

AMS Analysis Software Overview Squirrel 1.60

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Aerodyne

May 9, 2017



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 (main) or *_p (for PToF 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)

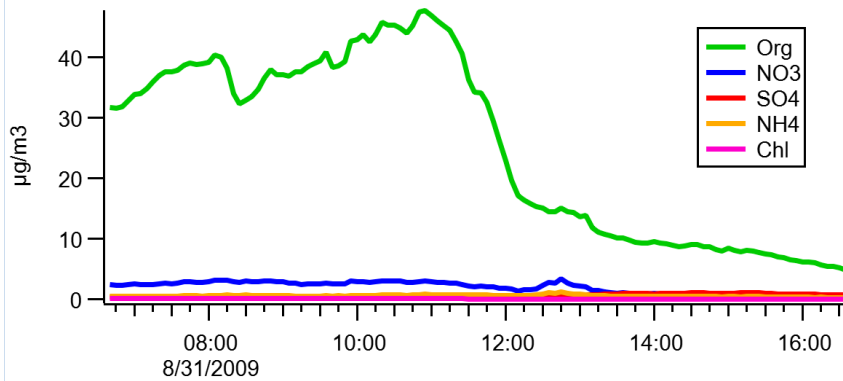
| Name | Date modified | Type | Size |
|---------------------|-------------------|-------------|-----------|
| PToF | 5/7/2017 8:01 PM | File folder | |
| 090831_044847_m.hdf | 6/29/2016 1:31 AM | HDF File | 18,769 KB |
| 090831_044887_m.hdf | 10/4/2014 9:14 AM | HDF File | 18,769 KB |
| 090831_044927_m.hdf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

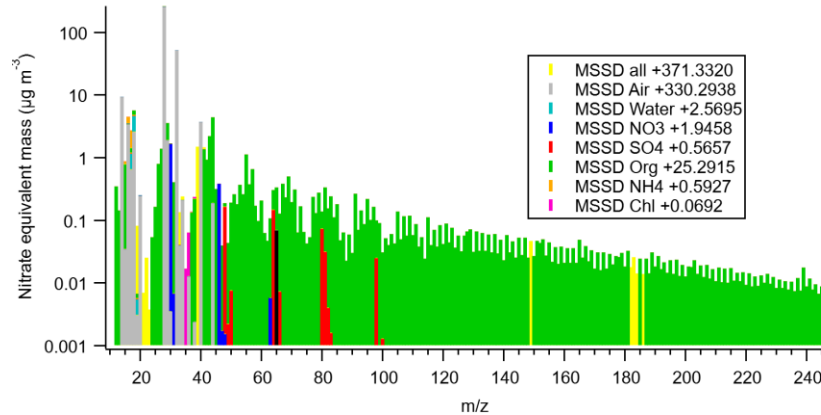
Goal for UMR (Unit Mass Resolution) data:

To generate the most precise loadings of:

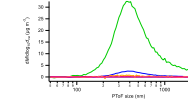
Organics (Org), **Nitrates (NO₃)**, **Chloride (Cl)**, **Sulfate (SO₄)**, **Ammonium (NH₄)**
in mainly 3 types of plots:



MS Time Series



Average Mass Spectra



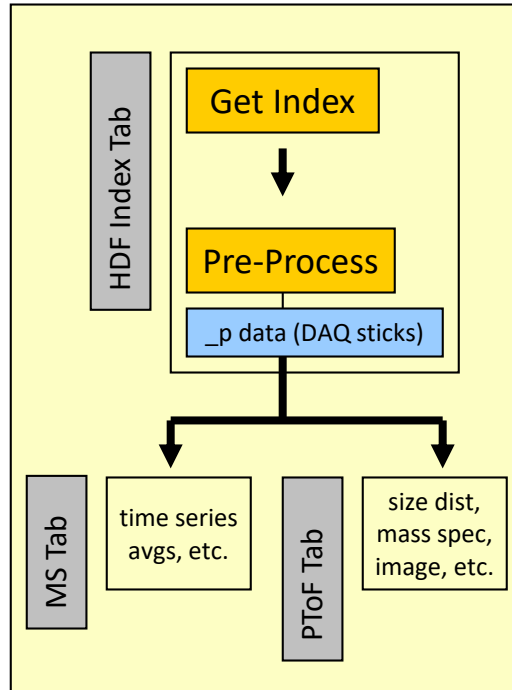
PToF Size Distribution

What is needed to achieve this goal:

