

# Introduction to Software for ACSM

# Data Analysis Software

- New release: Tofware v2.5.13
- Runs in Igor 6 and Igor 7
- Download from <https://sites.google.com/site/ariacsm/>
- Please update! Many bug fixes and new features.
- More information in manual -- TofwareManual.pdf
- Tofware is encrypted – need license for your instrument in order to analyze data
- TofwareLicence\_ACSMXXX.ibw needs to be in:
  - ...\\Documents\\WaveMetrics\\Igor Pro 6 User Files
  - OR ...\\Documents\\WaveMetrics\\Igor Pro 7 User Files

# Data Analysis – 2 levels of complexity

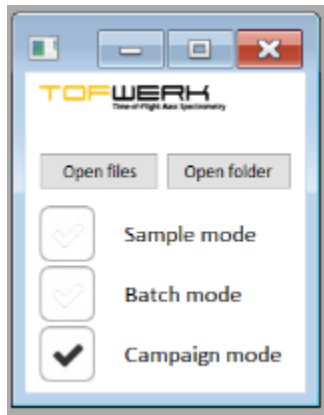
- Level 1: Use the native (e.g., 10 min), hourly .txt files as is.
  - Sticks calculated in Acquility, corrected for instrument calibrations
  - Gives you species mass loading
  - May be issues with native data before Acquility 2.3.1/Tofware 2.5.13 – be careful
- Level 2: Load .h5 data into Tofware and recalculate sticks
  - Check m/Q cal, baseline settings, peakwidth
  - Integrate peaks to get sticks
  - Analyze species mass loadings and mass spectra
  - Gives you Diff (Sample-Filter) on write timebase (e.g., 10 min)
  - Diagnostics
  - PMF Export

# Good housekeeping – check your detection limits

- Put a filter on your inlet
- Take  $\sim \frac{1}{2}$  -1 hour of data
- Look at the standard deviation of the Diff data in Tofware
- Gives an estimate of detection limit for your instrument at this point in time
- You will need your detection limit for  $\text{NH}_4$  if you want to calculate composition dependent collection efficiency (CDCE)

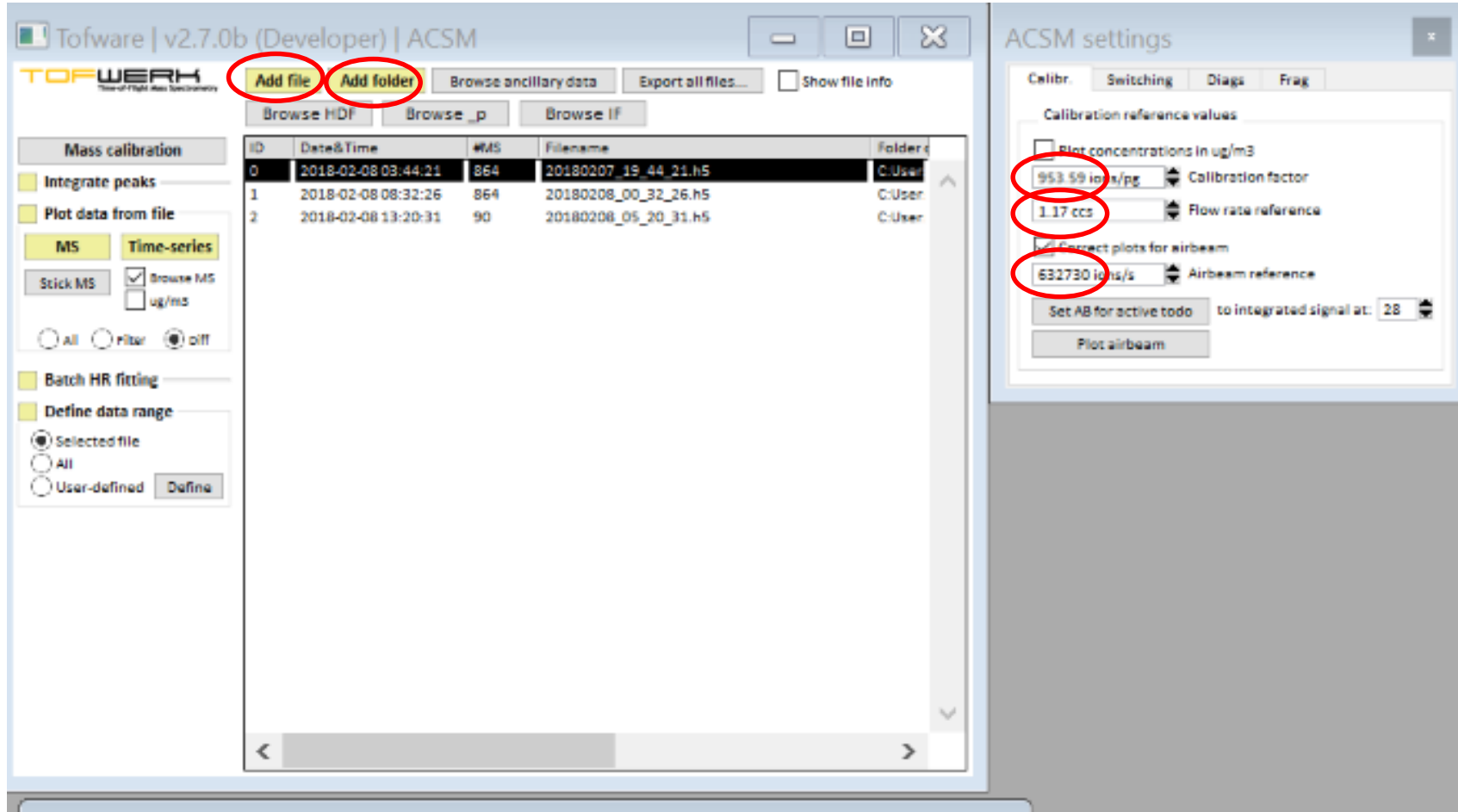
# Start Tofware

- Click on Tofware\_2\_5\_13\_ACSM.pxt, shortcuts get put in correct folders, then have to click on pxt again to start.



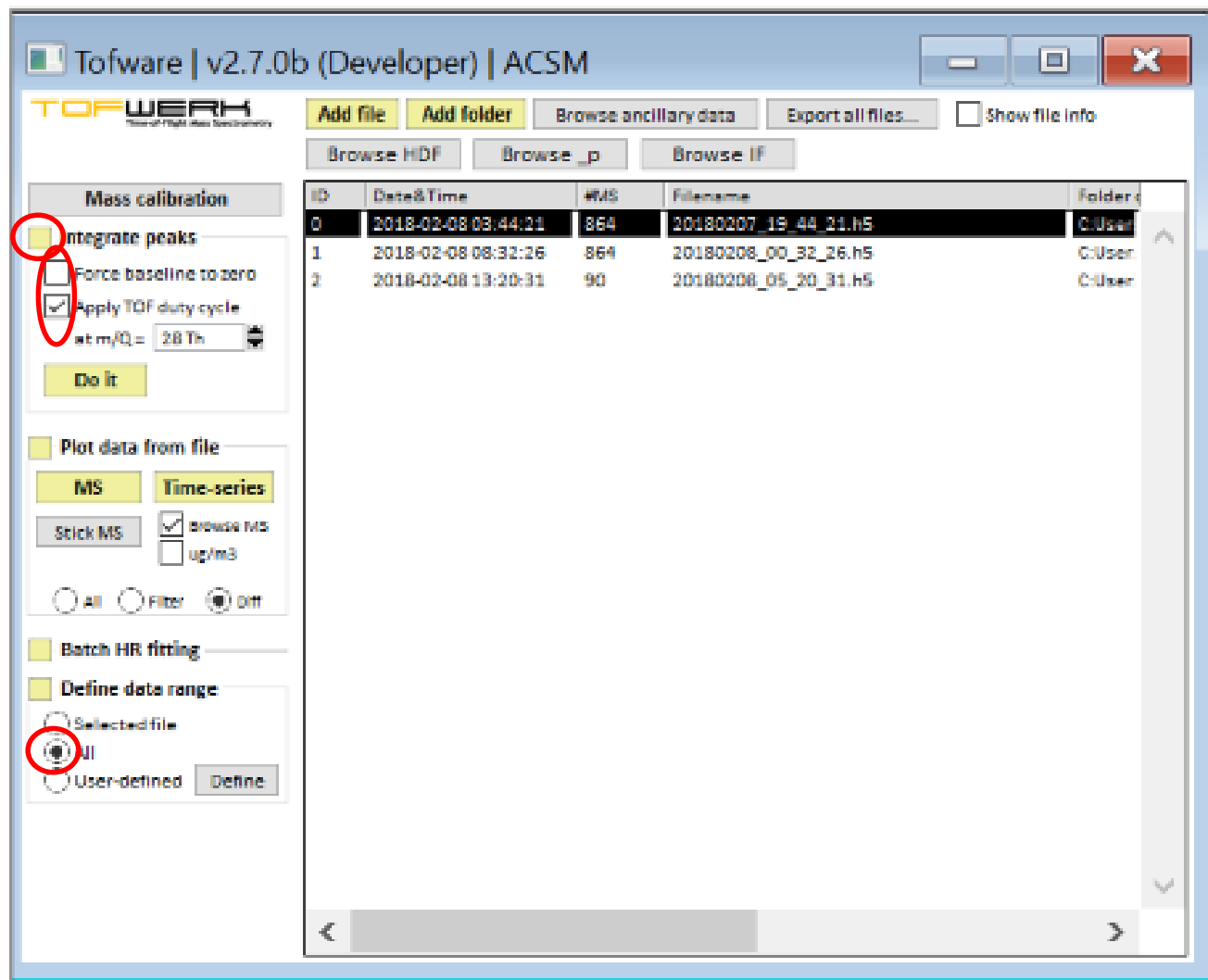
- ToF-ACSM data will always be in Campaign mode (multiple files acquired under same conditions)
- Open files – load one file
- Open folder – load all files in a folder

