ACSM Analysis Tutorial

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Wavemetrics Igor Pro

Aerodyne offers software analysis tools for its mass spectrometer products without charge to our users. Our software tools run inside the Wavemetrics, Inc. Igor application software which is not freely distributed. We remind you that Aerodyne instruments are delivered with a single-seat Igor license that can be used for running Aerodyne data analysis tools available on this page or any other data analysis. The Wavemetrics license is limited to one user at any given time, but can involve multiple computers. Users who need more seats should acquire additional licenses from Wavemetrics. (https://www.wavemetrics.com/order/order.htm)

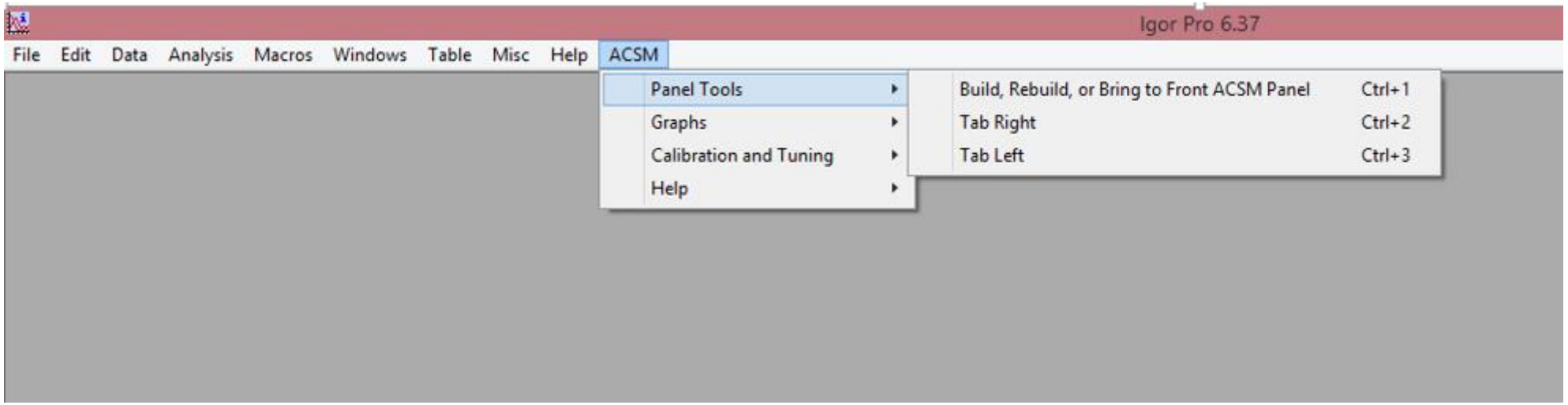
Basic Analysis Software

- acsm_local_abcd.ipf (version a.b.c.d) most recent is 1.6.0.3
  - Bulk of ACSM Specific routines for real-time and off-line analysis
- GlobalUtils.ipf
  - General purpose Igor utilities originally written by Scott Herndon, now maintained by Tara Yacovitch
- Both of these are required for ACSM analysis
- Compatible with Igor 6 and Igor 7

Other random tools

- ACSM_ExtraProcs_0000.ipf
- ACSM_ErrorCalculator_0101.ipf
- ACSM_Export_0022.ipf
- ACSM_mzScatterPlotMaker_1001.ipf
- ACSM_CMSMatrices.ipf

- This summer will see a push on integrating these into main package.



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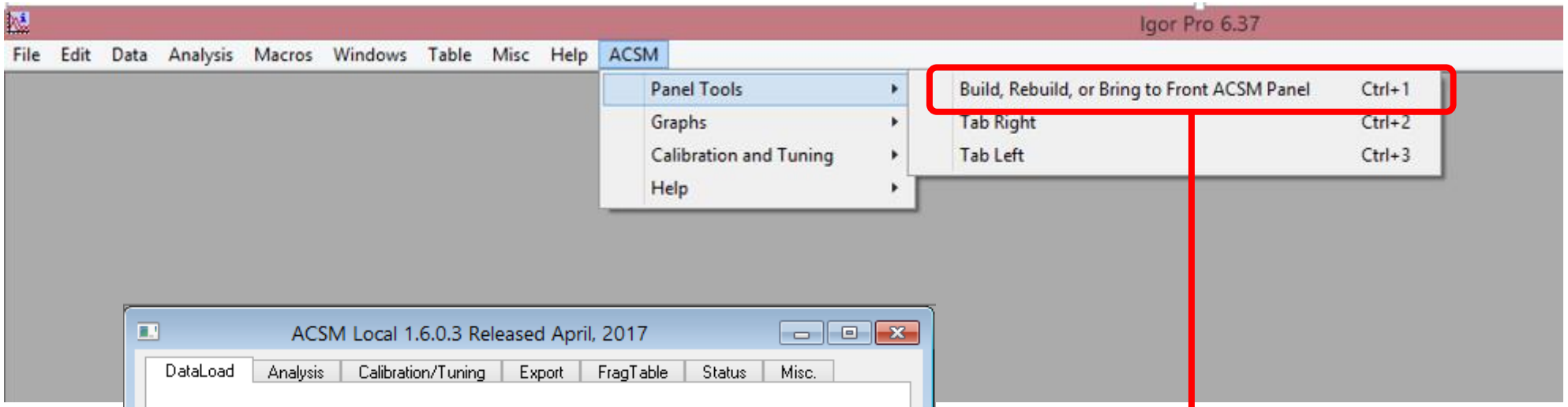
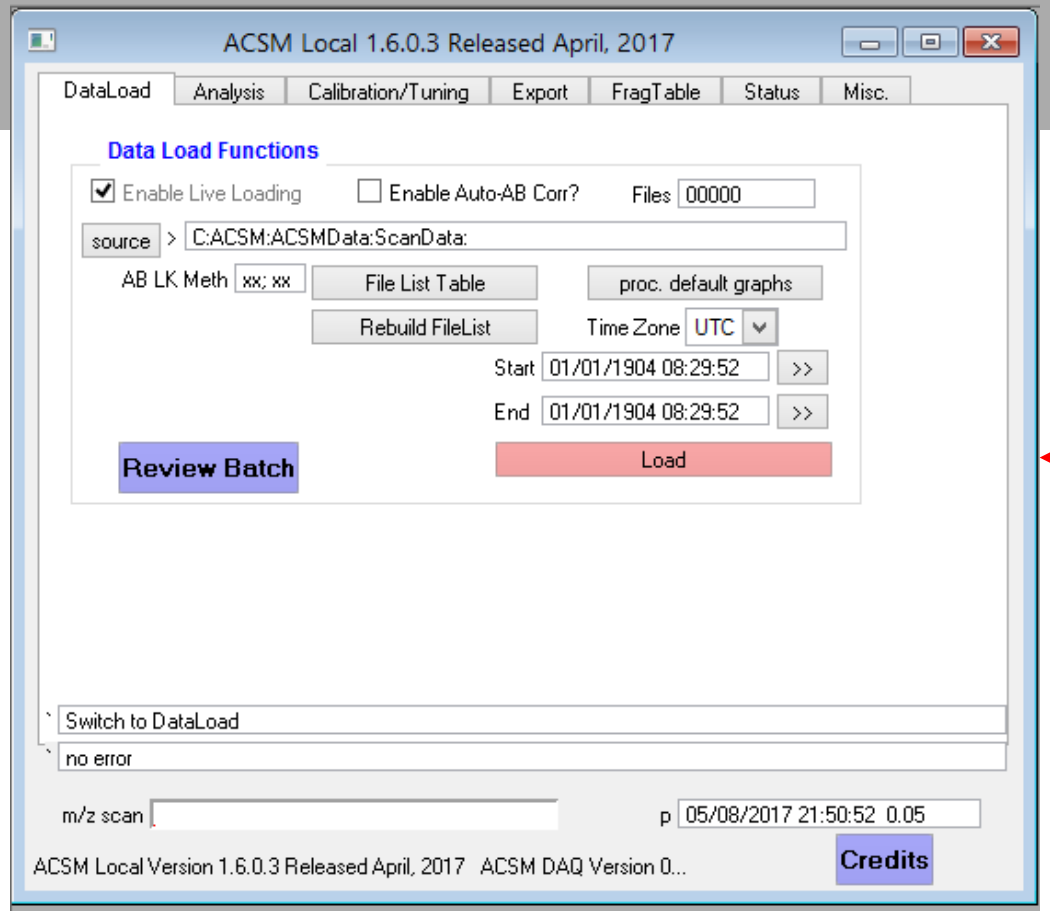
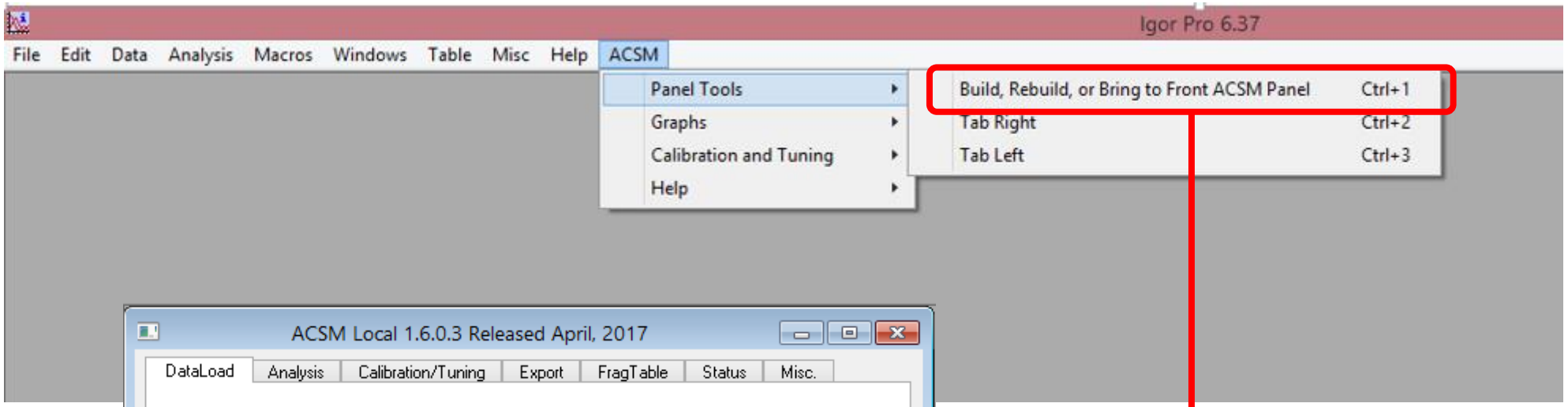
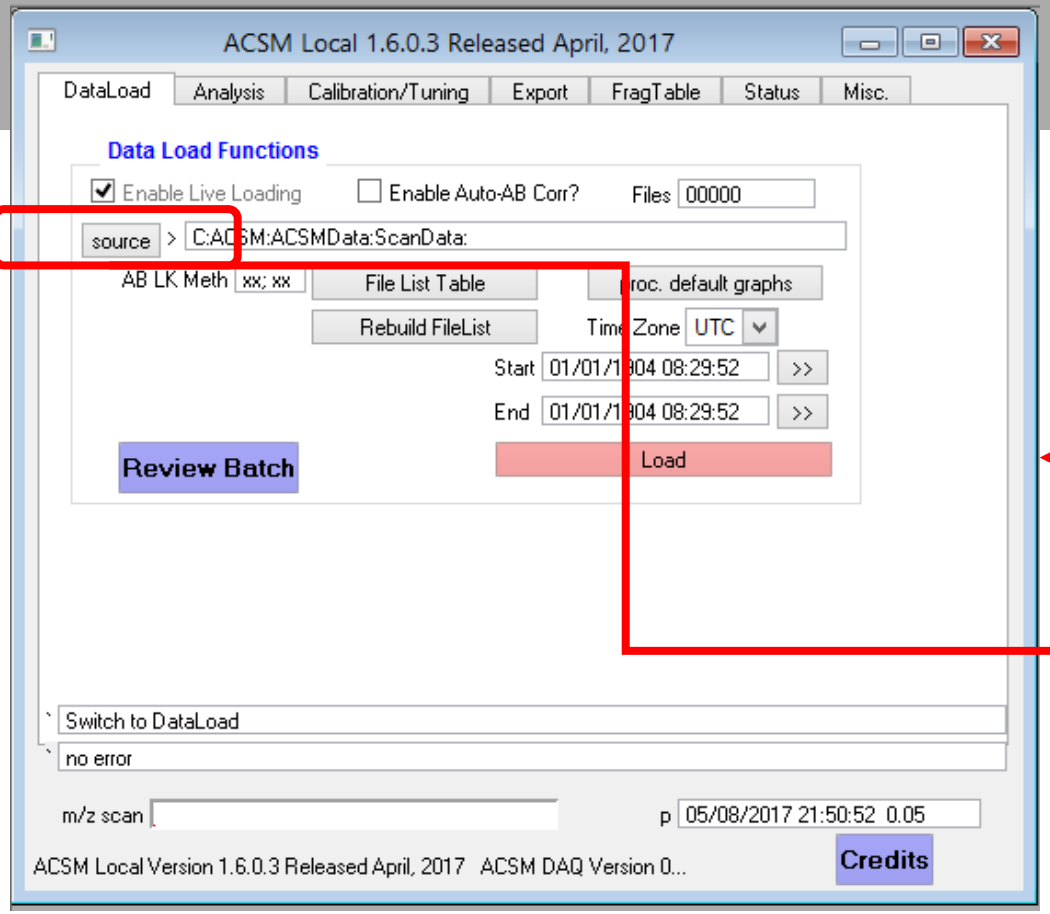
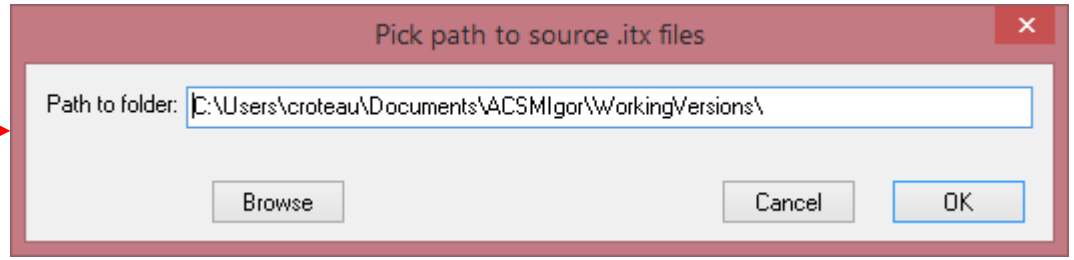
In Igor with ACSM_Local and GlobalUtils loaded in, we have an ACSM drop down menu with a bunch of tools.
First step is Build the Panel, you can click or hit Ctrl+1


