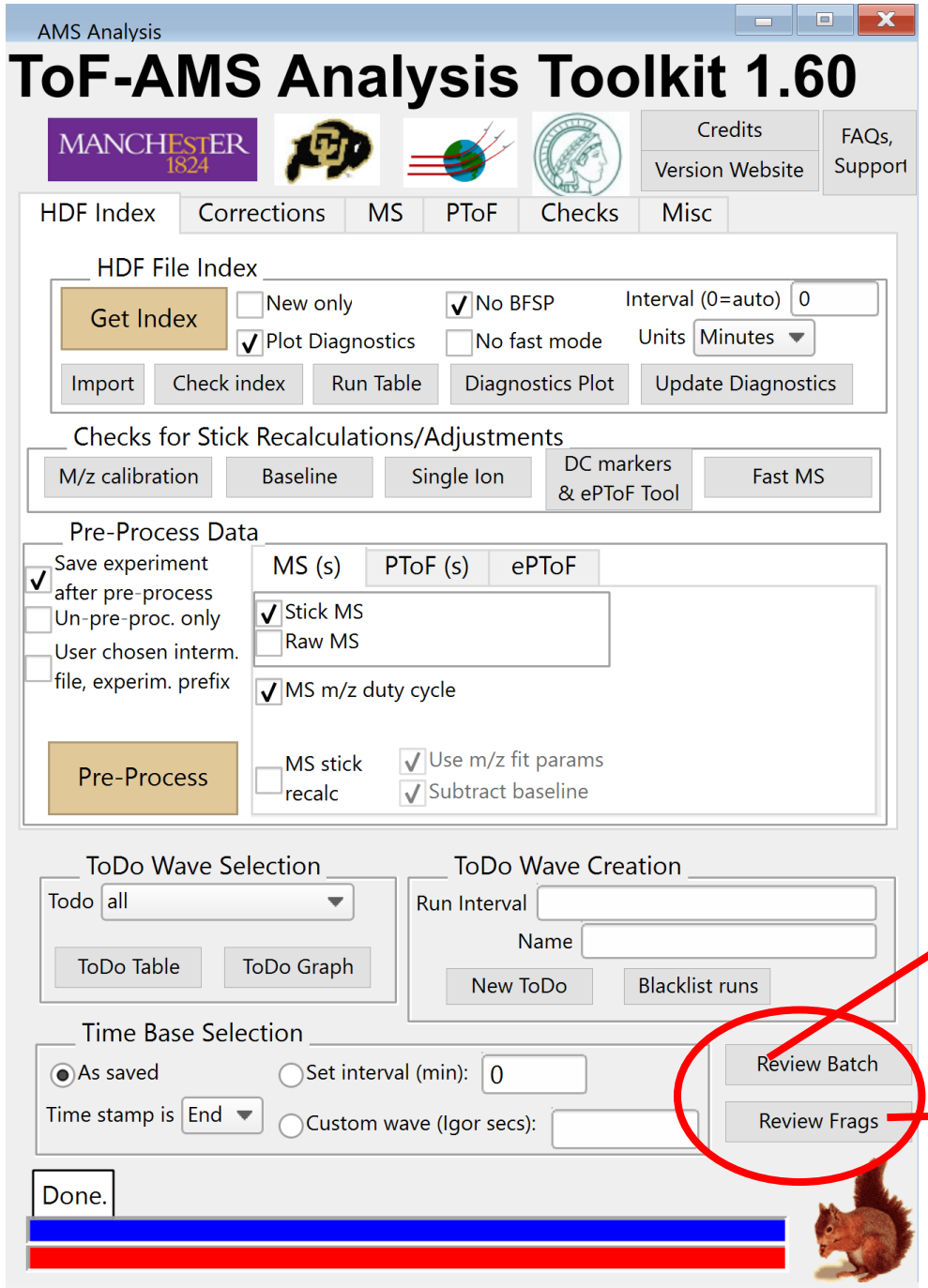


ReviewBatchTable

R10 | frag_organic

Point	specname_list	spec_list	frag_list	IEfac_list
3	CO\B2\M (air)	CO2_air	frag_CO2	1
4	Water	Water	frag_water	1
5	Ammonium	NH4	frag_NH4	4
6	Nitrate	NO3	frag_nitrate	1.1
7	Sulphate	SO4	frag_sulphate	1.2
8	SO\B3\M	SO3	frag_SO3	1.2
9	H\B2\MSO\B4\M	H2SO4	frag_H2SO4	1.2
10	Organics	Org	frag_organic	1.4
11	Chloride	Chl	frag_chloride	1.3