# Data Loading Panel



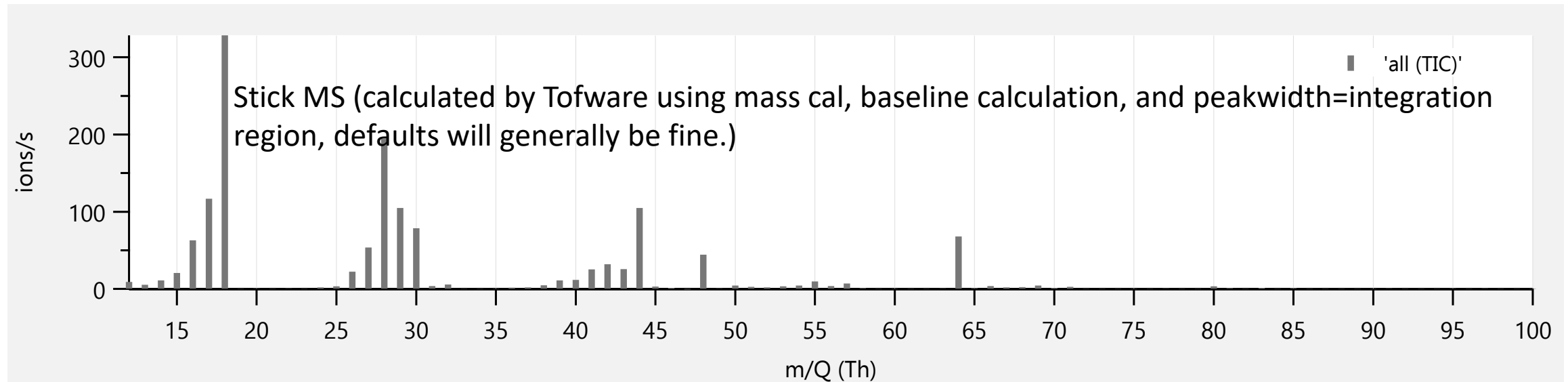
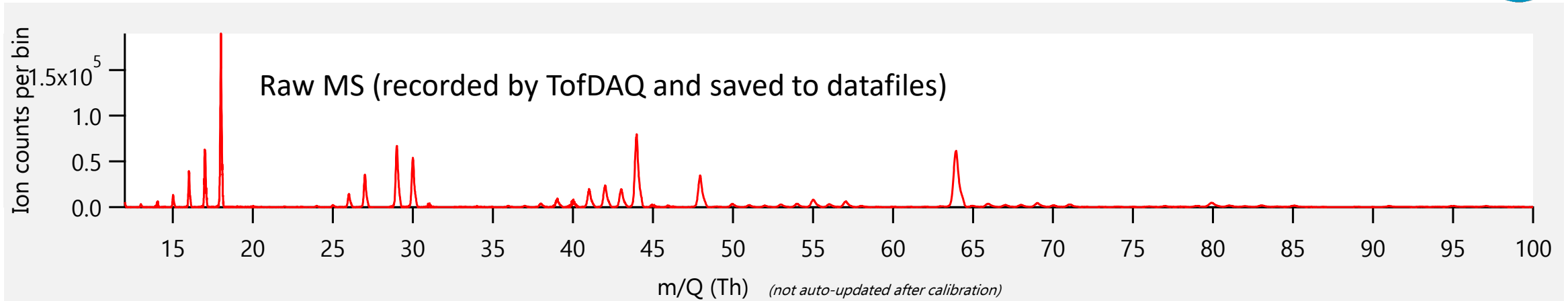
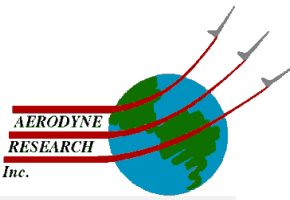
- Can add data folder or datafiles.
- Note that Tofware indexes the data, it does not actually load data until you look at it.
- Check that ions/pg, flow rate and AB are what you expect.

# Quick look at data: Integrate peaks



- Click Integrate Peaks
- Default: Do NOT Force baseline to zero
- Default: DO Apply ToF duty cycle
  - Accounts for the fact that lighter ions travel faster through the extraction region and are less likely to be extracted relative to heavier ions.
- Click All to do all files
- Click Do It

# This step integrates across each peak to give you the stick MS





# Plot time-series for species, in $\mu\text{g}/\text{m}^3$ , with AB correction

The screenshot displays the TOFWERK v2.5.13 ACSM software interface. The main window shows a file list with columns: ID, Date&Time, #MS, Filename, and Folder. The file list contains 11 entries, with the first entry (ID 0) highlighted. The 'Plot data from file' section on the left has 'Time-series' selected. The 'ACSM settings' dialog box is open, showing the 'Calibr.' tab. In this tab, 'Plot concentrations in ug/m3' and 'Correct plots for airbeam' are checked. The 'all' dialog box is also open, showing a list of species with 'all (TIC)' selected. The 'Species' list includes: all (TIC), Org, NO3, SO4, Chl, NH4, H2O, and K.

**TOFWERK v2.5.13 | ACSM**

**Mass calibration**

- ☐ Integrate peaks
- ☐ Force baseline to zero
- ☒ Apply TOF duty cycle at  $m/Q = 28 \text{ Th}$
- Do it**

**Plot data from file**

- MS** **Time-series**
- ☐ Stick MS
- ☐ browse MS
- ☒  $\mu\text{g}/\text{m}^3$
- ☐ All ☐ Filter ☒ Diff

**Batch HR fitting**

**Define data range**

- ☐ Selected file
- ☒ All
- ☐ User-defined **Define**

ID	Date&Time	#MS	Filename	Folder
0	2016-03-25 15:51:44	4320	20160325_16_51_44.h5	C:\User
1	2016-03-26 15:52:35	4320	20160326_16_52_35.h5	C:\User
2	2016-03-27 15:53:26	4320	20160327_17_53_26.h5	C:\User
3	2016-03-28 15:54:23	4320	20160328_17_54_23.h5	C:\User
4	2016-03-29 15:55:14	4320	20160329_17_55_14.h5	C:\User
5	2016-03-30 15:56:05	4320	20160330_17_56_05.h5	C:\User
6	2016-04-01 15:57:48	4320	20160401_17_57_48.h5	C:\User
7	2016-04-02 15:58:39	4320	20160402_17_58_39.h5	C:\User
8	2016-04-03 15:59:36	4320	20160403_17_59_36.h5	C:\User
9	2016-04-04 16:00:27	4320	20160404_18_00_27.h5	C:\User
10	2016-04-05 16:01:21	4320	20160405_18_01_21.h5	C:\User

**ACSM settings**

Calibr. Switching Diags Frag

Calibration reference values

- ☒ Plot concentrations in  $\mu\text{g}/\text{m}^3$
- 150 ions/pg Calibration factor
- 1.33 ccs Flow rate reference
- ☒ Correct plots for airbeam
- 355000 ions/s Airbeam reference
- Set AB for active todo** to integrated signal
- Plot airbeam**

**all**

- ☐ Plot sum of all peaks
- ☐ Plot base peak
- ☐ Browse all peaks
- ☒ Plot peaks in this list:
- chl;nh4;no3;org;so4; ? Clear
- 1 Rolling average (1 = no effect)
- Plot** **Cancel**