Igor Pro 6.37
File Edit Data Analysis Macros Windows Table Misc Help ACSM
Panel Tools
Graphs
Calibration and Tuning
Help
Build, Rebuild, or Bring to Front ACSM Panel Ctrl+1
Tab Right Ctrl+2
Tab Left Ctrl+3

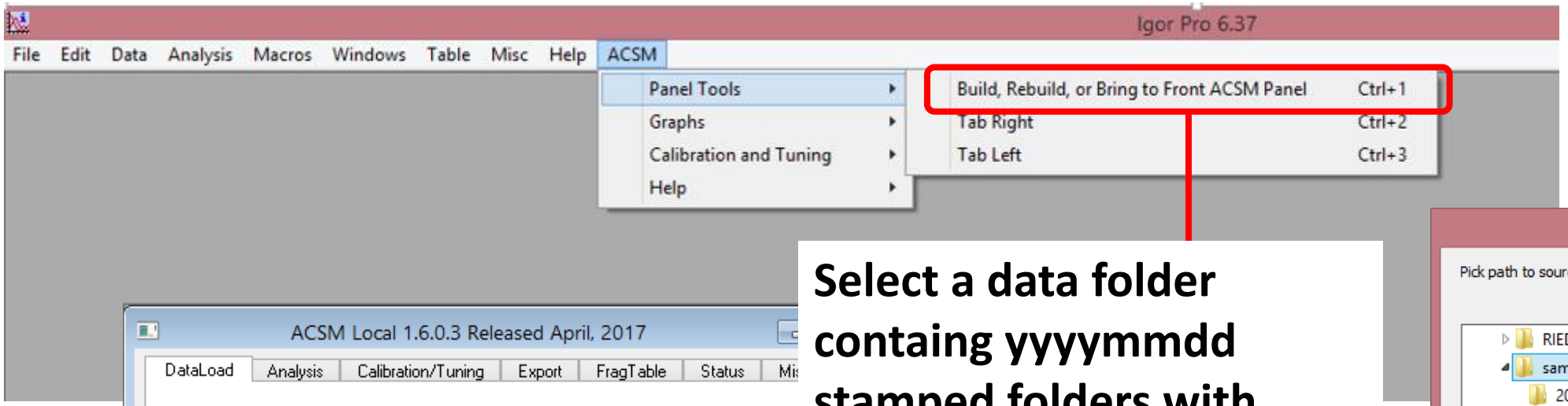

ACSM Local 1.6.0.3 Released April, 2017
DataLoad
Analysis
Calibration/Tuning
Export
FragTable
Status
Misc.
Data Load Functions
Enable Live Loading
Enable Auto-AB Corr?
Files 00000
source
C:ACSM:ACSMData:ScanData:
AB LK Meth xx; xx
File List Table
proc. default graphs
Rebuild FileList
Time Zone UTC
Start 01/01/1904 08:29:52
End 01/01/1904 08:29:52
Review Batch
Load
Switch to DataLoad
no error
m/z scan
p 05/08/2017 21:50:52 0.05
ACSM Local Version 1.6.0.3 Released April, 2017 ACSM DAQ Version 0...
Credits