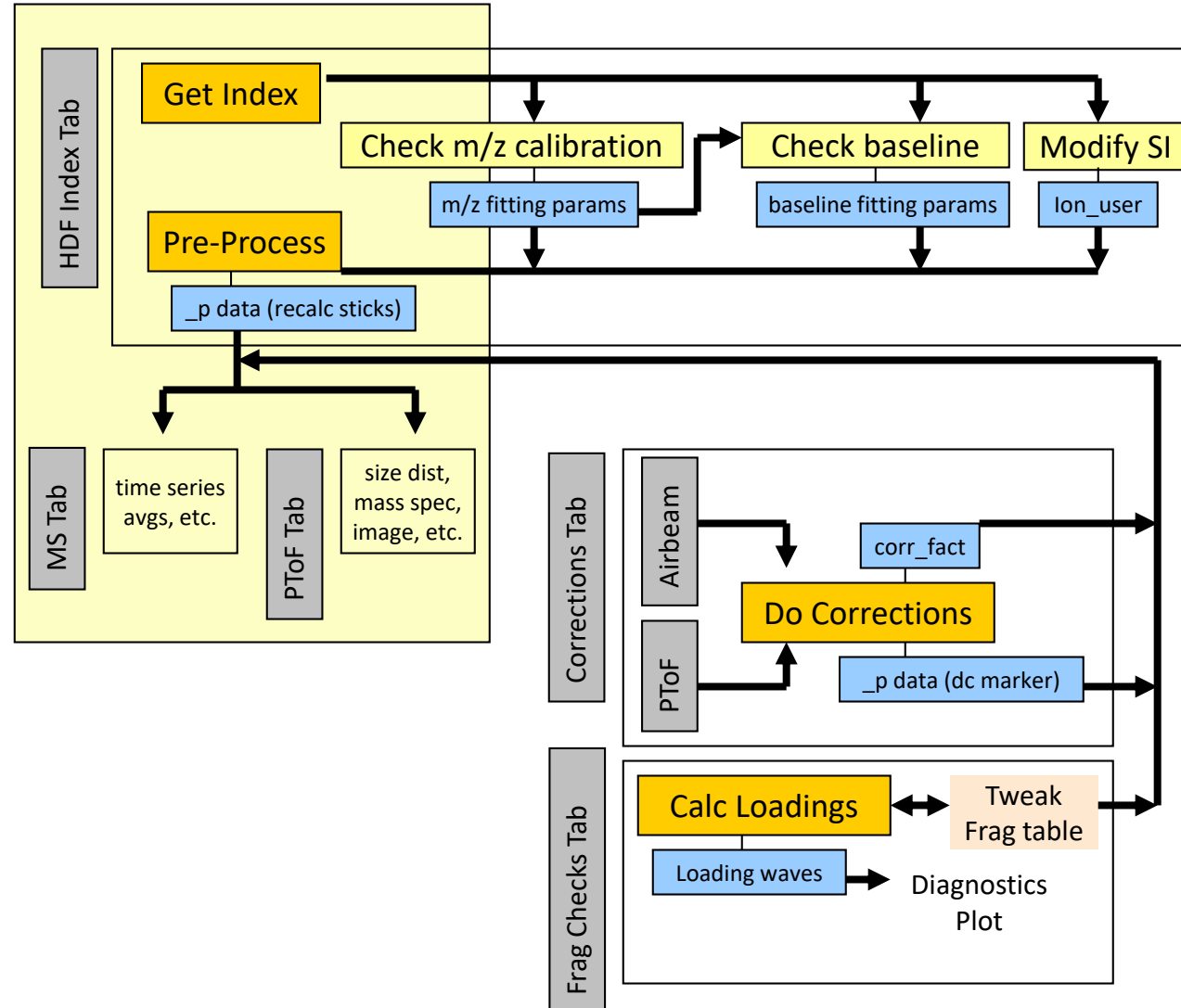
- ✓ Accurate UMR integrated spectrum
- ✓ Accurate method for grouping UMR signal to different species
- ✓ Accurate conversion to $\mu\text{g}/\text{m}^3$