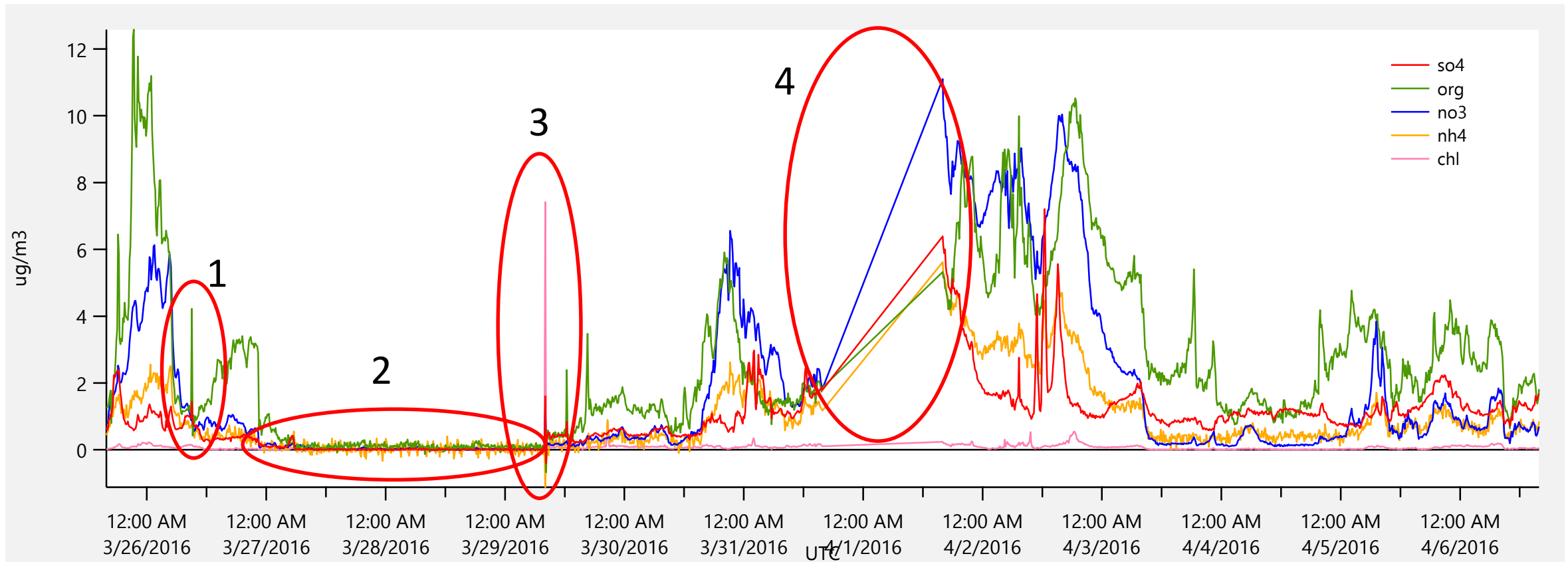
ion	x0
m/Q 1	1.0000000000
m/Q 2	2.0000000000
m/Q 3	3.0000000000
m/Q 4	4.0000000000
m/Q 5	5.0000000000
m/Q 6	6.0000000000
m/Q 7	7.0000000000
m/Q 8	8.0000000000
m/Q 9	9.0000000000
m/Q 10	10.0000000000
m/Q 11	11.0000000000
m/Q 12	12.0000000000
m/Q 13	13.0000000000
m/Q 14	14.0000000000
m/Q 15	15.0000000000
m/Q 16	16.0000000000
m/Q 17	17.0000000000
m/Q 18	18.0000000000
m/Q 19	19.0000000000
m/Q 20	20.0000000000
m/Q 21	21.0000000000
m/Q 22	22.0000000000

**Species**

- ☒ Show species panel
- ☒ Calculate frag. patterns
- all (TIC)
- Org
- NO3
- SO4
- Chl
- NH4
- H2O
- K

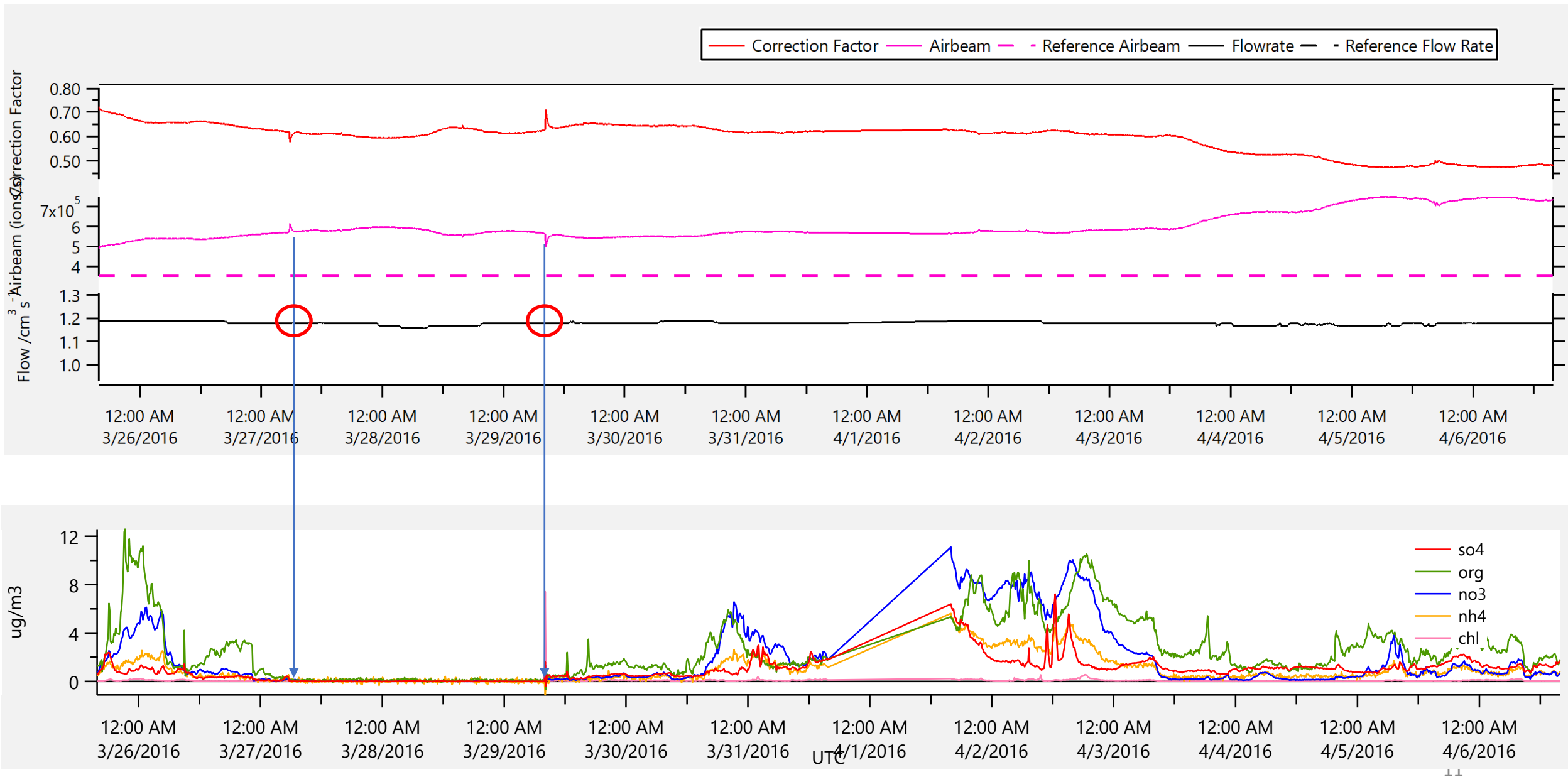
# Sample data from ACTRIS Paris intercomparison, March 2016.

## Some parts of data look suspicious – let's investigate



- 1 and 3: Very narrow spikes (1 point wide) sometimes mean air burps from o-rings. Let's look at AB.
- 2: Very low signal with no diurnal variation looks suspicious. Let's look at instrument parameters.
- 4: Missing 24 hours of data. Turned out to be corrupted datafile.

See blips in AB, but flow rate looks steady. So, not critical orifice clogging.