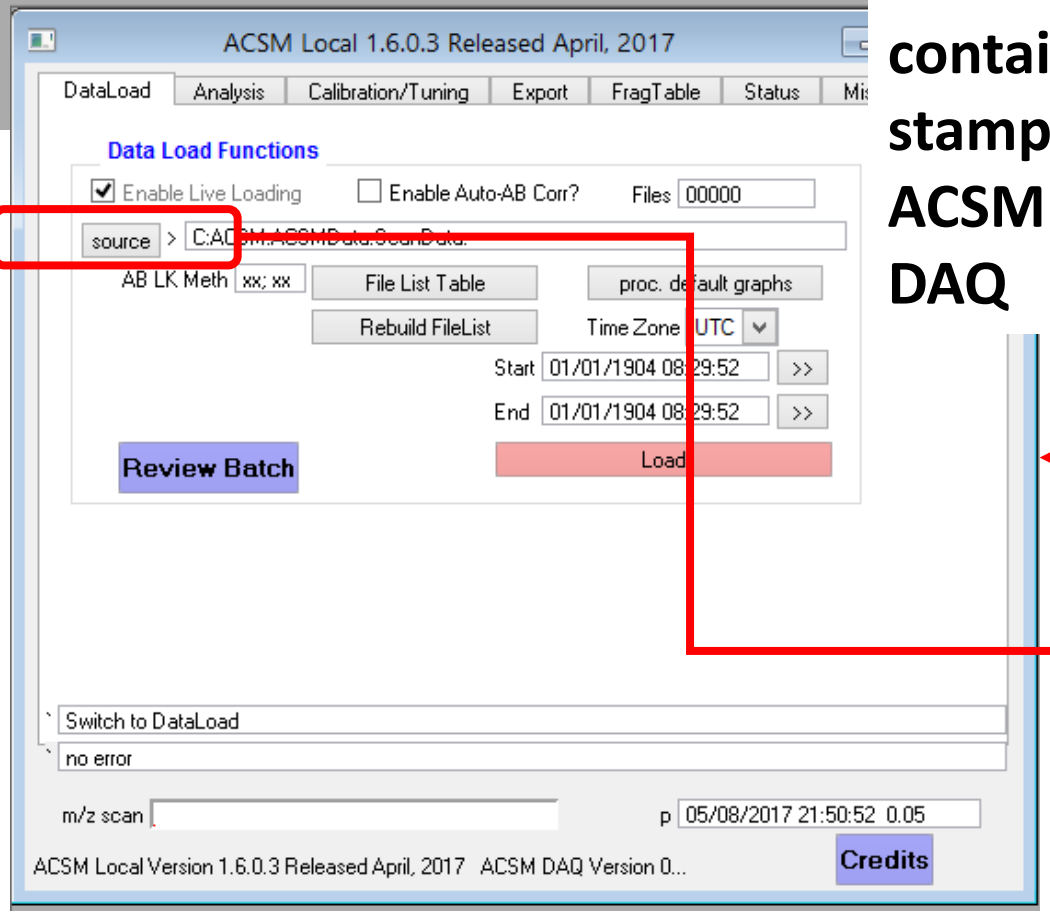


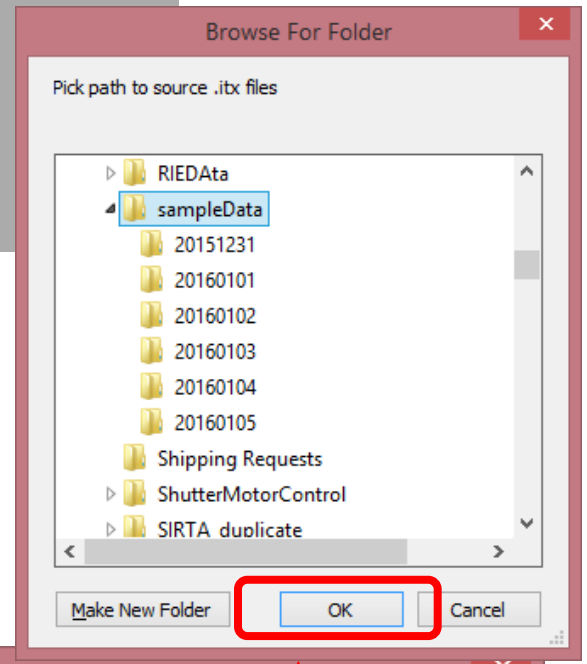


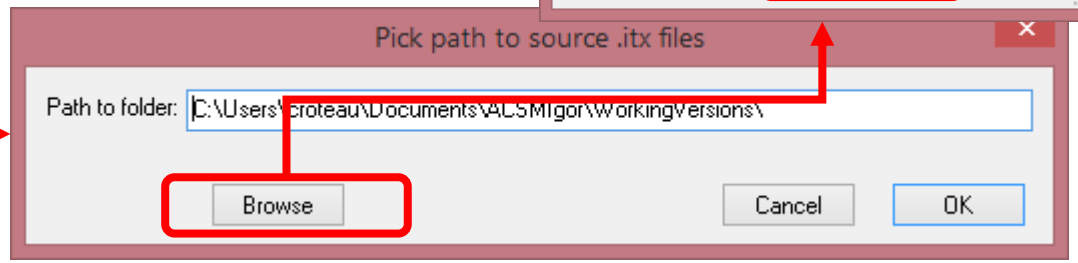
Source button allows us to load from directory that is not the default DAQ directory

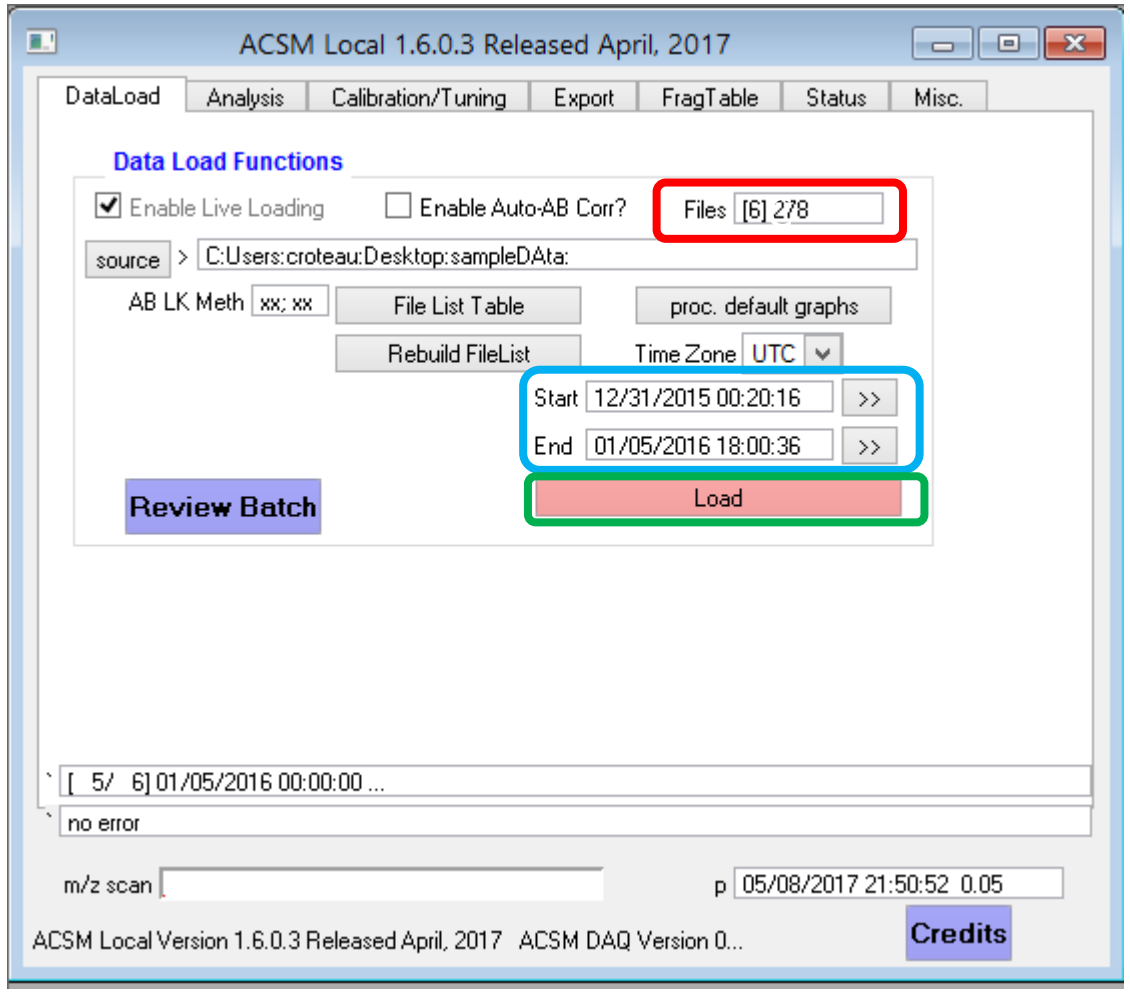


Select a data folder containg yyyymmdd stamped folders with ACSM Data as written by DAQ









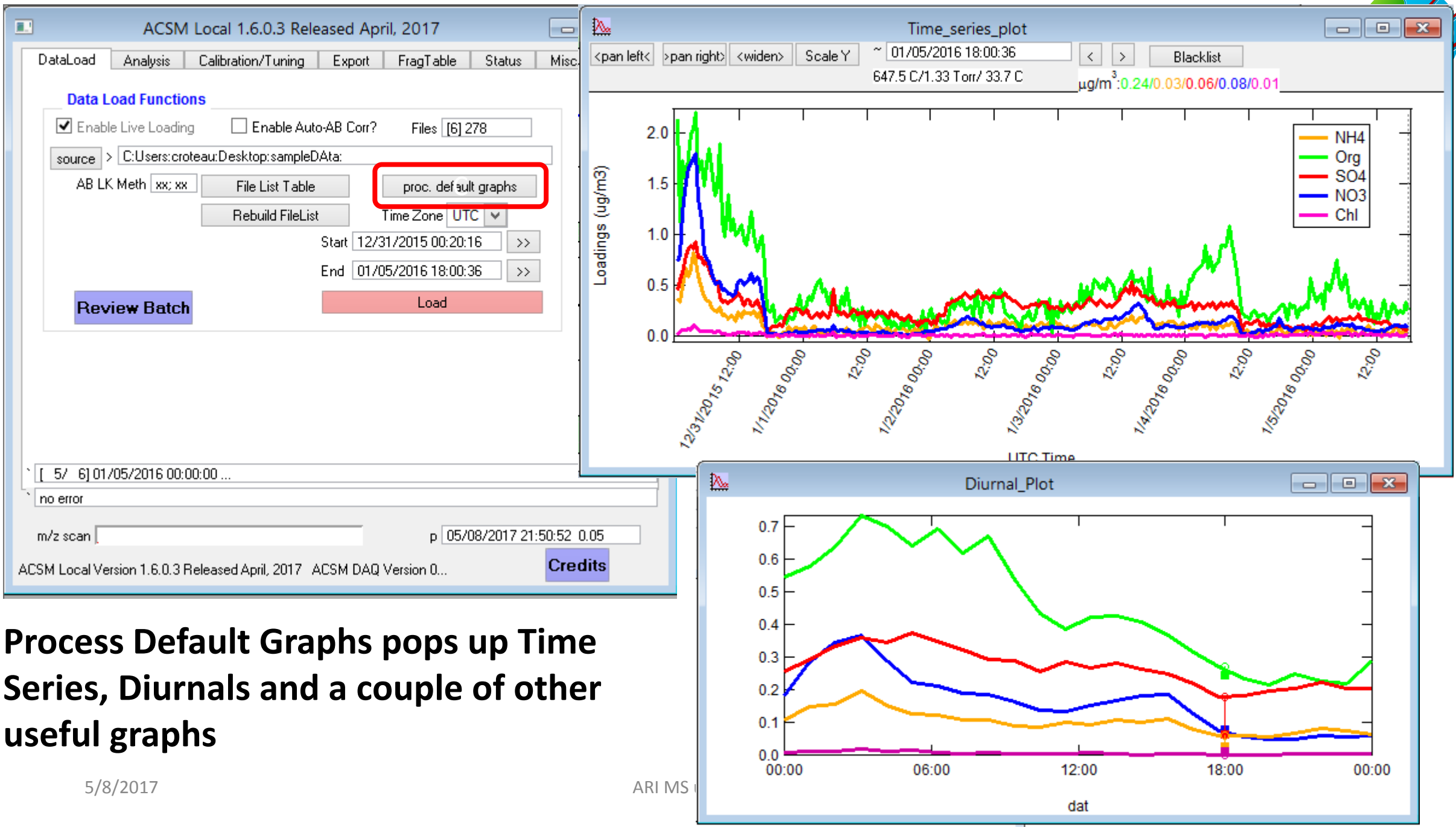
[number of folders (days)] total number of files

Start and end date of data set in source folder These can be manually edited or you can use calendar tool to select a subset of the data