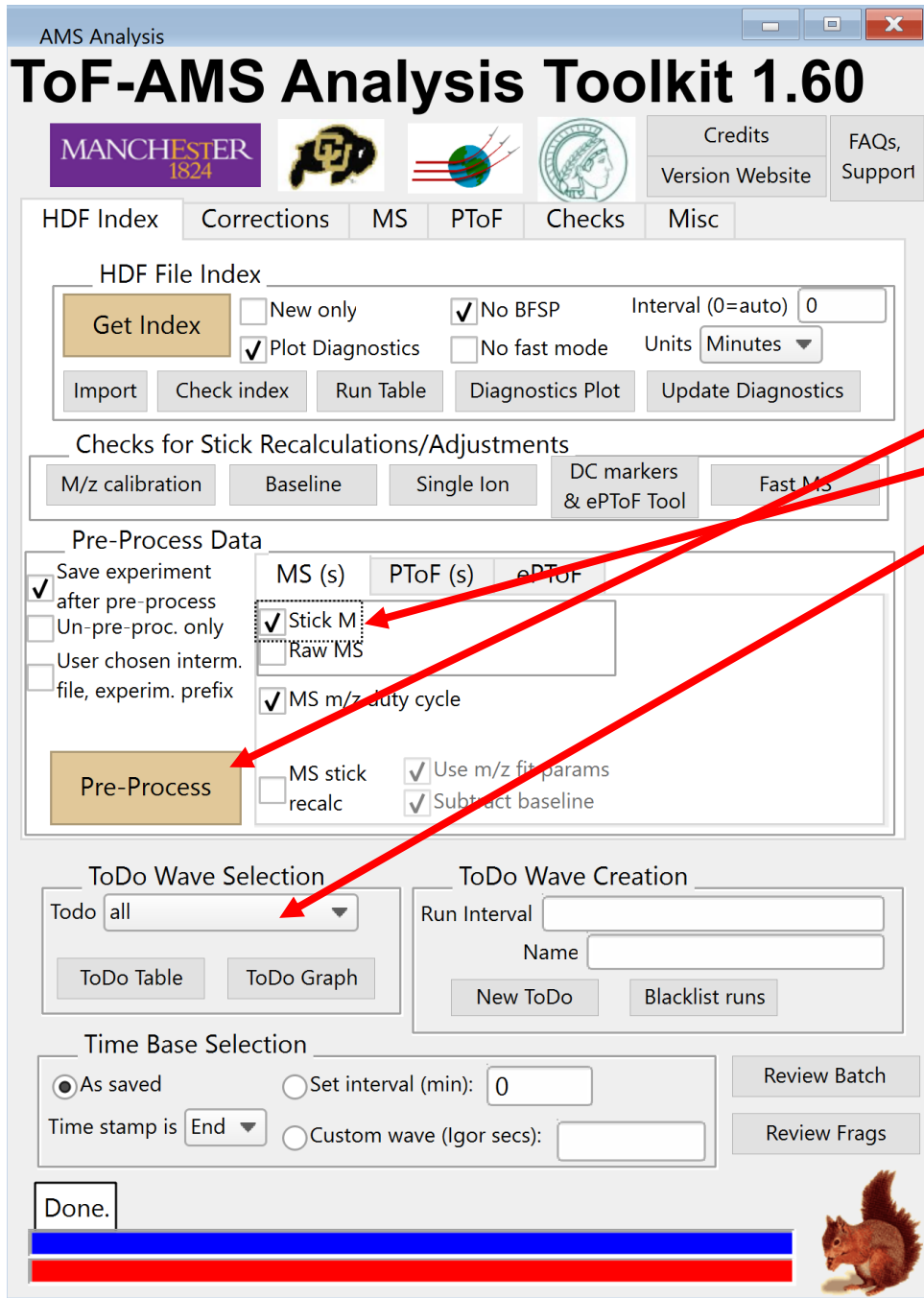
Squirrel Analysis Flow Charts

Quick-Look



Complete Analysis





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:



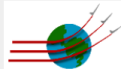

http://cires1.colorado.edu/jimenez-group/wiki/index.php/ToF-AMS_Analysis_Software

Web site that describes analysis steps:

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

AMS Analysis

ToF-AMS Analysis Toolkit 1.60

Credits
Version Website

FAQs,
Support

HDF Index
Corrections
MS
PToF
Checks
Misc

HDF File Index

Get Index

☐ New only
☒ No BFSP
Interval (0=auto) 0
☒ Plot Diagnostics
☐ No fast mode
Units Minutes

Import
Check index
Run Table
Diagnostics Plot
Update Diagnostics

Checks for Stick Recalculations/Adjustments

M/z calibration
Baseline
Single Ion
DC markers & ePToF Tool
Fast MS

Pre-Process Data

☒ Save experiment after pre-process
☐ Un-pre-proc. only
☐ User chosen interm. file, experim. prefix

MS (s)
PToF (s)
ePToF

☒ Stick MS
☐ Raw MS
☒ MS m/z duty cycle

☐ MS stick recalc
☒ Use m/z fit params
☒ Subtract baseline

Pre-Process

ToDo Wave Selection

Todo all

ToDo Table
ToDo Graph

ToDo Wave Creation

Run Interval
Name


New ToDo
Blacklist runs

Time Base Selection

☒ As saved
☐ Set interval (min): 0

Time stamp is End
☐ Custom wave (Igor secs):

Review Batch
Review Frags

Done.