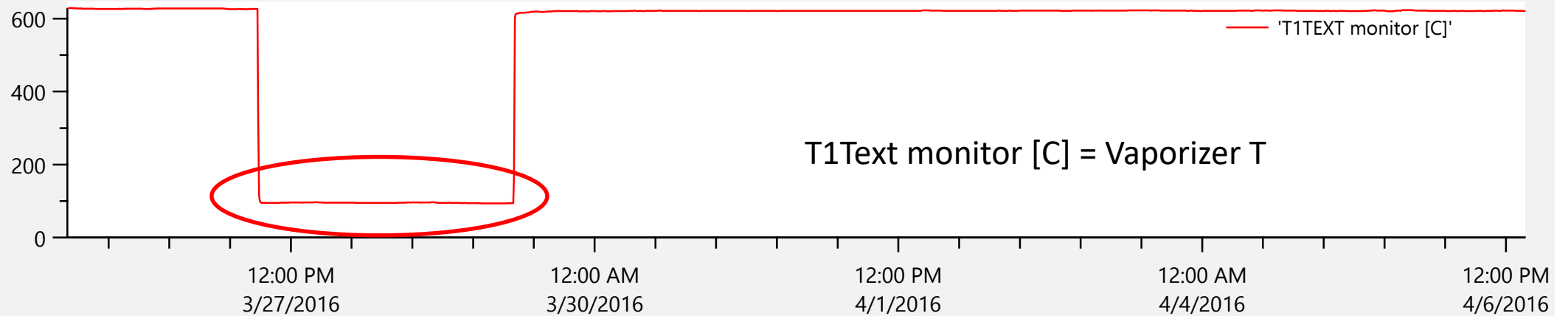
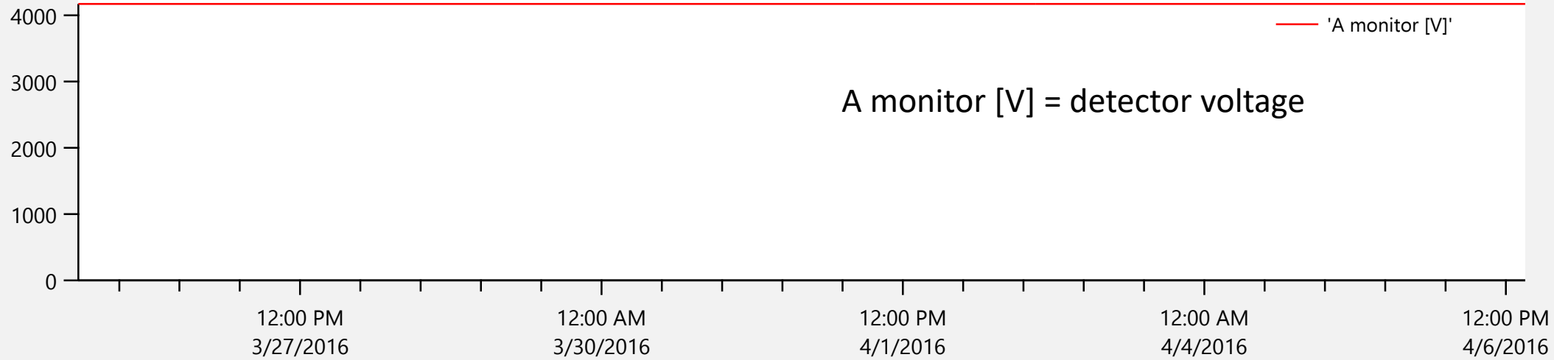


# Take a look at ancillary data – detector voltage, vaporizer temperature

The screenshot displays the TOFWERK v2.5.13 ACSM software interface. On the left, the 'Ancillary' window shows a list of available data points under the '/TPS2' header. The 'T1TEXT monitor [C]' is selected. On the right, the main window shows the 'Mass calibration' and 'Integrate peaks' sections. The 'Browse ancillary data' button is circled in red, and a red arrow points from it to the 'T1TEXT monitor [C]' in the left window. The 'Integrate peaks' section includes options for 'Force baseline to zero' and 'Apply TOF duty cycle' at m/Q = 28 Th. The 'Plot data from file' section has 'MS' and 'Time-series' tabs, with 'ug/m3' selected. The 'Batch HR fitting' and 'Define data range' sections are also visible. A table of files is shown on the right, with columns for ID, Date/Time, #MS, Filename, and Folder.

ID	Date/Time	#MS	Filename	Folder
1	2016-03-25 15:51:44	4320	20160325_16_51_44.h5	C:\User...
2	2016-03-26 15:52:35	4320	20160326_16_52_35.h5	C:\User...
3	2016-03-27 15:53:26	4320	20160327_17_53_26.h5	C:\User...
4	2016-03-28 15:54:23	4320	20160328_17_54_23.h5	C:\User...
5	2016-03-29 15:55:14	4320	20160329_17_55_14.h5	C:\User...
6	2016-03-30 15:56:05	4320	20160330_17_56_05.h5	C:\User...
7	2016-04-01 15:57:48	4320	20160401_17_57_48.h5	C:\User...
8	2016-04-02 15:58:39	4320	20160402_17_58_39.h5	C:\User...
9	2016-04-03 15:59:36	4320	20160403_17_59_36.h5	C:\User...
10	2016-04-04 16:00:27	4320	20160404_18_00_27.h5	C:\User...
11	2016-04-05 16:01:21	4320	20160405_18_01_21.h5	C:\User...

Aha! Vaporizer turned off for a few days. Need to remove these runs.



- **Todo concept:** Set of data that you perform operations on.

The screenshot displays the Tofware v2.5.13 ACSM interface. The main window shows a list of files and a table of data points. A 'Create todo' dialog box is open, allowing users to create a new todo set. The dialog includes several options for creating a todo set, such as 'From point', 'From selected files in table', 'From todo', 'Every N writes', 'By time of day', and 'By key wave'. The 'From todo' option is selected, and the 'all' todo is chosen. The dialog also shows a list of todos and a table of data points. Red circles highlight the 'New...' button in the top left, the 'AND NOT' button in the logic section, and the 'Create new todo' button at the bottom.

**File List:**

- Get List
- all
- HDF\_fileID\_0
- HDF\_fileID\_1
- HDF\_fileID\_2
- HDF\_fileID\_3
- HDF\_fileID\_4
- HDF\_fileID\_5
- HDF\_fileID\_6
- HDF\_fileID\_7
- HDF\_fileID\_8
- HDF\_fileID\_9
- HDF\_fileID\_10
- new
- NoVap

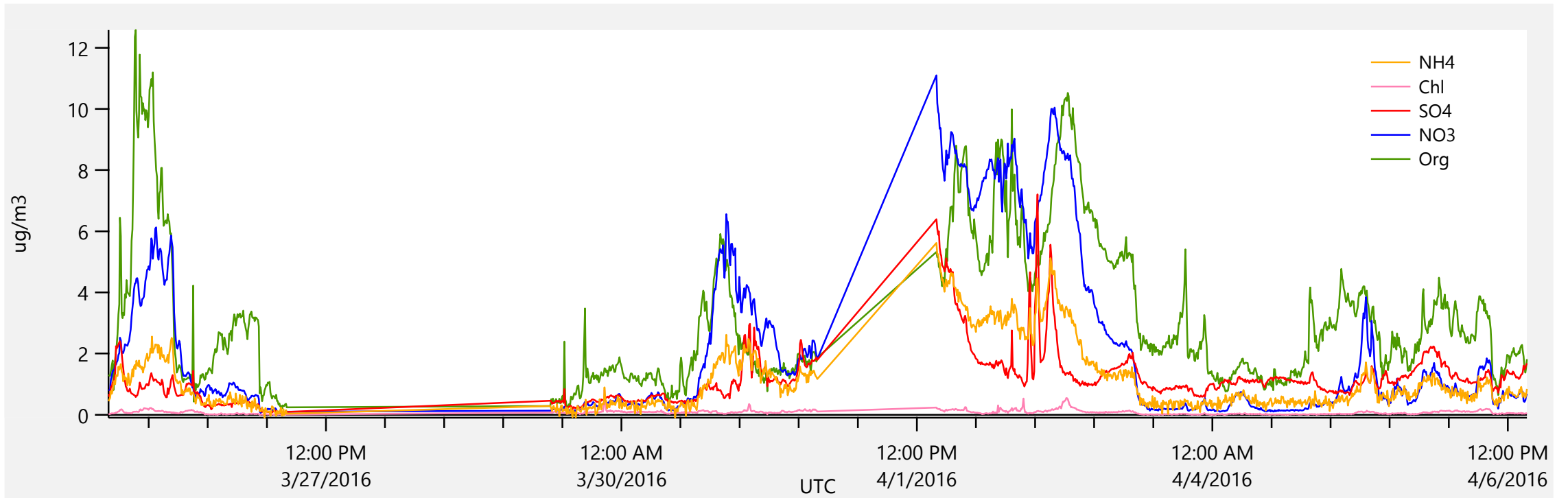
**Table:**

ID	Date&Time	#MS	Filename	Folder
0	2016-03-25 15:51:44	4320	20160325_16_51_44.h5	C:\User...
1	2016-03-26 15:52:35	4320	20160326_16_52_35.h5	C:\User...
2	2016-03-27 15:53:26	4320	20160327_17_53_26.h5	C:\User...
3	2016-03-28 15:54:23	4320	20160328_17_54_23.h5	C:\User...
4	2016-03-29 15:55:14	4320	20160329_17_55_14.h5	C:\User...
5	2016-03-30 15:56:05	4320	20160330_17_56_05.h5	C:\User...
6	2016-04-01 15:57:48	4320	20160401_17_57_48.h5	C:\User...
7	2016-04-02 15:58:39	4320	20160402_17_58_39.h5	C:\User...