12	Total	Total	$NH4,$NO3,$SO4	1
13	NH\B4\M 16	NH4_16	frag_NH4[16]	4
14	NH\B4\M 17	NH4_17	frag_NH4[17]	4
15	SO\B4\M 48	SO4_48	frag_sulphate[48]	1.2
16	SO\B4\M 64	SO4_64	frag_sulphate[64]	1.2
17	SO\B4\M 80	SO4_80	frag_sulphate[80]	1.2





✓ **Accurate method for grouping UMR signal to different species**

Batch table defines species

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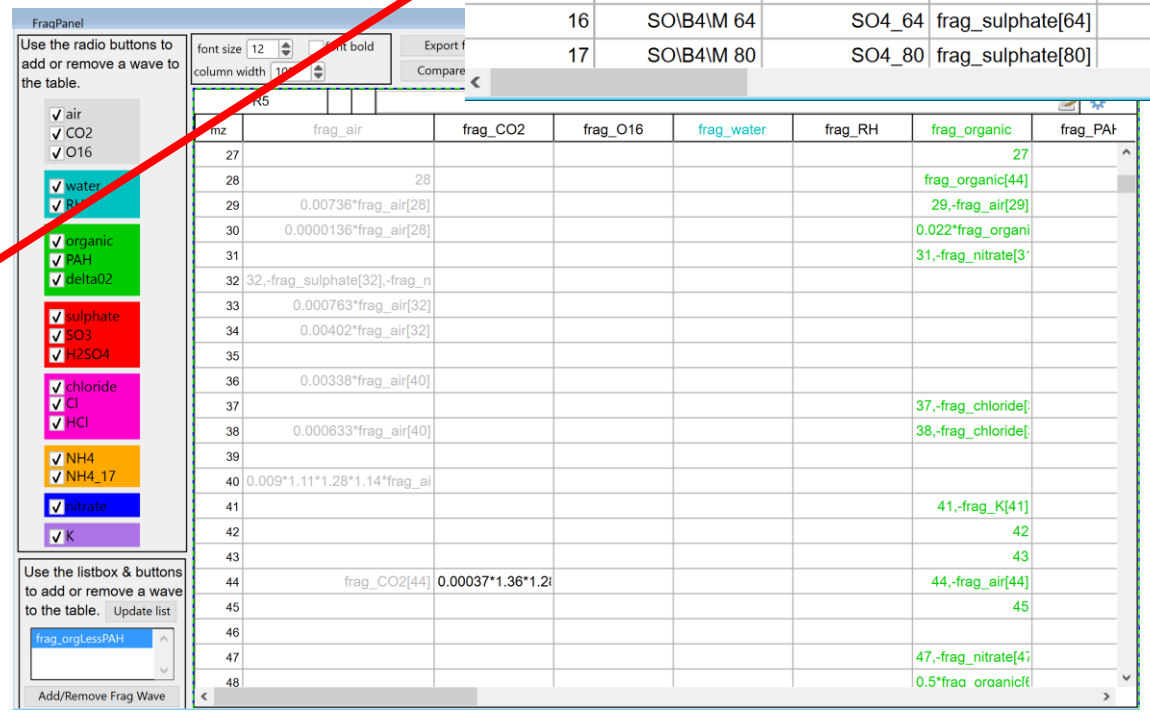
ReviewBatchTable