“Load” loads and processes all of the data in Start-to-End time range

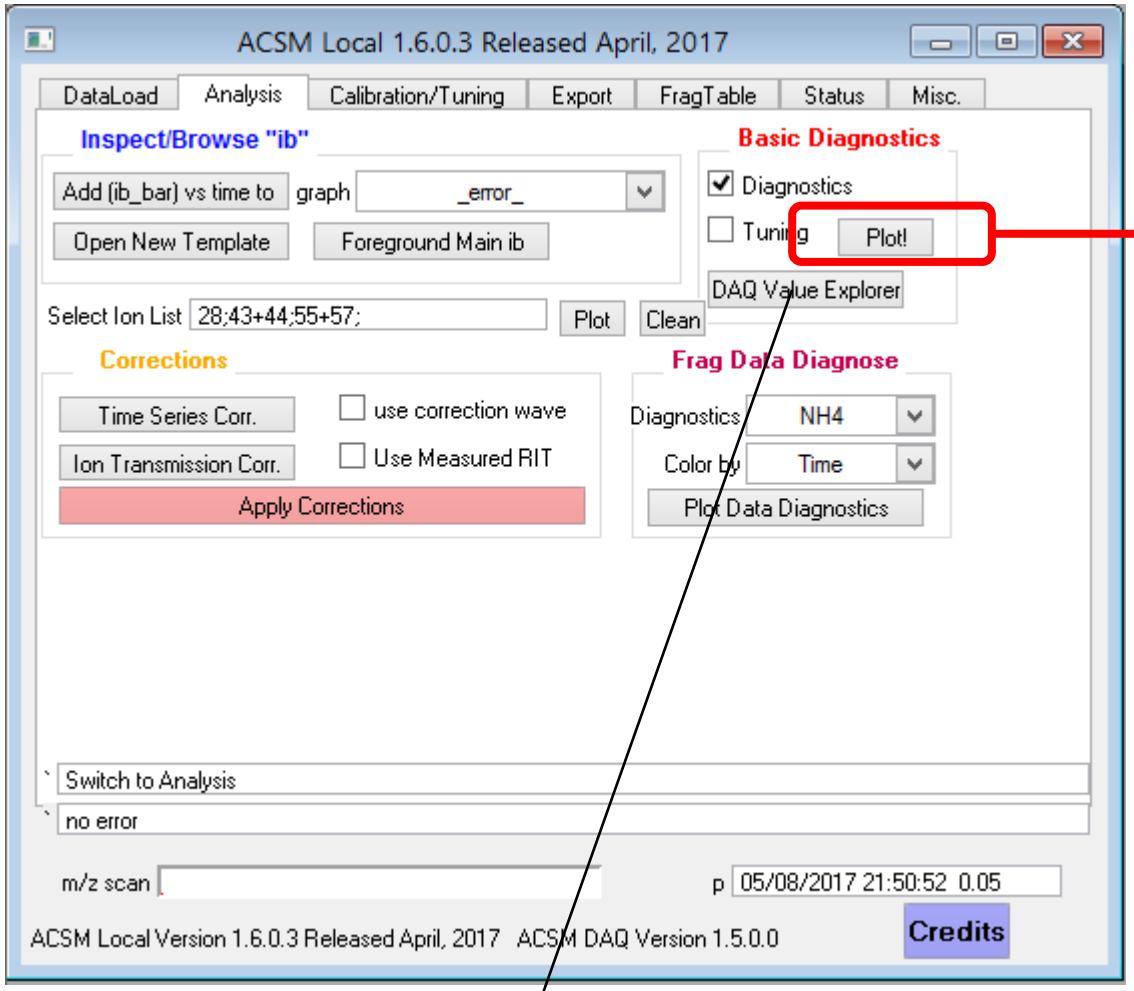
What ACSM Local does when it loads a file

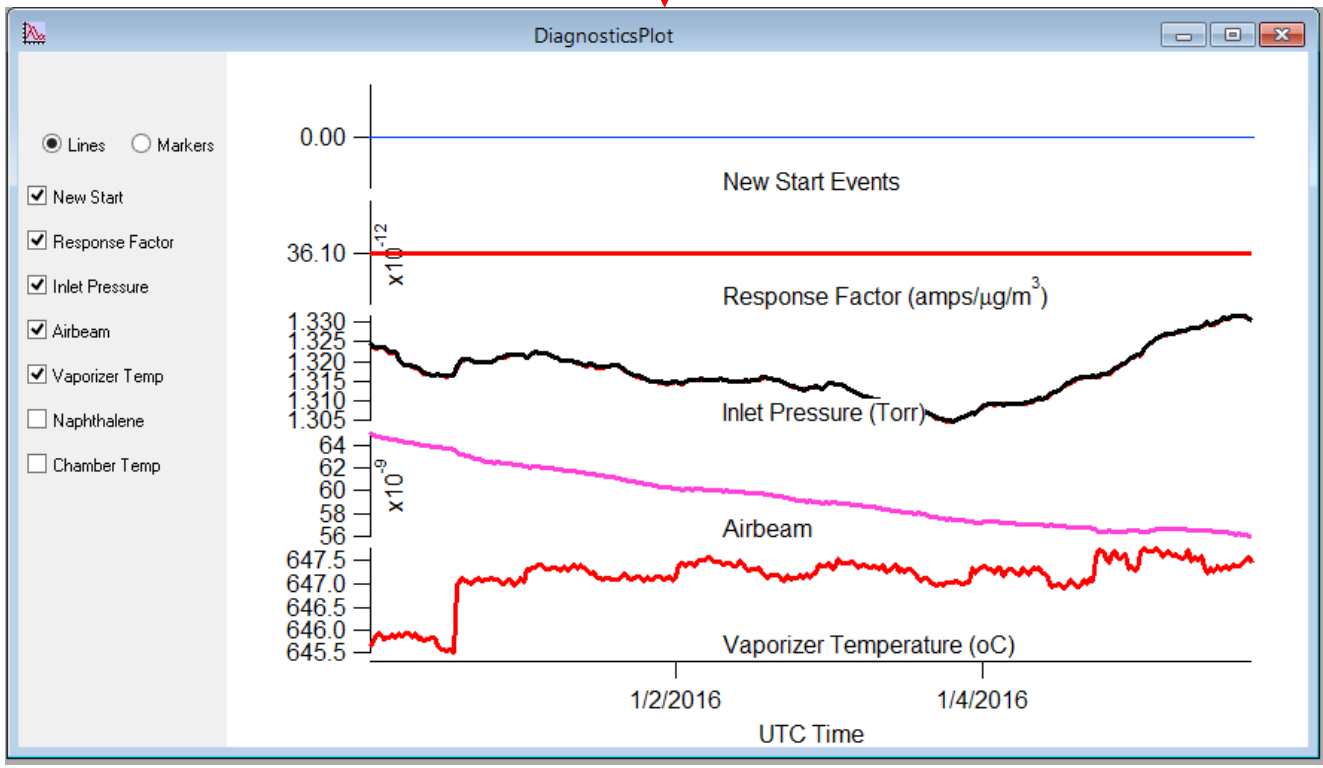
- Load Raw MS Data (sample and filter)
- Auto locate air and naphthalene peaks and do m/z calibration
- Apply default ion transmission correction (more later)
- Calculate peak intensities in sample and filter
- Take difference (MSSDiff)
- Apply fragmentation patterns to get species mass spectra
- Sum all peaks in species mass spectra
- Apply calibration factors to calculate loadings



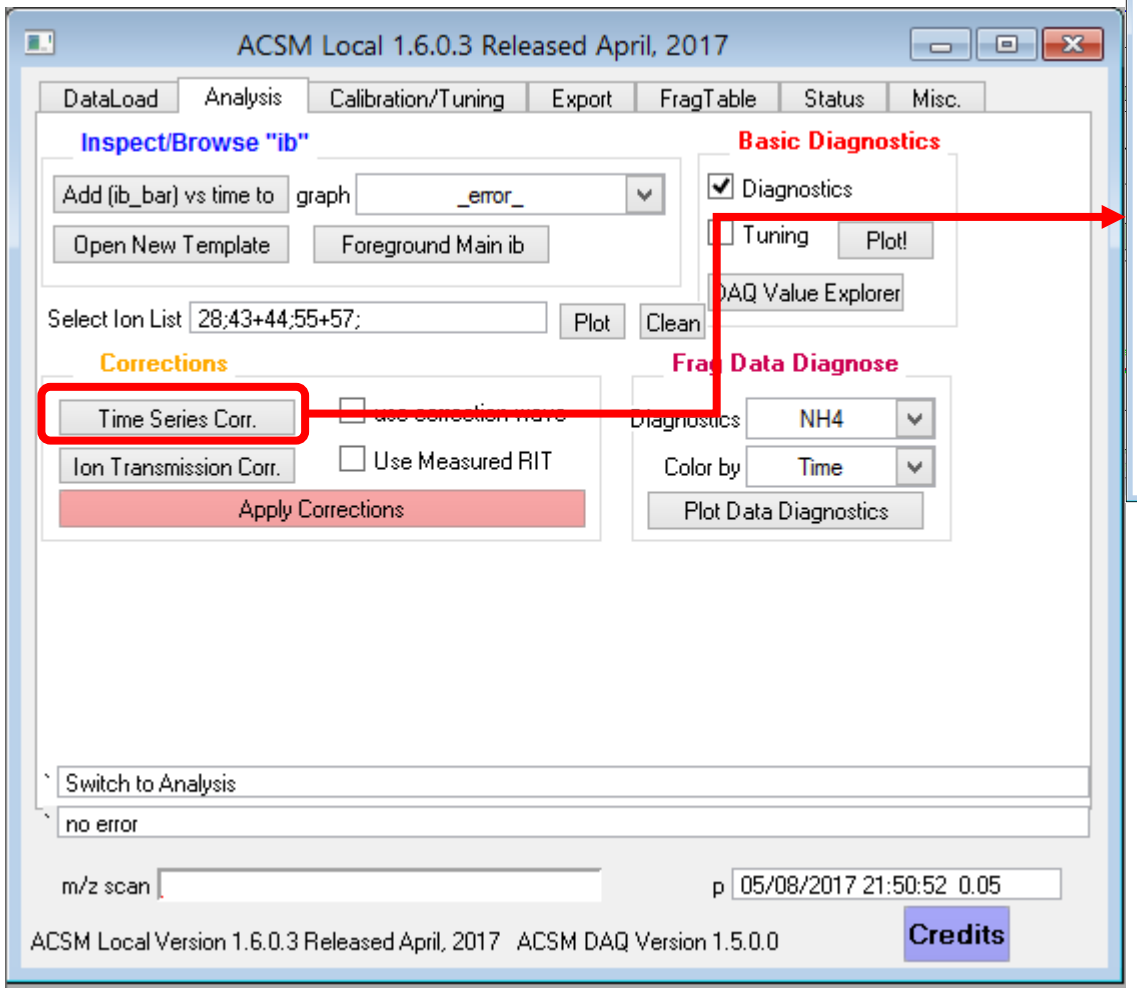
Process Default Graphs pops up Time Series, Diurnals and a couple of other useful graphs