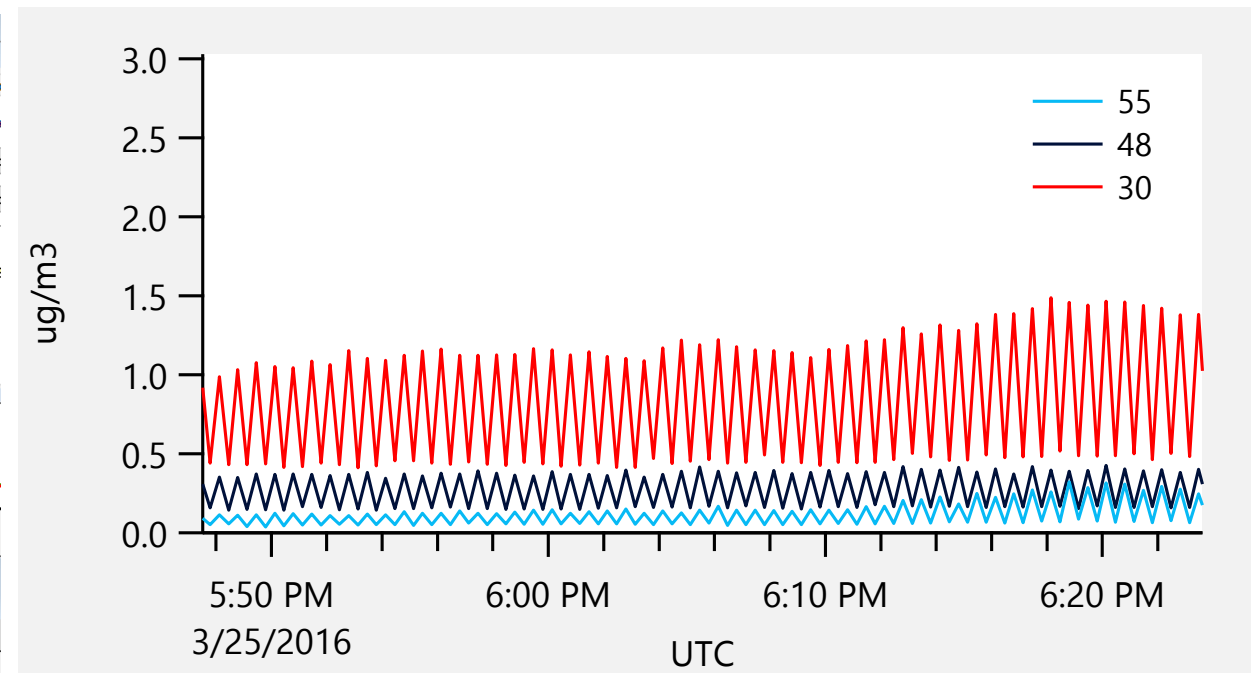
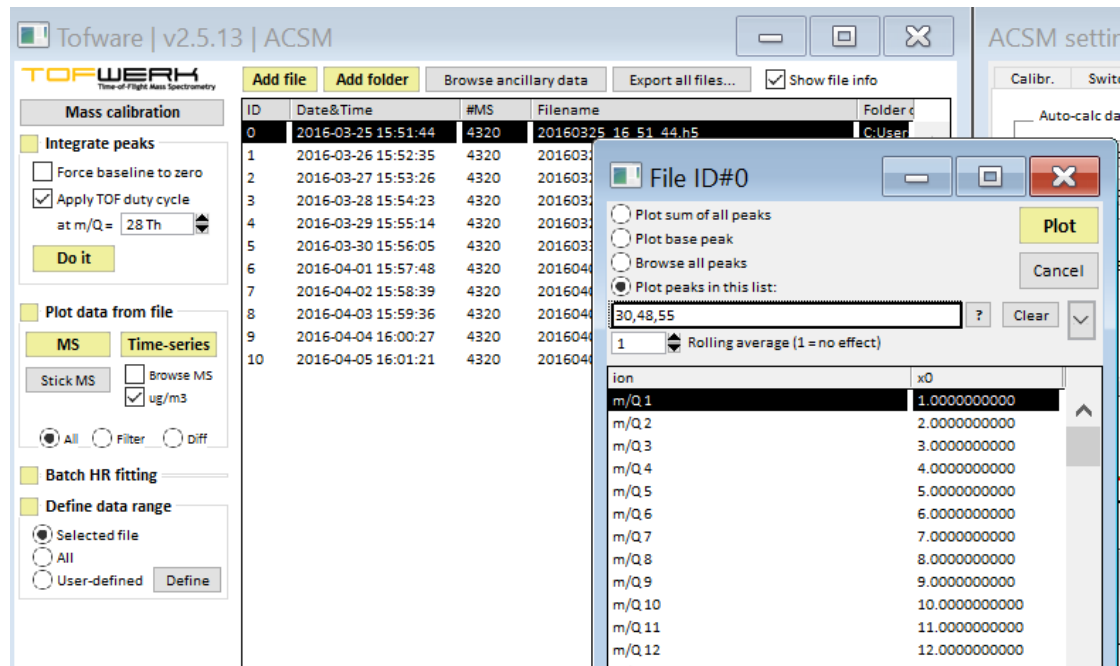
**Create todo dialog options:**

- ☐ From point 0 to point 1583
- ☐ From selected files in table
- ☒ From todo: all
- ☐ Every N writes: 10
- ☐ By time of day: From (hr): 0 To (hr): 0
- ☐ By key wave: make new
- ☐ Save buf indices with todos (BufTodos)
- Logic: AND OR AND NOT Clear
- all ANDNOT Novap
- Overwrite selected
- Create new todo: Good

Now we have a todo with good ambient data.

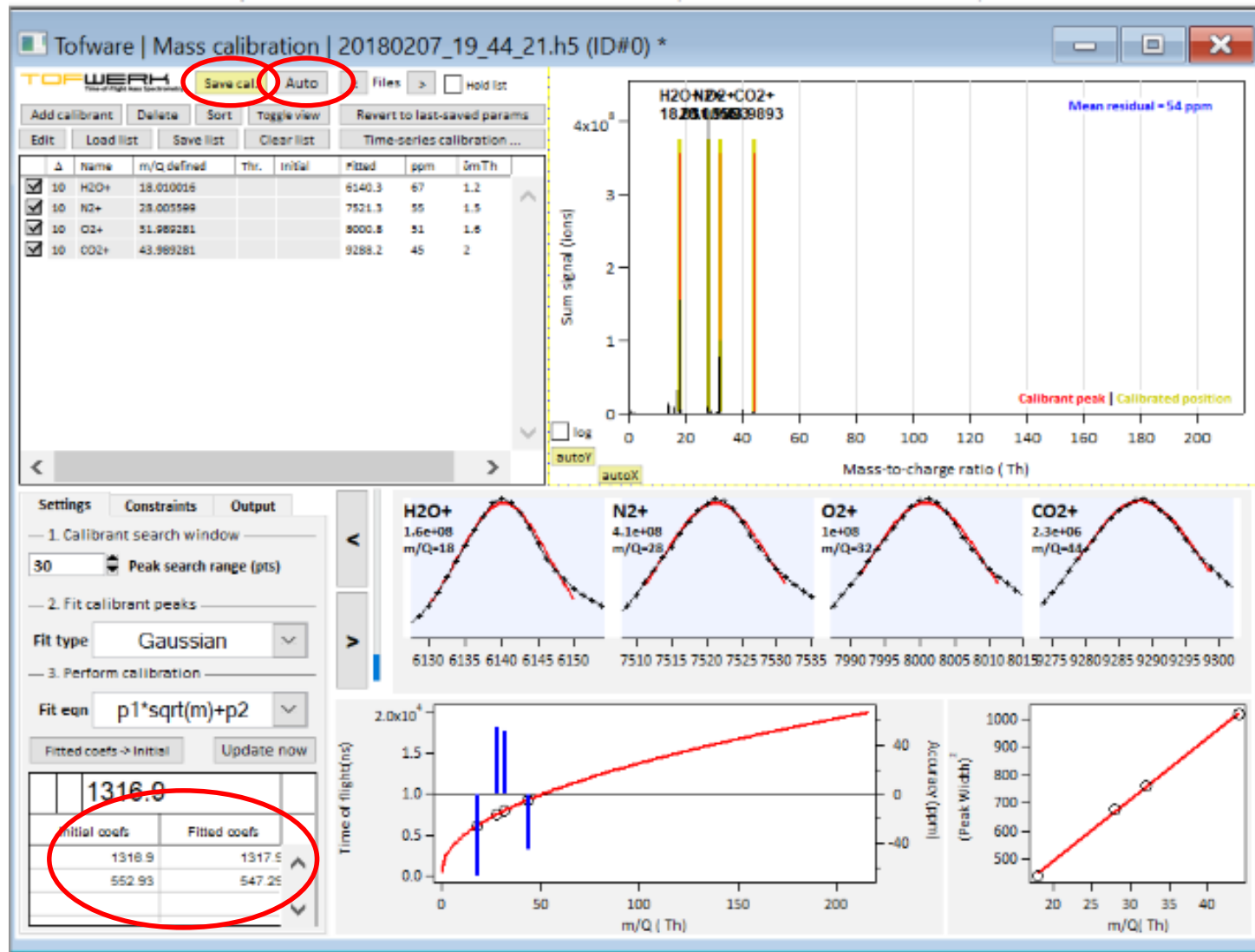


- Now that we have taken a quick look, we can go through the mass calibration, baseline fitting and peakwidth more carefully (optional).
- If your quick look shows very noisy or negative data, worth looking at the all time-series to see if valve switching was ok. Look at m/Q's where you expect signal. Also look at 18. Highly variable H<sub>2</sub>O can cause problems. Using a dryer on your inlet can help, but most of water is in the vacuum chamber.