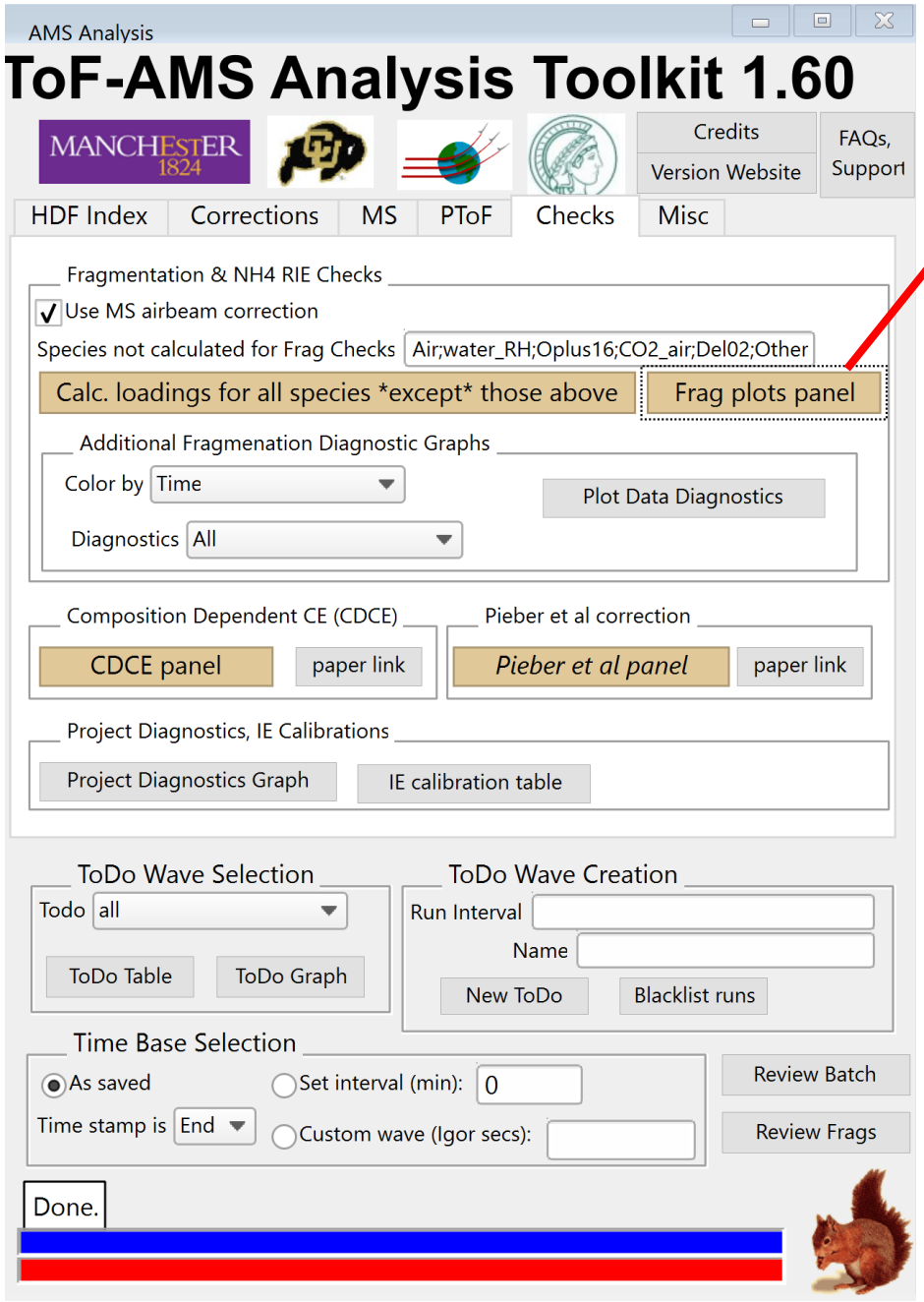
R10 | frag_organic

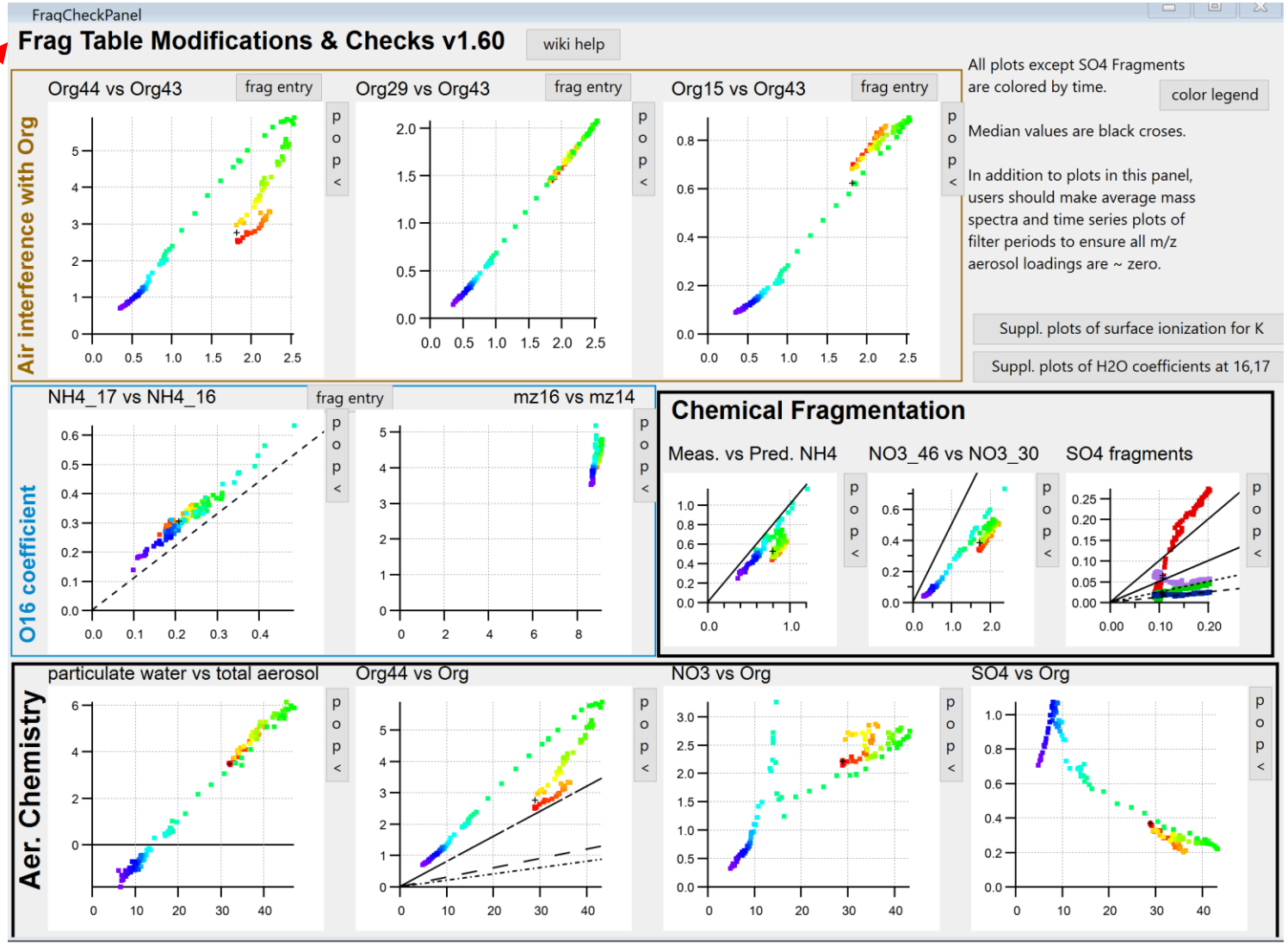
Point	specname_list	spec_list	frag_list	IEfac_list
3	CO\B2\M (air)	CO2_air	frag_CO2	1
4	Water	Water	frag_water	1
5	Ammonium	NH4	frag_NH4	4
6	Nitrate	NO3	frag_nitrate	1.1
7	Sulphate	SO4	frag_sulphate	1.2
8	SO\B3\M	SO3	frag_SO3	1.2
9	H\B2\MSO\B4\M	H2SO4	frag_H2SO4	1.2
10	Organics	Org	frag_organic	1.4
11	Chloride	Chl	frag_chloride	1.3
12	Total	Total	$NH4,$NO3,$SO4	1
13	NH\B4\M 16	NH4_16	frag_NH4[16]	4
14	NH\B4\M 17	NH4_17	frag_NH4[17]	4
15	SO\B4\M 48	SO4_48	frag_sulphate[48]	1.2
16	SO\B4\M 64	SO4_64	frag_sulphate[64]	1.2
17	SO\B4\M 80	SO4_80	frag_sulphate[80]	1.2