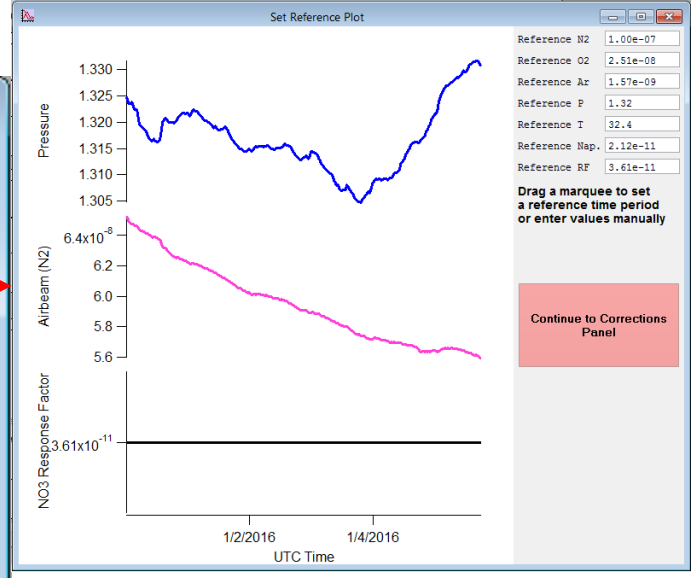
Diagnostics provides a quick view of our basic checks: airbeam, pressure, vaporizer temperature





Can also use DAQ Value Explorer to plot time series of the other ~80 housekeeping parameters recorded by DAQ





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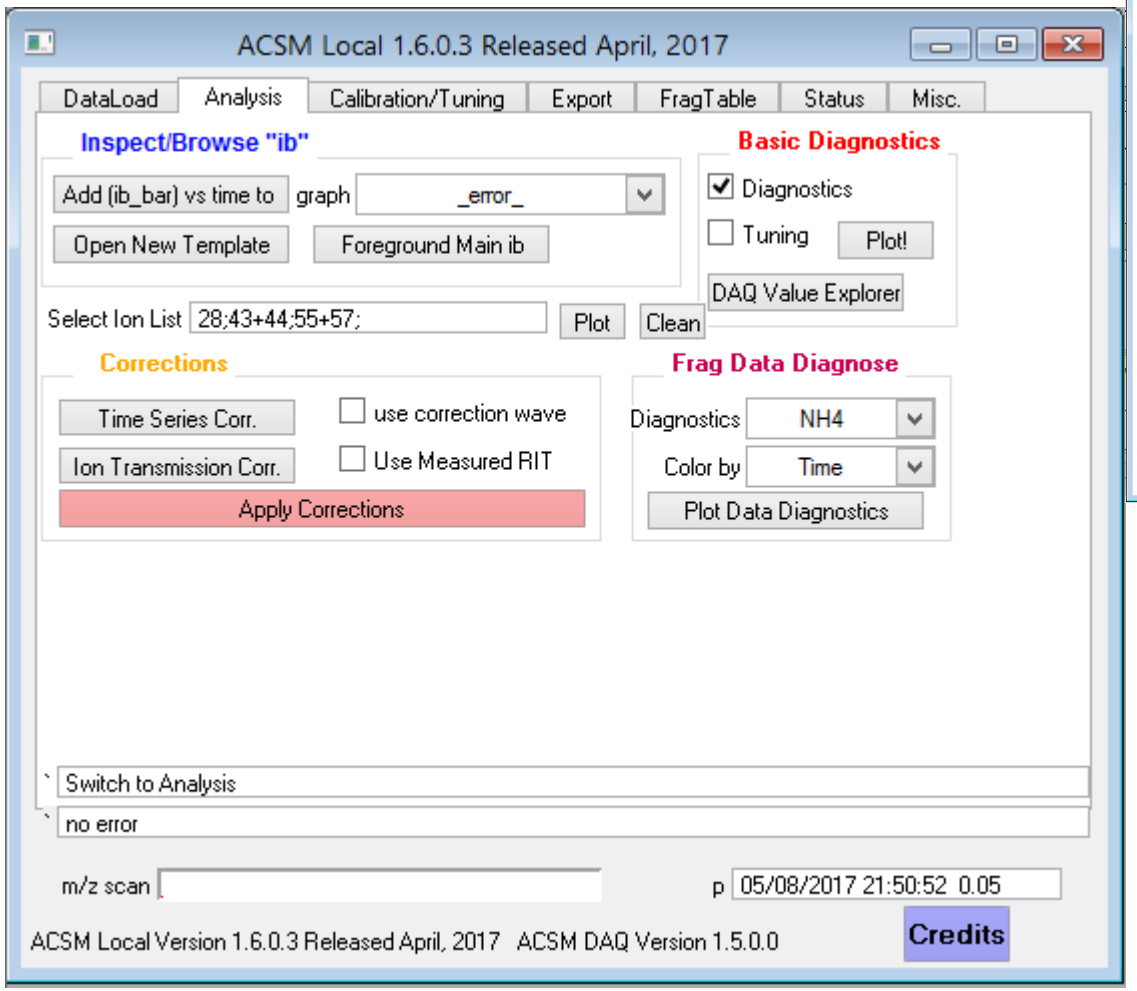
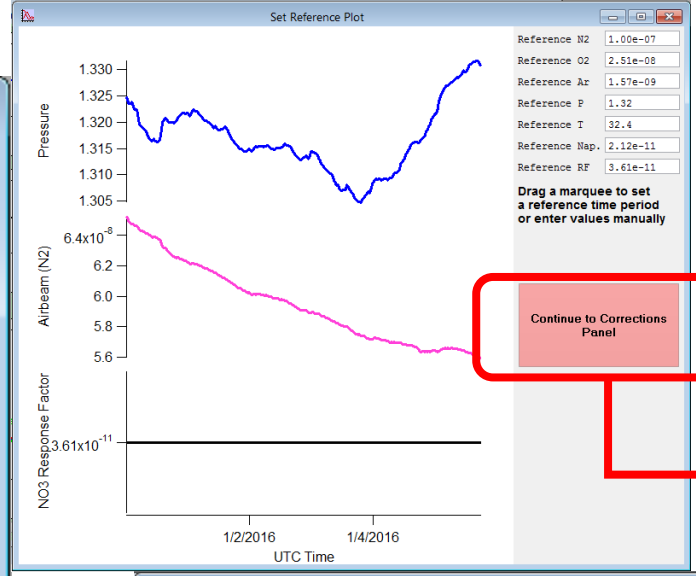
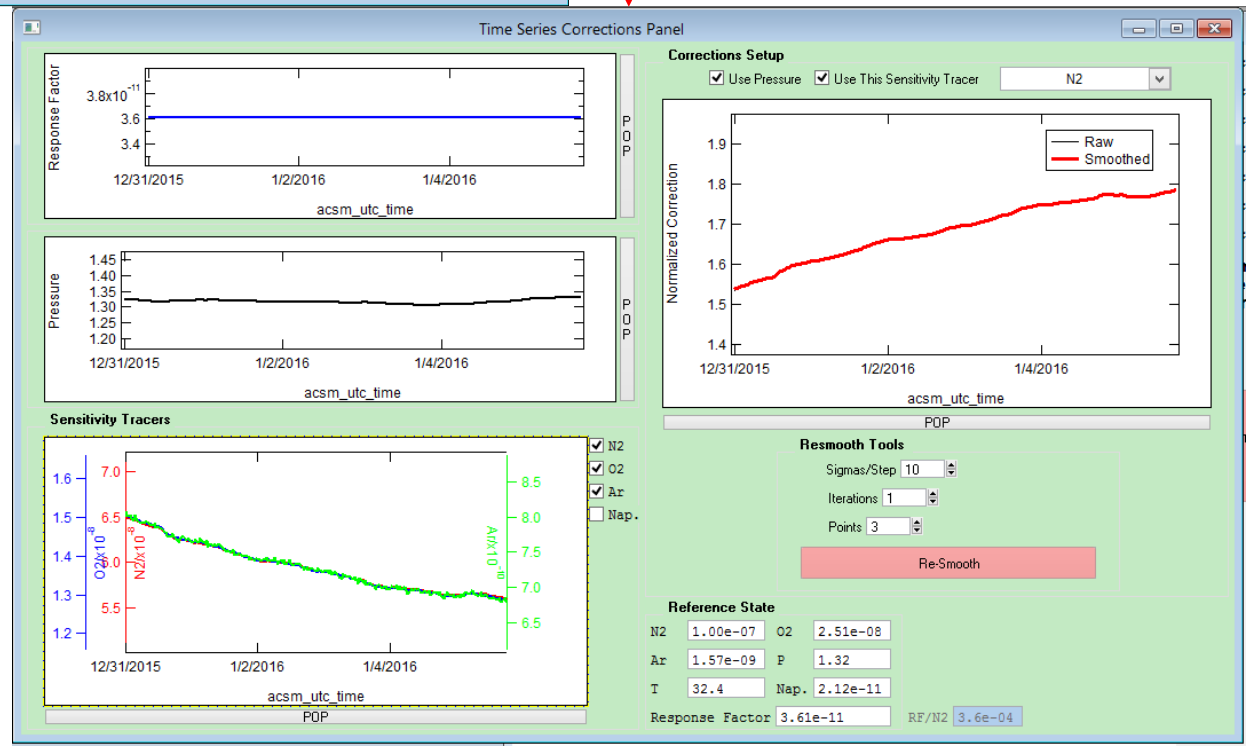
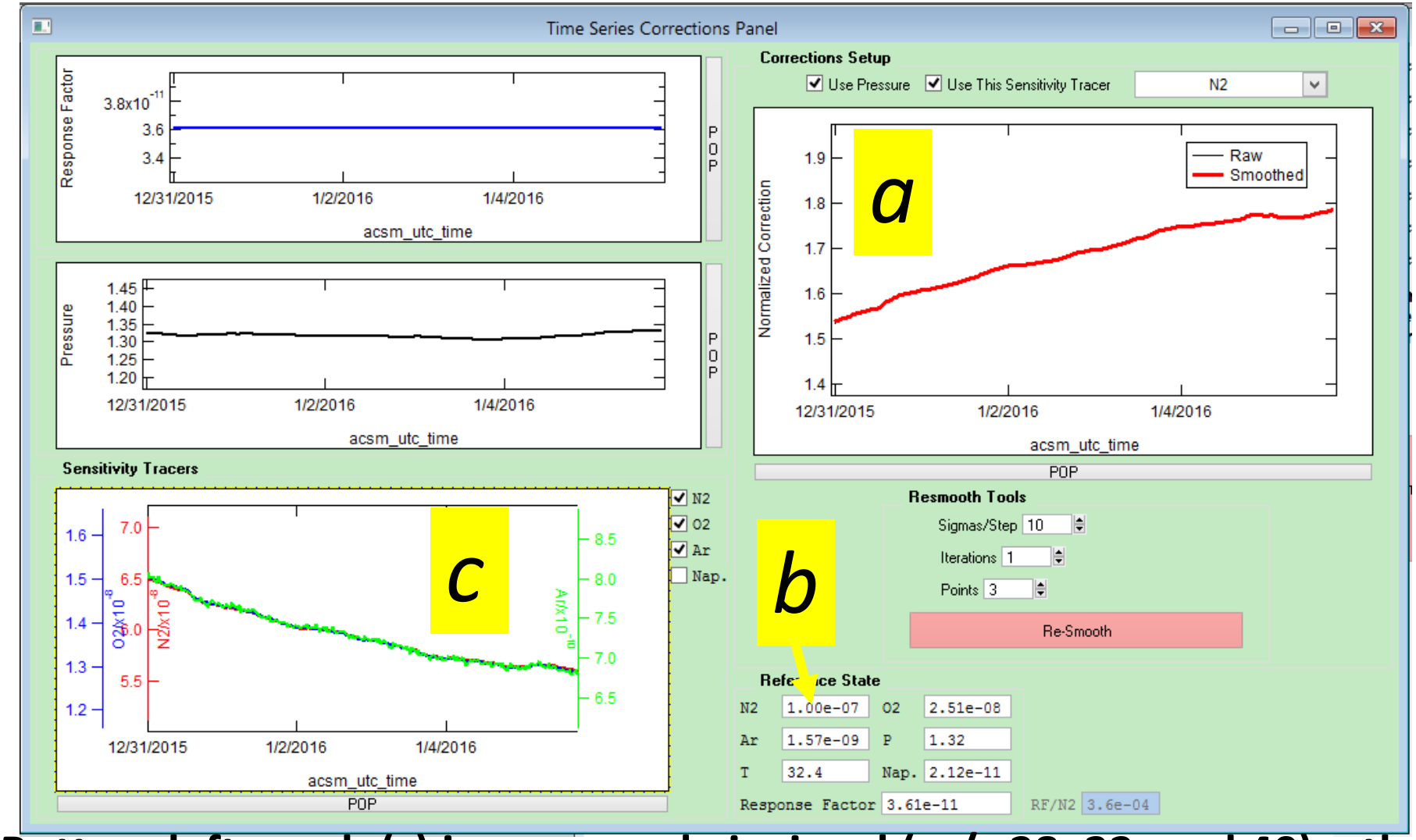
"Time Series Correction" corrects for time-dependent changes in sensitivity (SEM Decay) and/or flow rate by comparing measured air signal at a given point in time to air signal when calibration was performed