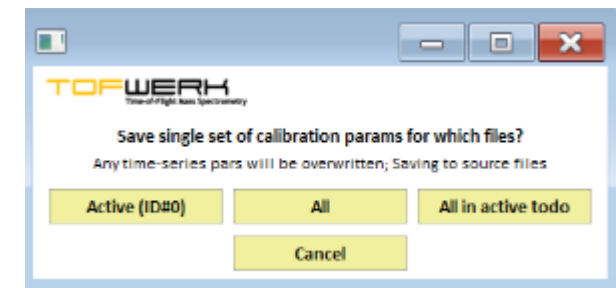




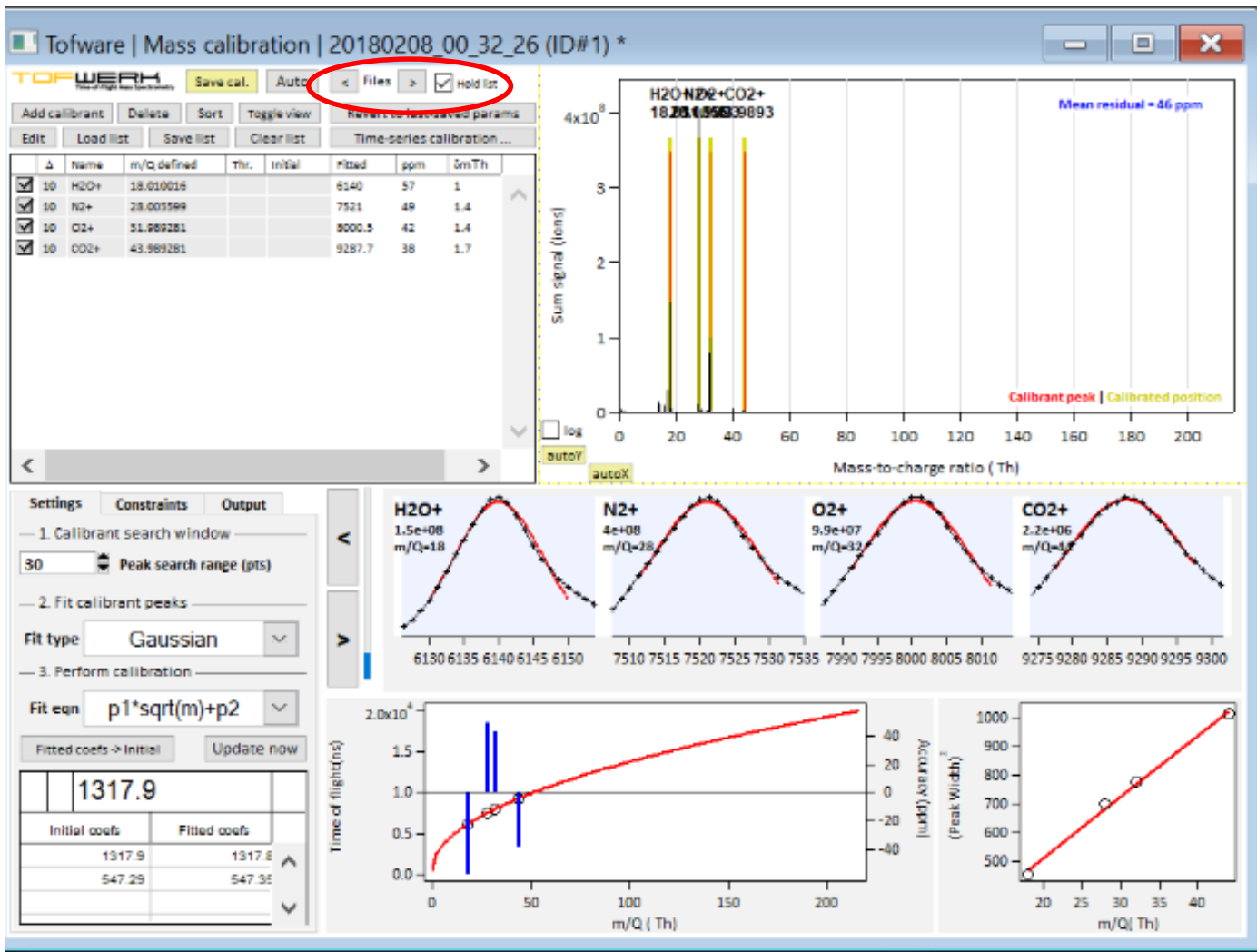
# Check Mass Calibration



- Click Auto to get same masses as in Acquility
- Should not be much change in mass cal parameters
- Click Save cal



# Mass Calibration on Multiple Files

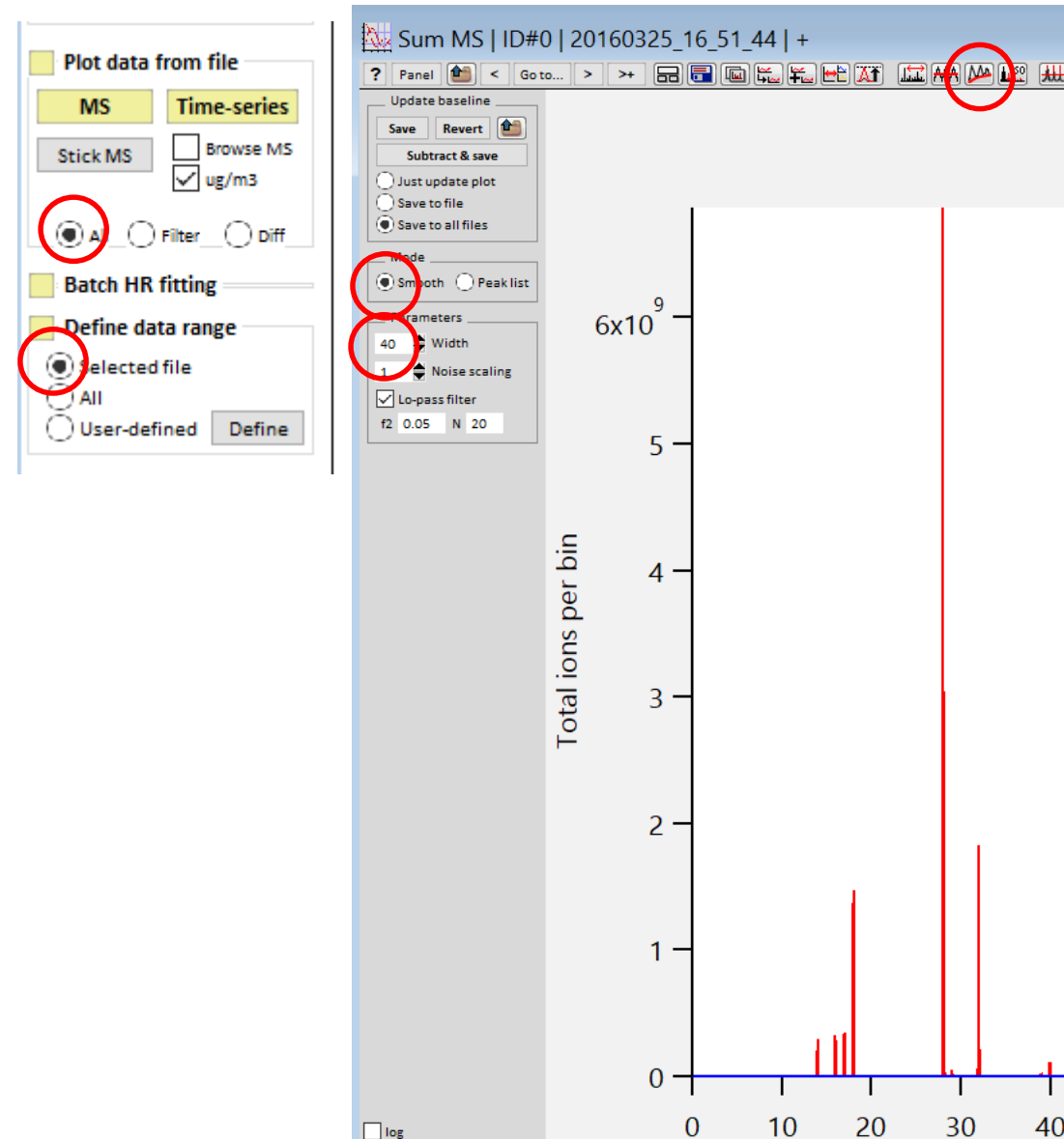


- Check Hold List box to keep same masses
- Click arrows to go forward and back in the file list
- Good idea to check each file
- Mass cal generally very stable in ToF-ACSM