Get Index

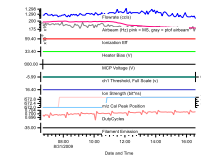
Always step #0

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



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Get Index

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☒ Plot Diagnostics ☐ No fast mode Units Minutes

Import Check index Run Table Diagnostics Plot Update Diagnostics

Checks for Stick Recalculations/Adjustments

M/z calibration Baseline Single Ion DC markers & ePToF Tool Fast MS

Pre-Process Data

☒ Save experiment after pre-process

☐ Un-pre-proc. only

☐ User chosen interm. file, experim. prefix

MS (s) PToF (s) ePToF

☒ Stick MS

☐ Raw MS

☒ MS m/z duty cycle

Pre-Process

☐ MS stick recalc ☒ Use m/z fit params ☒ Subtract baseline

ToDo Wave Selection

Todo all

ToDo Table ToDo Graph

ToDo Wave Creation

Run Interval

Name

New ToDo Blacklist runs

Time Base Selection


☒ As saved ☐ Set interval (min): 0

Time stamp is End ☐ Custom wave (Igor secs):

Review Batch

Review Frags

Done.



✓ **Accurate UMR integrated spectrum**

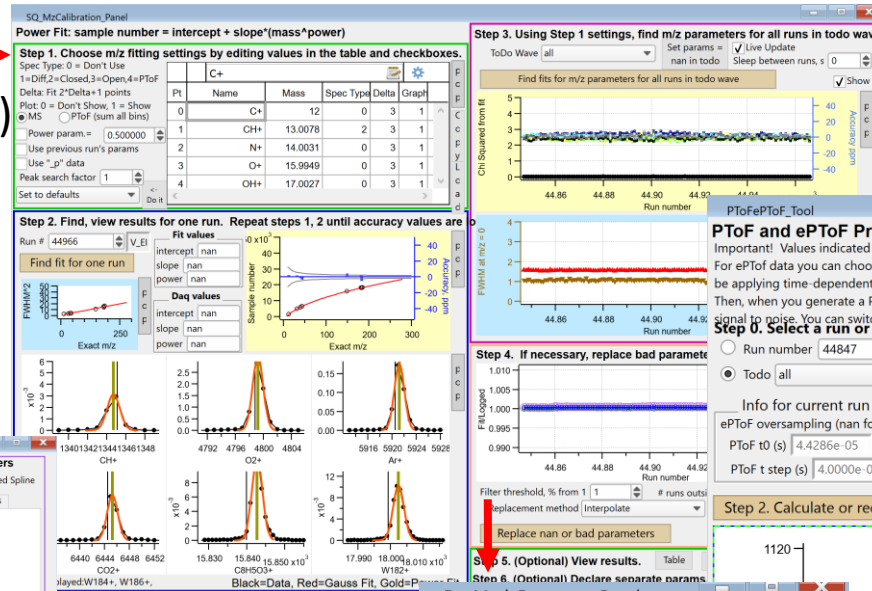
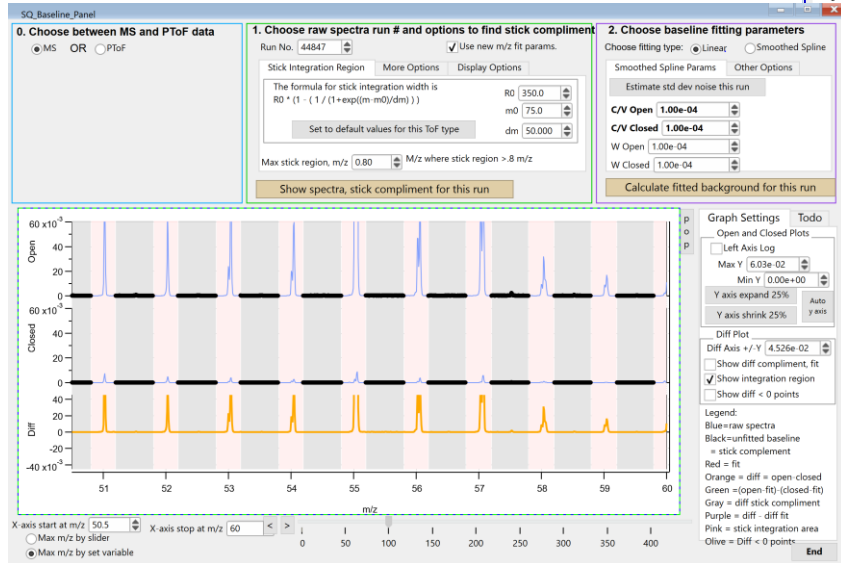
Requires:

- 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)

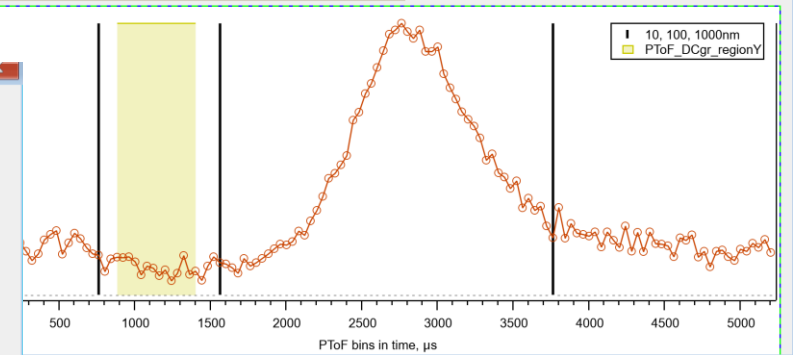
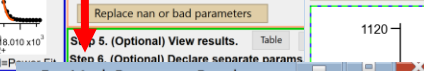
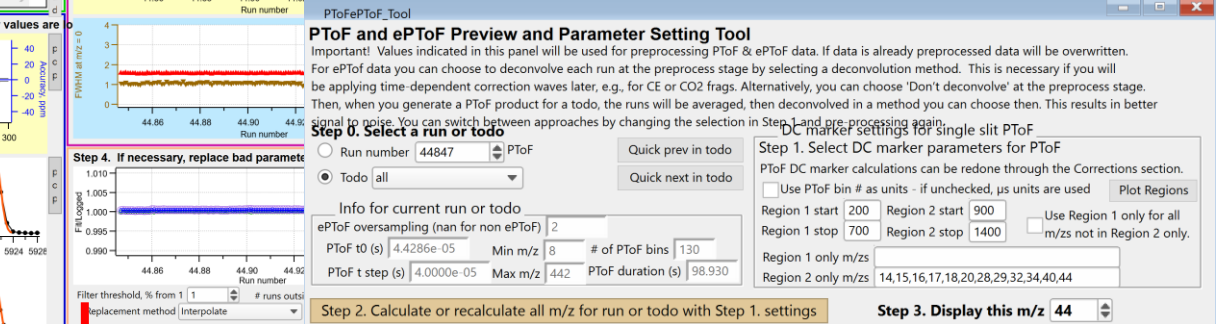
✓ Accurate UMR integrated spectrum 'finalize sticks'

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)



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 |

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

How to modify fast closed in fast closed run
☒ Average fast closed cycles
To view the non-averaged closed values one can preprocess without the fast mode settings checked on todo of fast closed run
☐ do m/z cal on avg fast closed and then interpolate m/z params across all fast runs
Extrapolate Slow/Fast transitions
☐ (if ending of fast cycle was in fast open not closed, use slow MS)

AMS Analysis

ToF-AMS Analysis Toolkit 1.60

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HDF File Index

Get Index

☐ New only ☒ No BFSP Interval (0=auto) 0

☒ Plot Diagnostics ☐ No fast mode Units Minutes

Import Check index Run Table Diagnostics Plot Update Diagnostics

Checks for Stick Recalculations/Adjustments

M/z calibration Baseline Single Ion DC markers & ePToF Tool Fast MS

Pre-Process Data

☒ Save experiment after pre-process

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☐ User chosen interm. file, experim. prefix

MS (s) PToF (s) ePToF

☒ Stick MS

☐ Raw MS

☒ MS m/z duty cycle

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☒ Use m/z fit params

☒ Subtract baseline

Pre-Process

ToDo Wave Selection

Todo all

ToDo Table ToDo Graph

ToDo Wave Creation

Run Interval

Name

New ToDo Blacklist runs

Time Base Selection


☒ As saved ☐ Set interval (min): 0

Time stamp is End ☐ Custom wave (Igor secs):

Review Batch

Review Frags

Done.