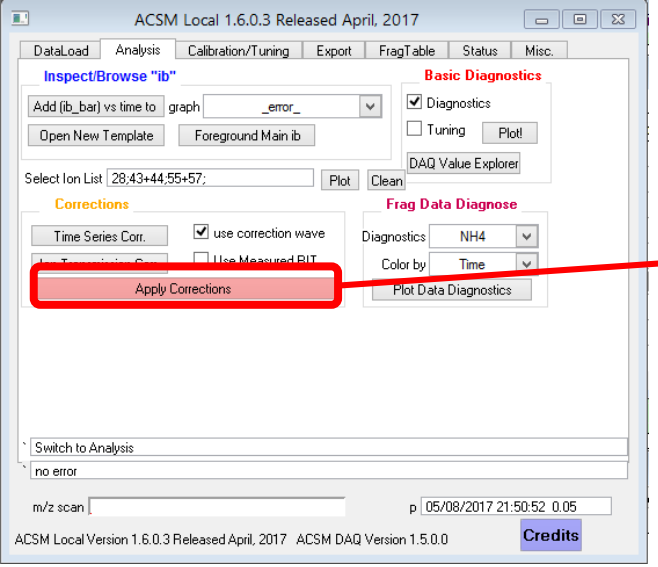
This first panel is obsolete unless analyzing data from early version of ACSM DAQ so just click big button

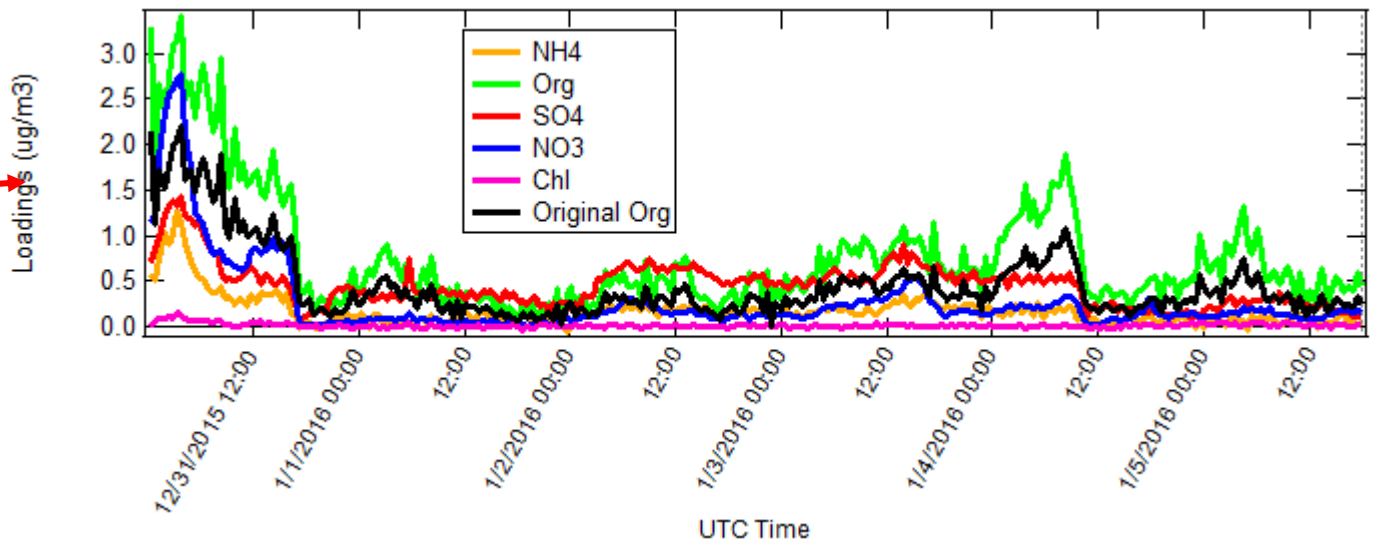


$$a = \frac{b}{c}$$

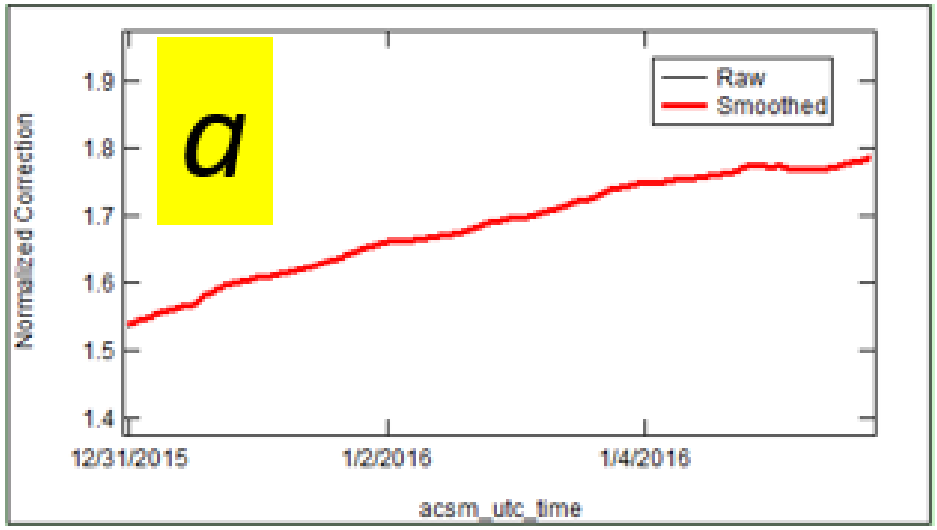
Bottom left graph (*c*) is measured air signal (m/z 28, 32, and 40) – these should do the same thing

Top right graph (*a*) is the actual "correction factor" – it is calculated as the ratio of the reference airbeam to the measured airbeam.