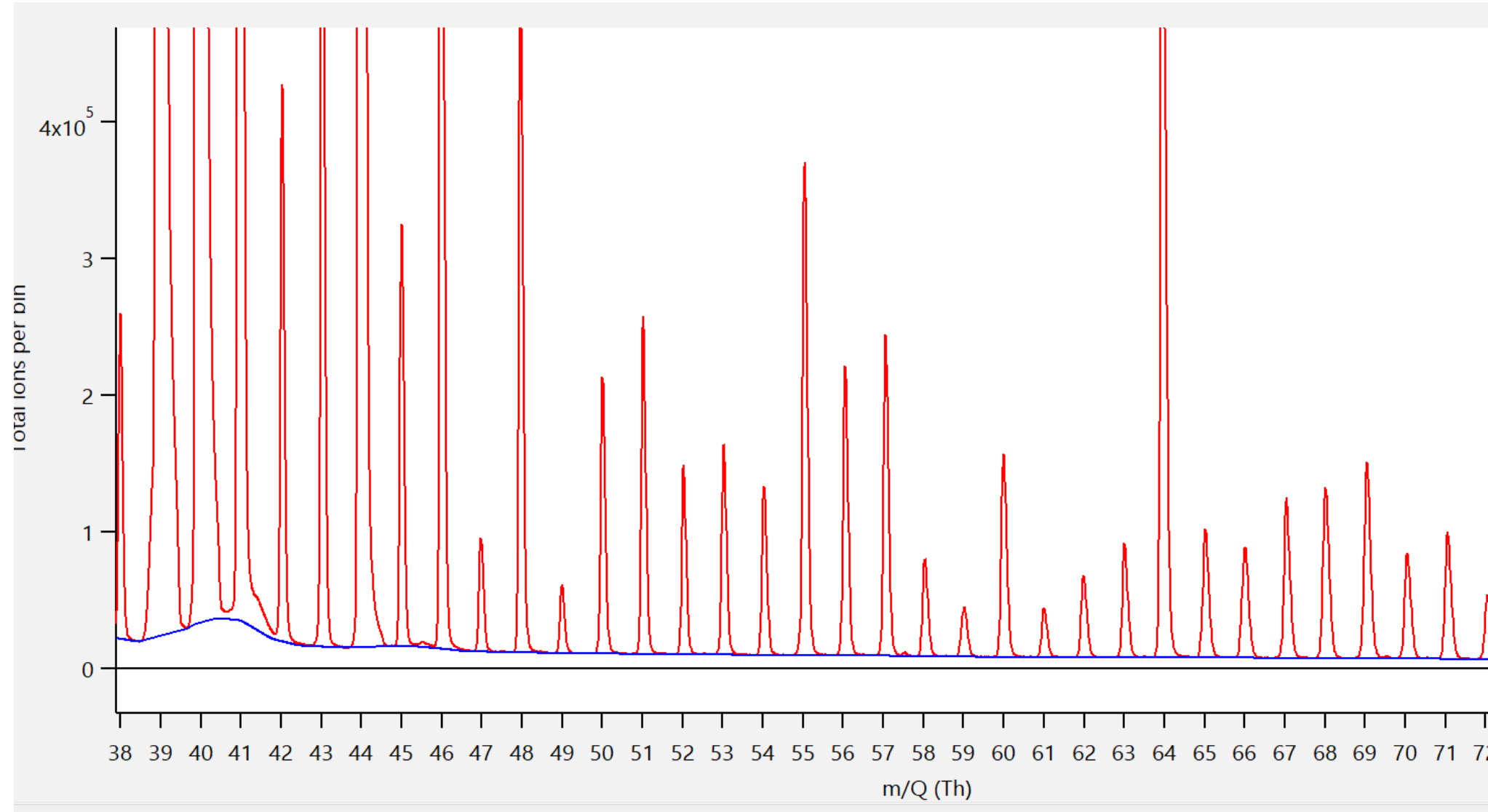
# Baseline Fitting (NOTE Do not use IF panel – has bugs)

On any All MS

- Click the baseline button
- Use Smooth Mode
  - Determines baseline by taking lowest point in a moving average window and smoothing
- Use Width of moving average = 40
- Estimates noise on baseline using regions with no peaks
- Adds noise to smoothed moving average to put baseline in the center of the noise
- Save to all files (saves the parameters that will be used to calculate the baseline when you integrate peaks.)



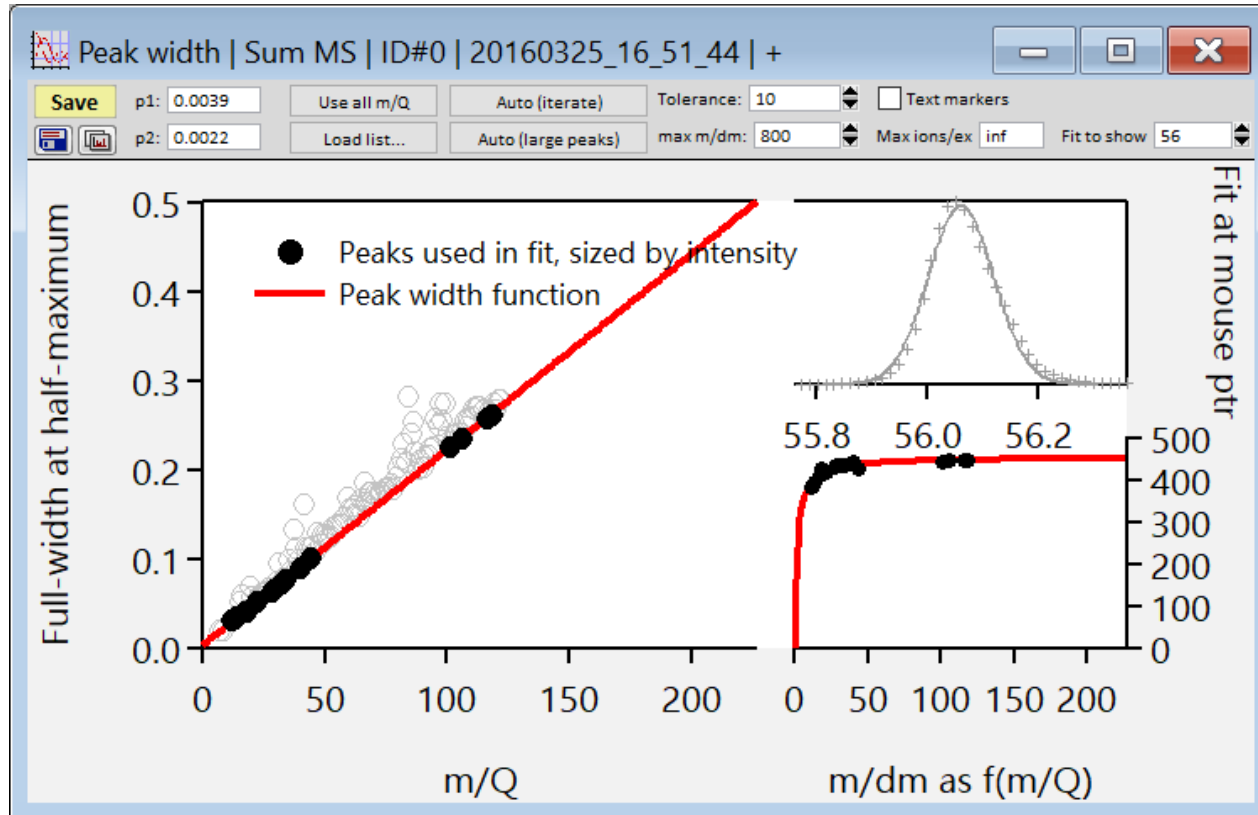
# Baseline Fitting cont.: Detector takes a while to recover after a large signal.