✓ 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 calibration, baseline, etc. steps

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

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Species ☒ Convert to $\mu\text{g}/\text{m}^3$
☐ Use MS AB correction
☐ Calc, plot 1s prec. err.
☐ Ask for wave name suffix

Data Plot

Time Series
Diurnal Time Series Whiskers
2-d Time Series Spectra

Average Mass Spectrum
 ☒ Graph controls ☒ Truncate sticks to 0 for stacking
Spectra Type
m/z base for raw spectra
☒ As saved ☐ Defined grid: Min Max Res28 ☒ Conserve areas
☐ Custom: ☒ New m/z fit params

ToDo Wave Selection
Todo

ToDo Wave Creation
Run Interval
Name

Time Base Selection
☒ As saved ☐ Set interval (min):
Time stamp is ☐ Custom wave (Igor secs):

Done.

AMS Analysis

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Species ☒ Convert to $\mu\text{g}/\text{m}^3$
☐ Use MS AB correction
☐ Scale (normalize) to MS data
Max m/z (0 = default)
☒ Use nonzero frag_air (adv. users)
GP/PP boundary (nm)
☐ Ask for wave name suffix
☐ Show DC or ePTOF test regions
☐ Find, display mode, median stats

Default aerosol species Default MS species

Diameter axis

Plot ☐ Don't deconvolve ☒ Matrix inversion
Smooth BL region
☐ Tofwerk inversion ☒ Scale to EPTOFSumDiff

PTOF/EPTOF Info
ePTOF:N

PTOF:Y

Diameter Base
☒ As saved
☐ Set nm intervals # bins min max
☐ Custom nm wave (wave is in root) Wave name:

DVa Size and Time

Mass Spectra

MS vs PToF (not for ePTOF)

ToDo Wave Selection
Todo

ToDo Wave Creation
Run Interval
Name

Time Base Selection
☒ As saved ☐ Set interval (min):
Time stamp is ☐ Custom wave (Igor secs):

Done.

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Name

New ToDo Blacklist runs

Time Base Selection

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Time stamp is End ☐ Custom wave (lgor secs):

Review Batch

Review Frags

Done.

✓ 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\M\SO\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 |

FragPanel

Use the radio buttons to add or remove a wave to the table.

font size 12 font bold

Export f Compare

font size 12 column width 100

R5

mz frag_air frag_CO2 frag_O16 frag_water frag_RH frag_organic frag_PAH

27

28

29 0.00736*frag_air[28]

30 0.0000136*frag_air[28]

31

32 32,-frag_sulphate[32]-frag_n

33 0.000763*frag_air[32]

34 0.00402*frag_air[32]

35

36 0.00338*frag_air[40]

37

38 0.000633*frag_air[40]

39

40 0.009*1.11*1.28*1.14*frag_ai

41

42

43

44 frag_CO2[44] 0.00037*1.36*1.28

45

46

47

48

Use the listbox & buttons to add or remove a wave to the table. Update list

frag_orgLessPAH

Add/Remove Frag Wave

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Get Index ☐ New only ☒ No BFSP Interval (0=auto) 0

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Checks for Stick Recalculations/Adjustments

M/z calibration Baseline Single Ion DC markers & ePTof Tool Fast MS

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MS (s) PToF (s) ePTof

☒ Stick MS ☐ Raw MS

☒ MS m/z duty cycle

☐ MS stick recal ☒ Use m/z fit params ☒ Subtract baseline

Pre-Process

ToDo Wave Selection

ToDo all

ToDo Table ToDo Graph

ToDo Wave Creation

Run Interval

Name

New ToDo Blacklist runs

Time Base Selection

☒ As saved ☐ Set interval (min): 0

Time stamp is End ☐ Custom wave (lgor secs):

Done.