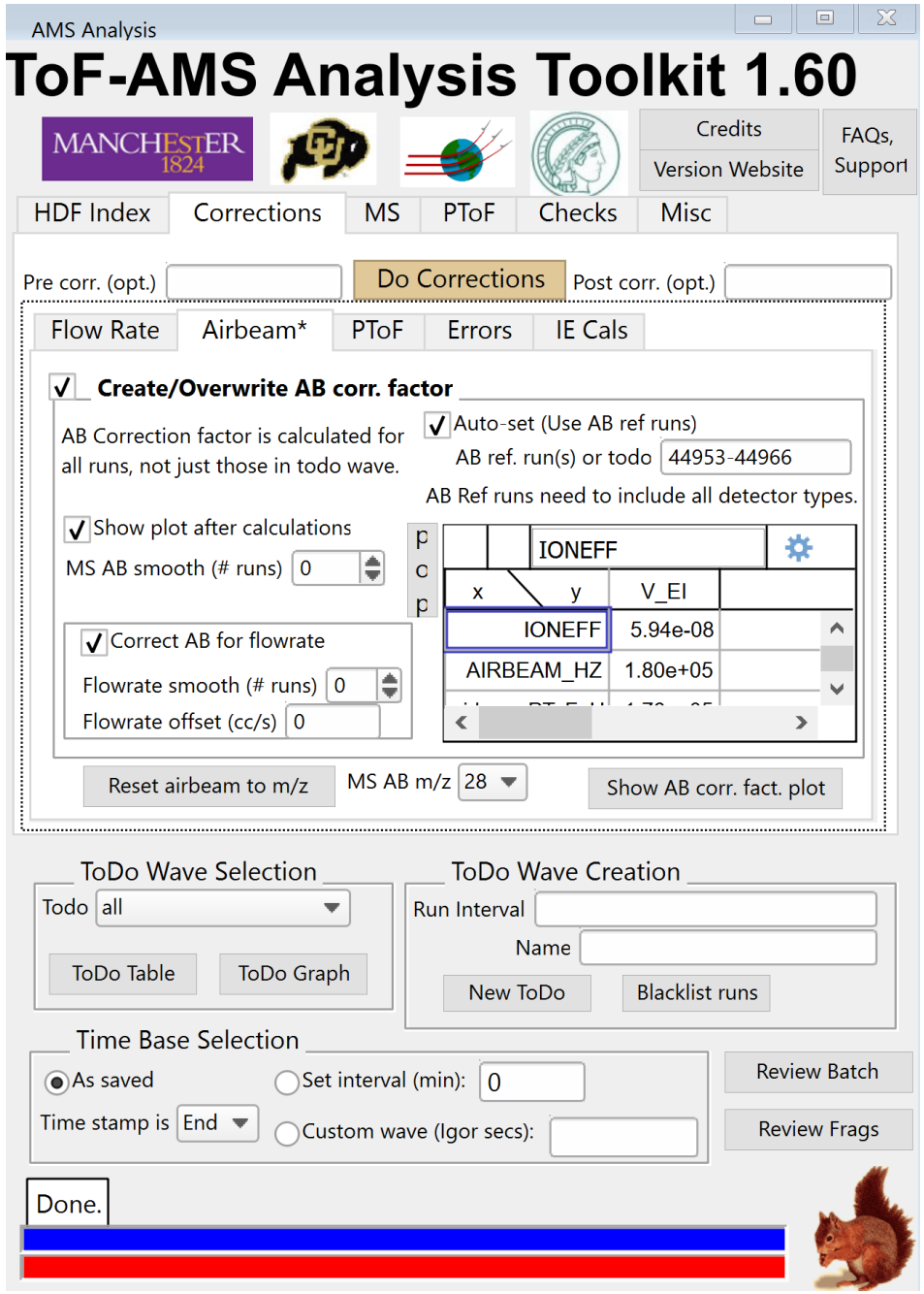


✓ Accurate method for grouping UMR signal to different species

Some frag table adjustments must be made for each instrument, data set
A panel is provided to guide you through the important correlations to examine.







- ✓ **Accurate conversion from ion counts to µg/m³**

Includes, but is not limited to

- AB (airbeam) correction factor
- RIE (relative ionization efficiency)
- CE (collection efficiency)
- PToF size calibration
- Flow calibration
- Perhaps other frag table adjustments (i.e. Time dependent CO2 frag wave)
- Perhaps Error calculation

See http://cires1.colorado.edu/jimenez-group/wiki/index.php/Field_Data_Analysis_Guide

Let the science begin!