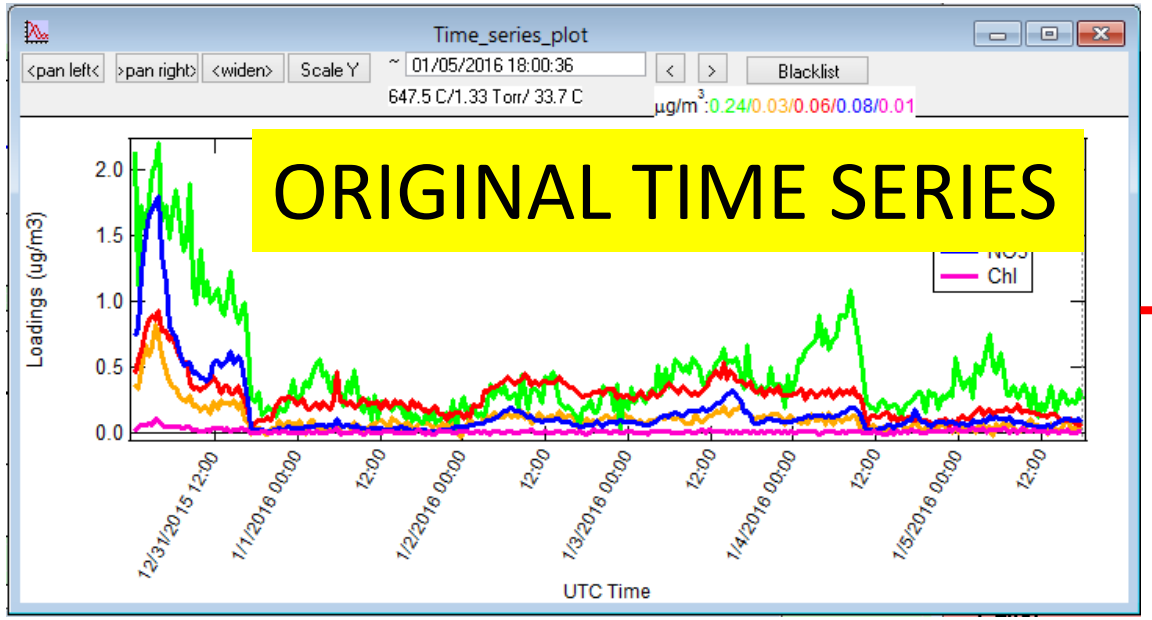




Time series correction can have a big effect on calculated mass loadings



X



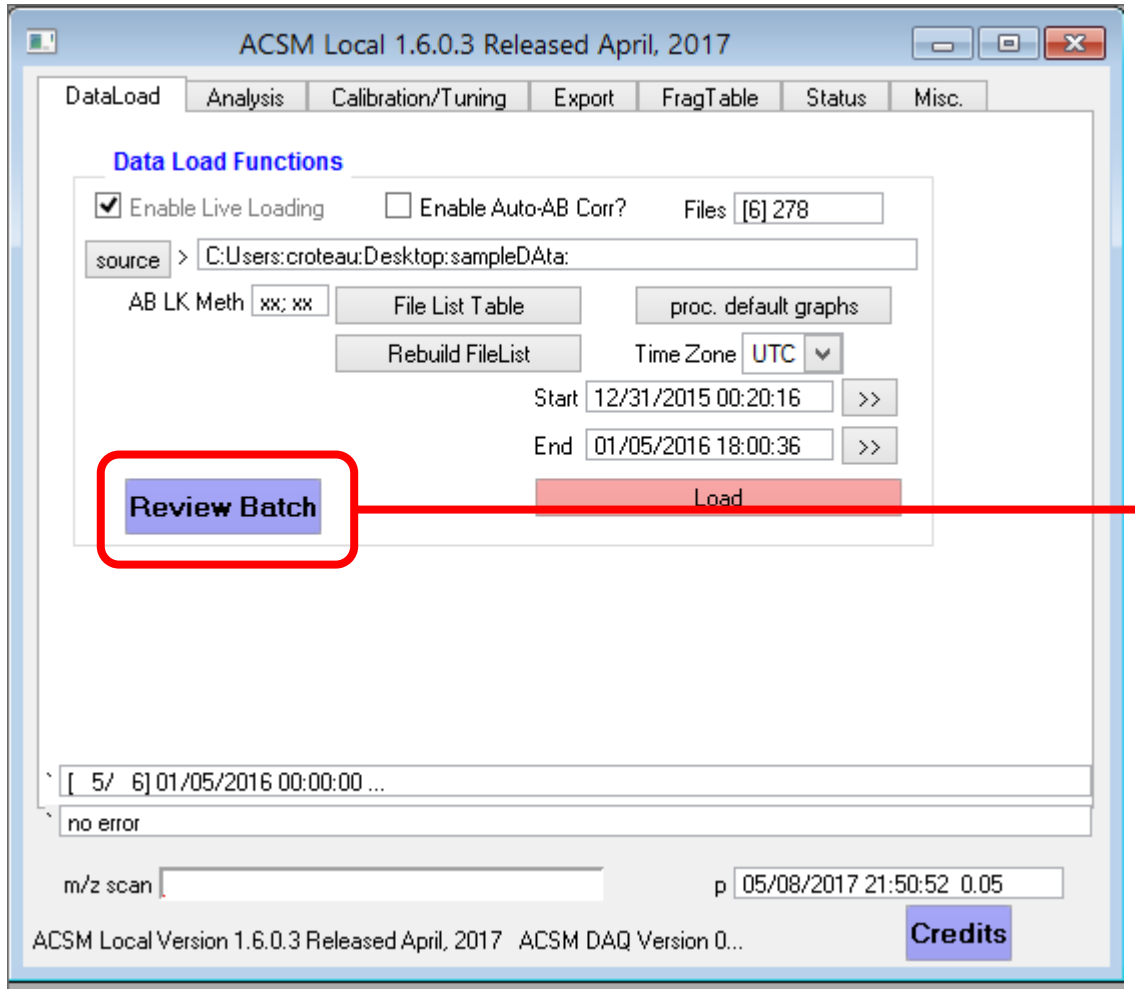
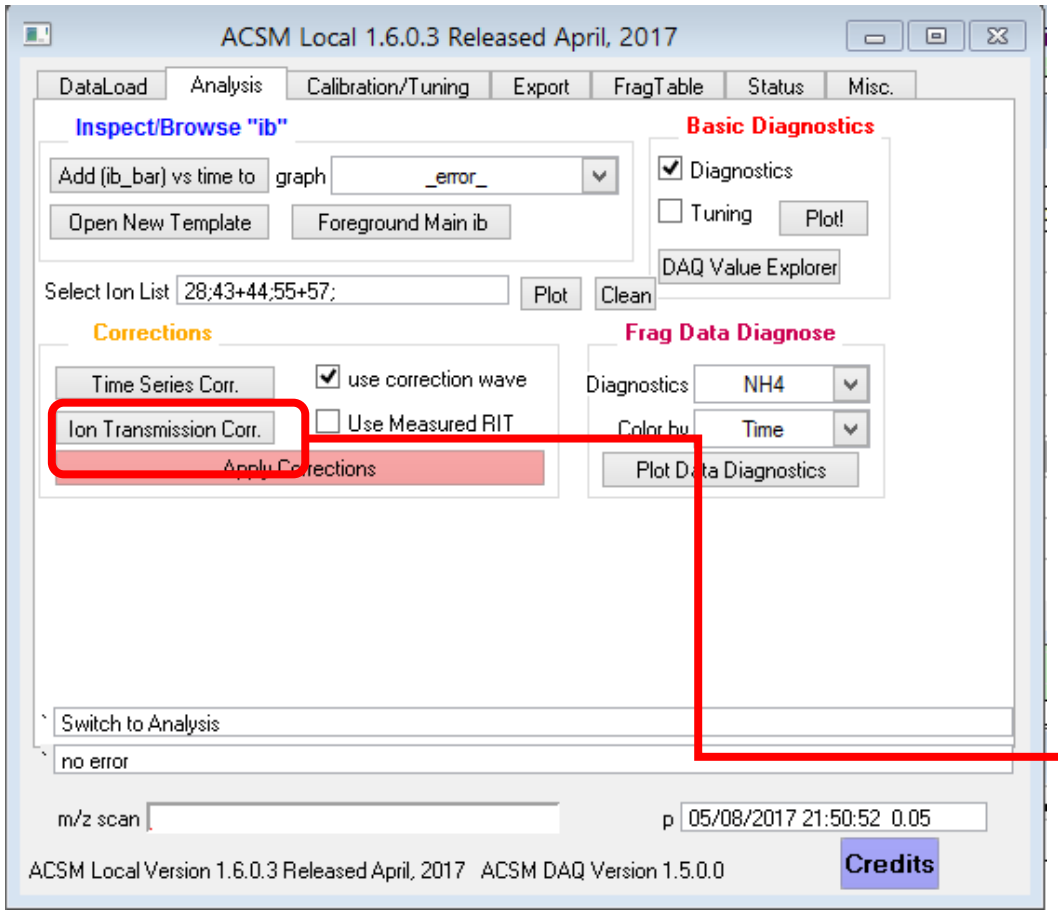


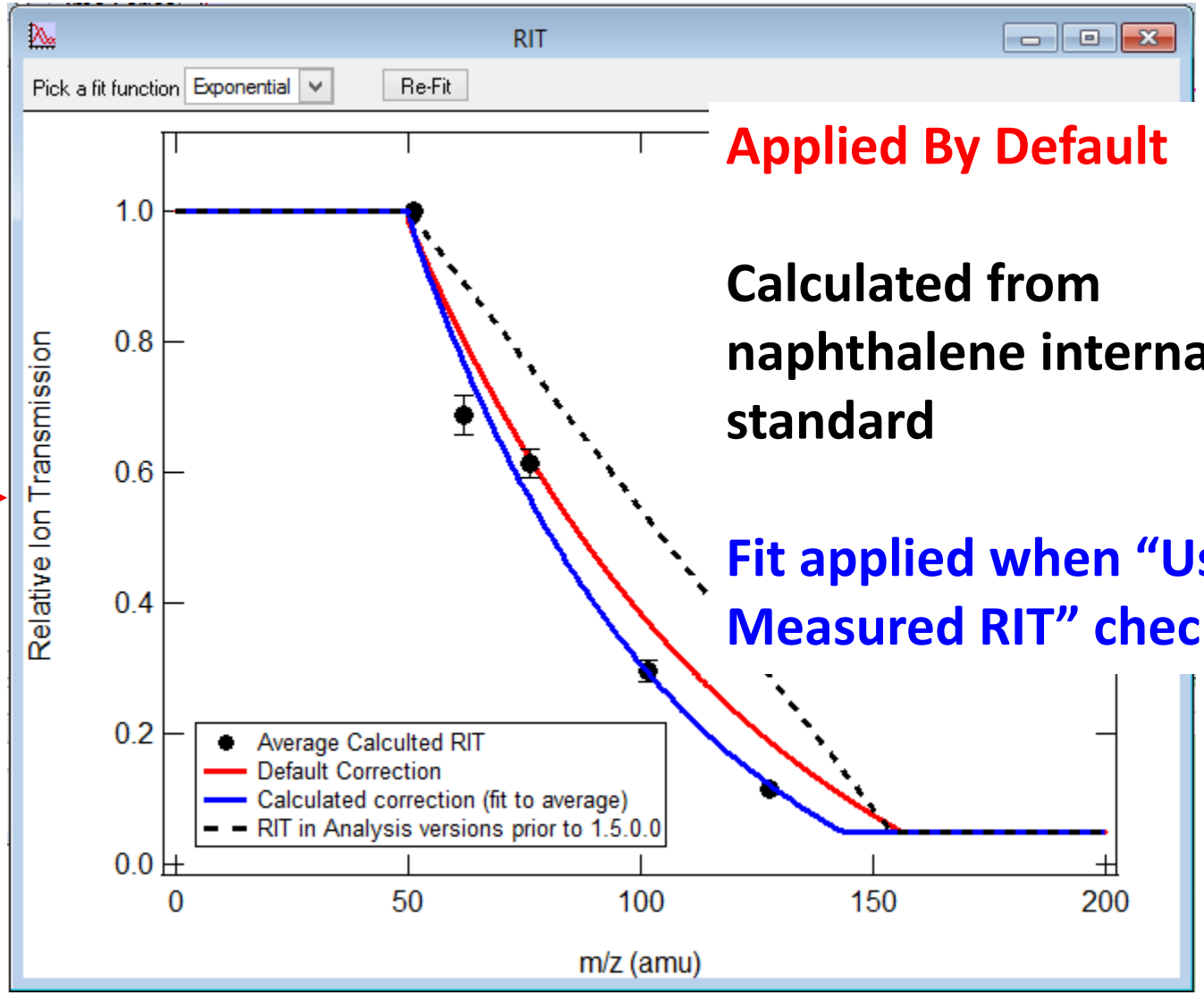
Table1:Specname,RIE,CE,Masscalib_nitrate