Review Batch

Review Frags

✓ 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\M\SO\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 |

FragPanel

Use the radio buttons to add or remove a wave to the table.

font size 12 column width 10

Export f Compare

Use the listbox & buttons to add or remove a wave to the table. Update list

frag_organicLessPAH

Add/Remove Frag Wave

| mz | frag_air | frag_CO2 | frag_O16 | frag_water | frag_RH | frag_organic | frag_PAT |
|----|-------------------------------|-------------------|----------|------------|---------|---------------------|----------|
| 27 | | | | | | 27 | |
| 28 | | | | | | frag_organic[44] | |
| 29 | 0.00736*frag_air[28] | | | | | 29,-frag_air[29] | |
| 30 | 0.0000136*frag_air[28] | | | | | 0.022*frag_organic | |
| 31 | | | | | | 31,-frag_nitrate[3] | |
| 32 | 32,-frag_sulphate[32],-frag_n | | | | | | |
| 33 | 0.000763*frag_air[32] | | | | | | |
| 34 | 0.00402*frag_air[32] | | | | | | |
| 35 | | | | | | | |
| 36 | 0.00338*frag_air[40] | | | | | | |
| 37 | | | | | | 37,-frag_chloride[| |
| 38 | 0.000633*frag_air[40] | | | | | 38,-frag_chloride[| |
| 39 | | | | | | | |
| 40 | 0.009*1.11*1.28*1.14*frag_ai | | | | | | |
| 41 | | | | | | 41,-frag_K[41] | |
| 42 | | | | | | 42 | |
| 43 | | | | | | 43 | |
| 44 | frag_CO2[44] | 0.00037*1.36*1.28 | | | | 44,-frag_air[44] | |
| 45 | | | | | | 45 | |
| 46 | | | | | | | |
| 47 | | | | | | 47,-frag_nitrate[4] | |
| 48 | | | | | | 0.5*frag_organic[4] | |

AMS Analysis

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HDF Index

Corrections

MS

PToF

Checks

Misc

Fragmentation & NH4 RIE Checks

☒ Use MS airbeam correction

Species not calculated for Frag Checks

Calc. loadings for all species *except* those above

Frag plots panel

Additional Fragmentation Diagnostic Graphs

Color by

Plot Data Diagnostics

Diagnostics

Composition Dependent CE (CDCE)

Pieber et al correction

CDCE panel

paper link

Pieber et al panel

paper link

Project Diagnostics, IE Calibrations

Project Diagnostics Graph

IE calibration table

ToDo Wave Selection

ToDo

ToDo Table

ToDo Graph

ToDo Wave Creation

Run Interval

Name

New ToDo

Blacklist runs

Time Base Selection

☒ As saved

☐ Set interval (min):

Time stamp is

☐ Custom wave (Igor secs):

