ACSM Analysis Tutorial

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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.
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
Source button allows us to load from directory that is not the default DAQ directory.
Select a data folder containing yyyyymmdd 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.
"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.
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.

\[ a = \frac{b}{c} \]
Time series correction can have a big effect on calculated mass loadings.
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”
Relative Ion Transmission:
Correct for poor transmission of larger m/z ions through the quadrupole.

Applied By Default
Calculated from naphthalene internal standard
Fit applied when “Use Measured RIT” checked
Effect of RIT is relatively small unless there are big deviations from the default.