R0 | Org

Point	Specname	RIE	CE	Masscalib_nitrate
0	Org	1.4	1	3.61e-11
1	NH4	7.99	1	
2	SO4	0.81	1	
3	NO3	1.1	1	
4	Chl	1.3	1	
5				

Review Batch allows user to edit RIE, CE, and NO3 Response Factor. Changes here also get applied when we click on "Apply Time Series Correction"



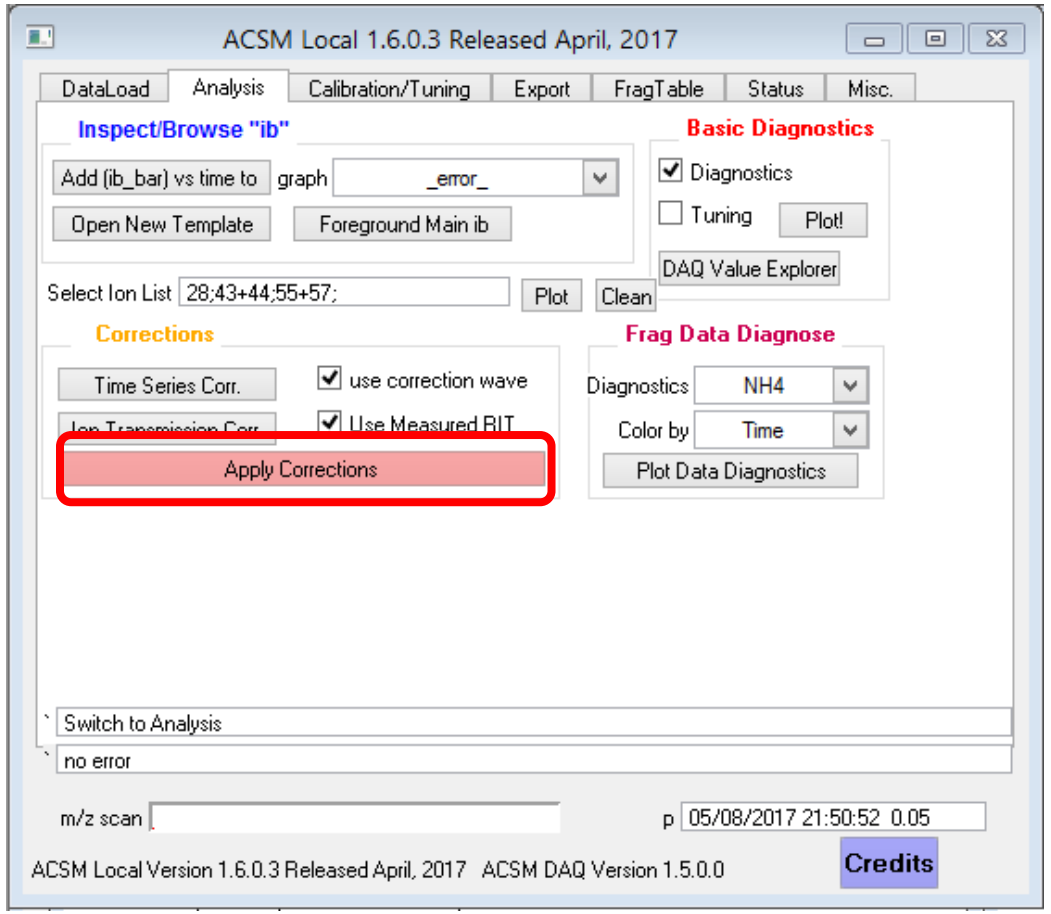


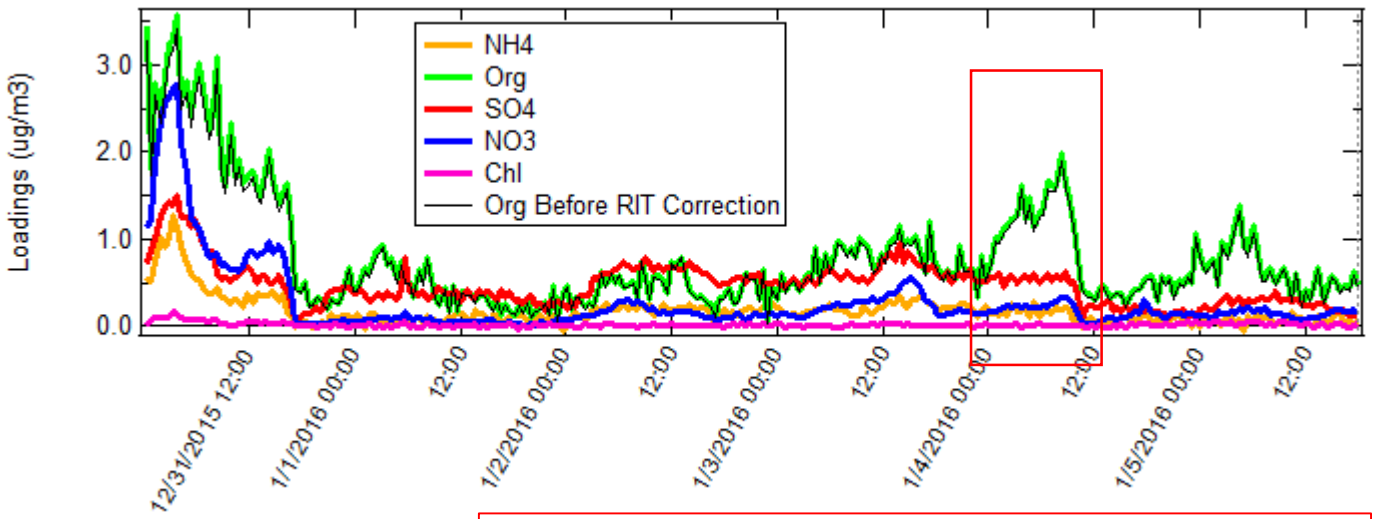
Applied By Default

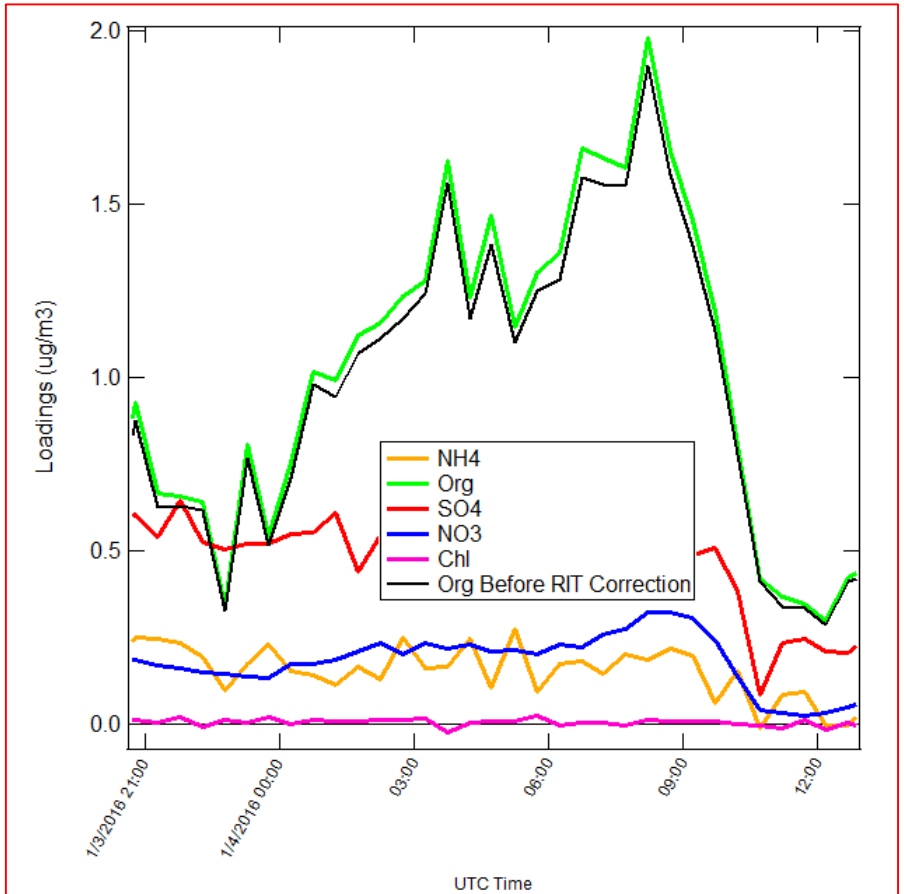
Calculated from naphthalene internal standard

Fit applied when "Use Measured RIT" checked

Relative Ion Transmission: Correct for poor transmission of larger m/z ions through the quadrupole.







Effect of RIT is relatively small unless there are big deviations from the default.