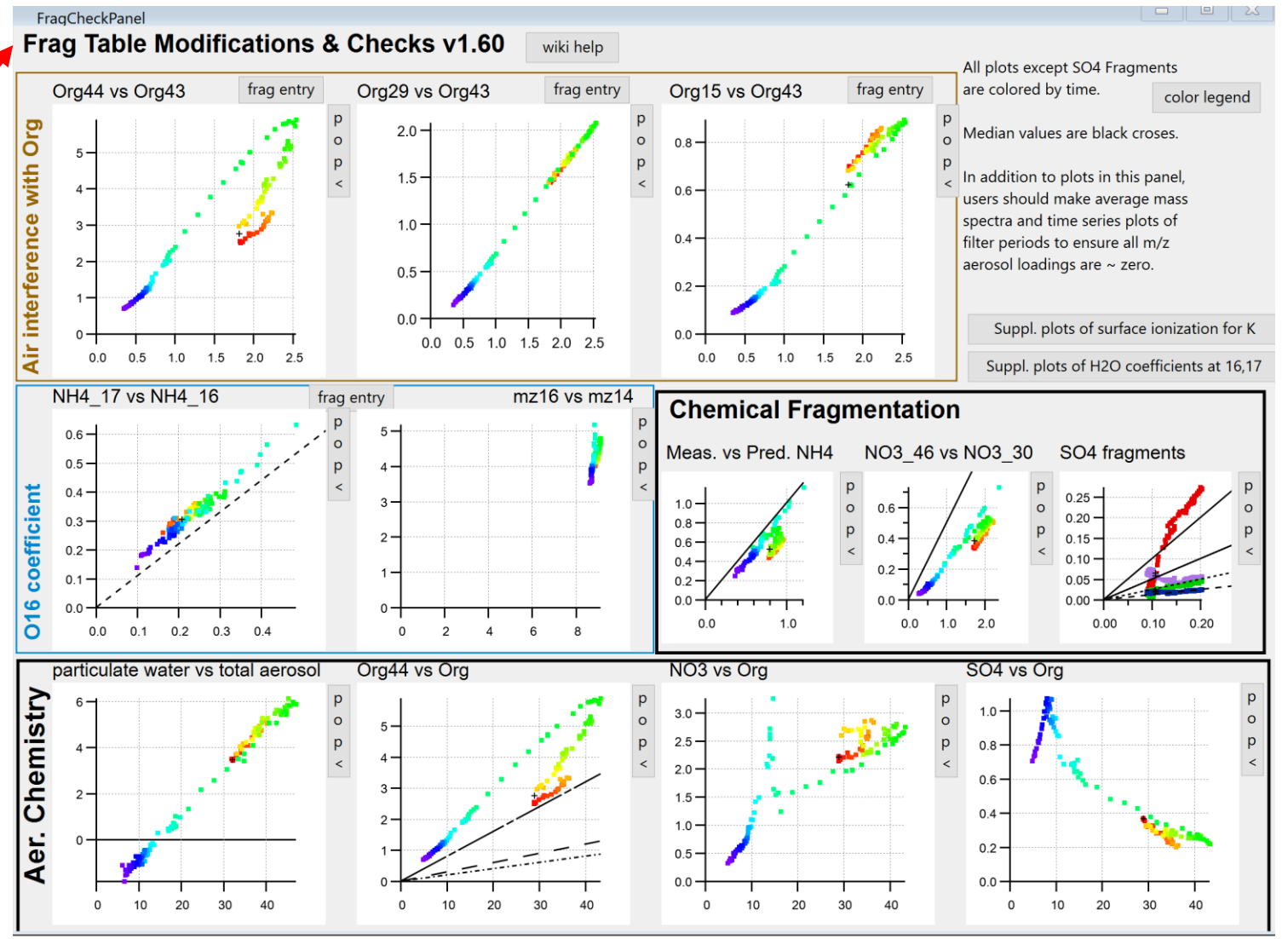
Review Batch

Review Frags

Done.

✓ 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.



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Pre corr. (opt.) Do Corrections Post corr. (opt.)

Flow Rate Airbeam* PToF Errors IE Cals

☒ **Create/Overwrite AB corr. factor**

AB Correction factor is calculated for all runs, not just those in todo wave.

☒ Auto-set (Use AB ref runs)
AB ref. run(s) or todo
AB Ref runs need to include all detector types.

☒ Show plot after calculations
MS AB smooth (# runs)

☒ Correct AB for flowrate
Flowrate smooth (# runs)
Flowrate offset (cc/s)

| x | y | V_EI |
|------------|---|----------|
| IONEFF | | 5.94e-08 |
| AIRBEAM_HZ | | 1.80e+05 |

Reset airbeam to m/z MS AB m/z Show AB corr. fact. plot


ToDo Wave Selection
Todo
ToDo Table ToDo Graph

ToDo Wave Creation
Run Interval
Name
New ToDo Blacklist runs

Time Base Selection
☒ As saved ☐ Set interval (min):
Time stamp is ☐ Custom wave (lg or secs):

Review Batch
Review Frags

Done.



✓ Accurate conversion from ion counts to $\mu\text{g}/\text{m}^3$

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!

AMS Analysis

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HDF Index Corrections MS PToF Checks Misc

Species: Org,NO3,SO4,NH4,Chl

Data: Diff Plot: Single

☒ Convert to $\mu\text{g}/\text{m}^3$

☐ Use MS AB correction

☐ Calc, plot 1s prec. err.

☐ Ask for wave name suffix

Time Series Diurnal Time Series

Default Species Whiskers: 5-95% f43 vs f44 f44 vs f60

Calculate Calc diurnal trends

2-d Time Series Spectra

Calc 2d matrix (not plotted)

☐ itx for PMF

Average Mass Spectrum

Species list to default ☒ Graph controls ☒ Truncate sticks to 0 for stacking

Spectra Type: Sticks

Calculate

Find raw baseline spectra

Export for AMS database

m/z base for raw spectra

☒ As saved ☒ Regrid

☐ Defined grid: Min 12 Max 500 Res28 10000 ☒ Conserve areas

☐ Custom: ☒ New m/z fit params

ToDo Wave Selection

ToDo: all

ToDo Table ToDo Graph

ToDo Wave Creation

Run Interval:

Name:

New ToDo Blacklist runs

Time Base Selection

☒ As saved ☐ Set interval (min): 0

Time stamp is: End ☐ Custom wave (lgor secs):

Review Batch

Review Frags

Done.