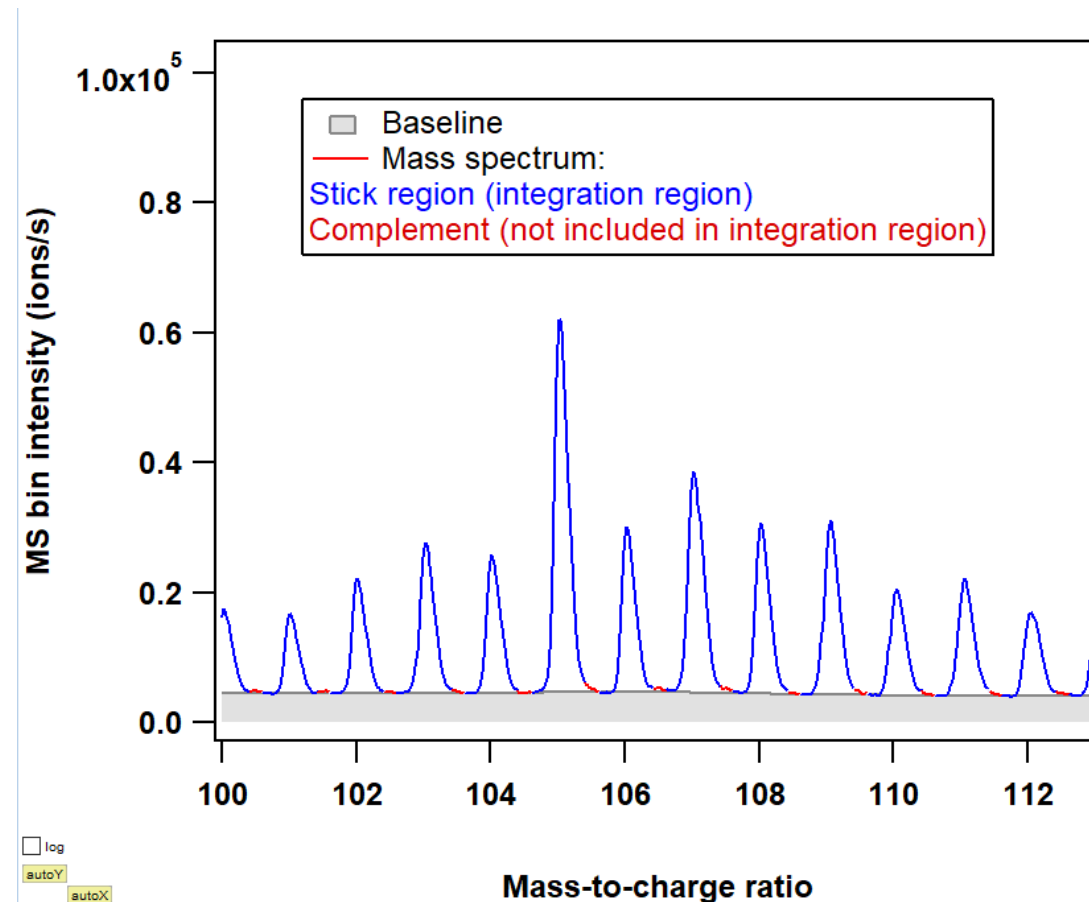
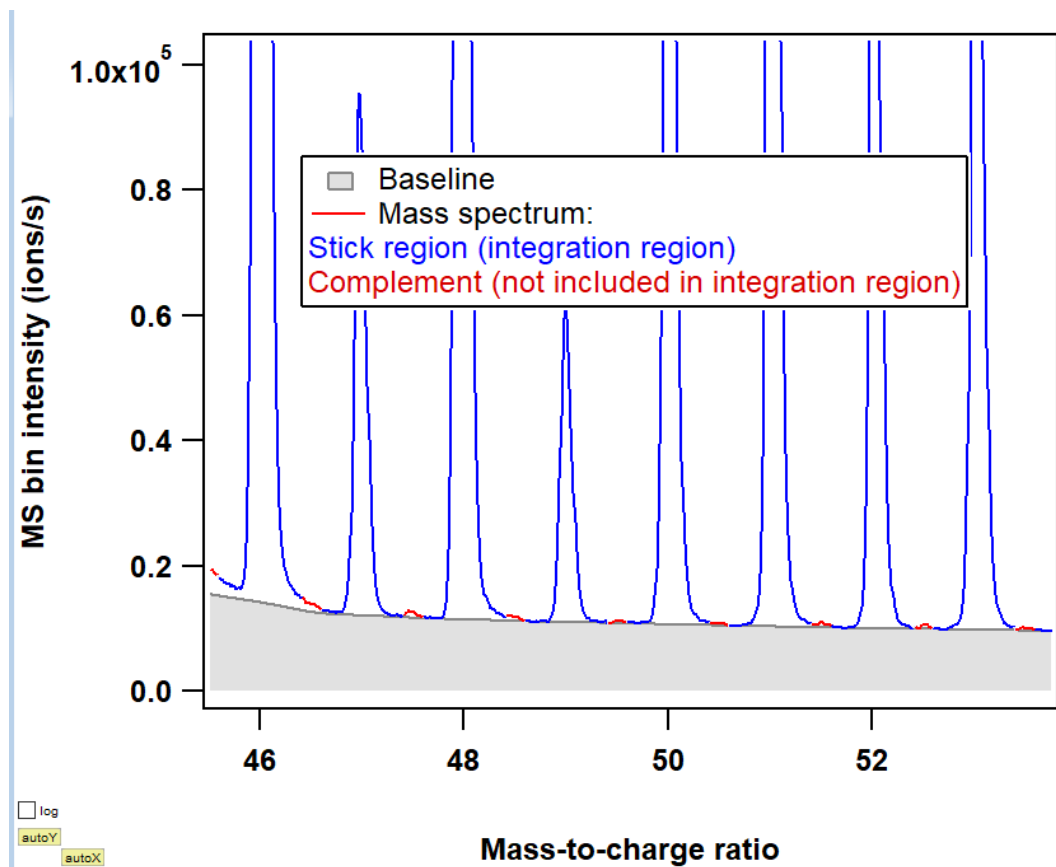
# Setting peakwidth (determines integration regions)

On any MS

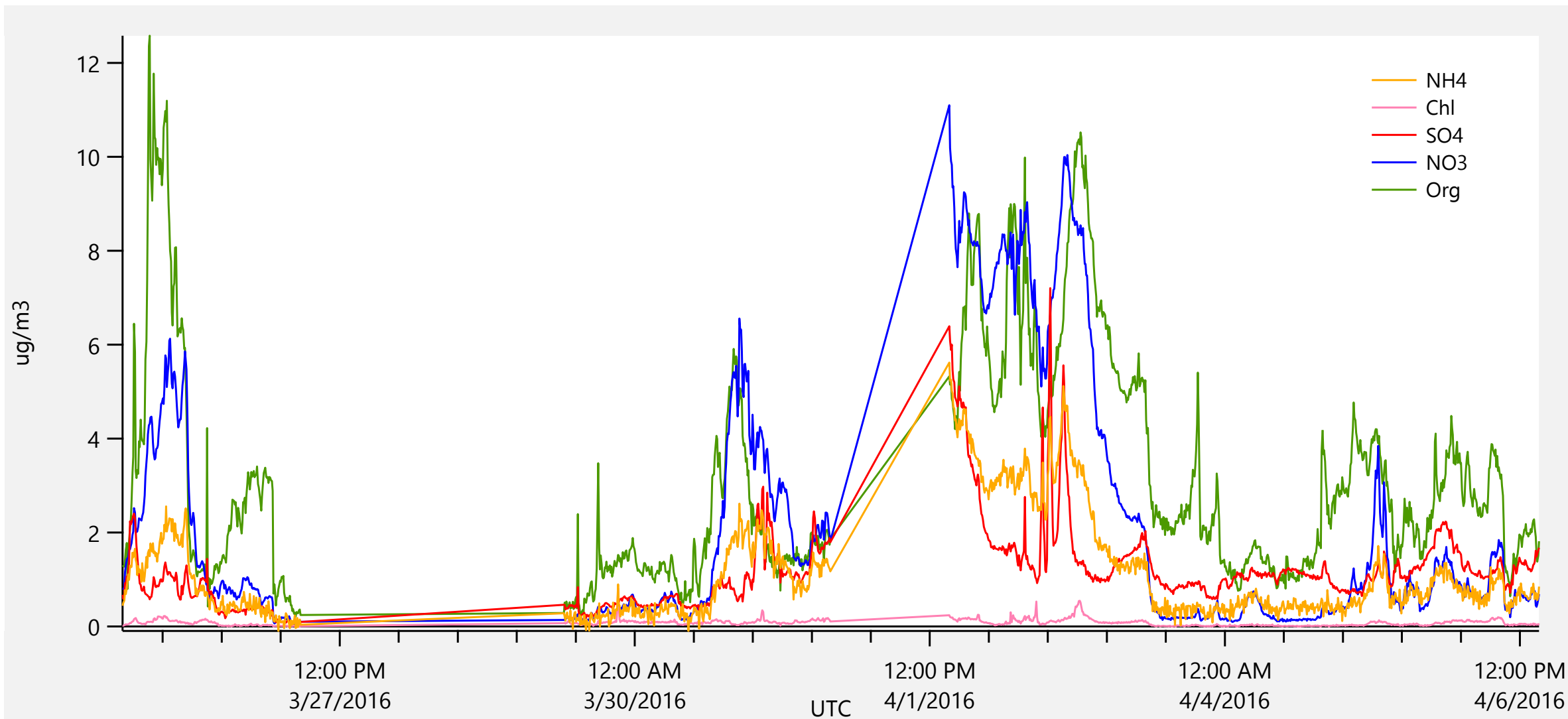
- Move cursor over a peak until it turns into a little hand and right click
- Choose peakwidth
  - Assumption: narrowest peaks are most likely to be a single ion fragment
  - Uses narrowest peaks to determine peakwidth as a function of  $m/Q$
- Save peakwidth function to all files
  - Peakwidth generally stable unless you tune HB or other voltages in mass spectrometer
- Lower right plot is instrument resolution in  $m/dm$



Stick integration regions are function of peakwidth up to a predefined maximum of 0.8 m/Q



# Integrate Peaks Again – Not Much Should Change



# Calculate an Average Stick Mass Spectrum

TOFWERK Time-of-Flight Mass Spectrometry

Mass calibration

Integrate peaks

☐ Force baseline to zero

☒ Apply TOF duty cycle

at m/Q = 28 Th

Do it

Plot data from file

MS Time-series

Stick MS ☐ Browse MS

☒ ug/m3

All Filter Diff

Batch HR fitting

Define data range

☐ Selected file

☐ All

☒ User-defined Define

ID	Date&Time	#MS	Filename	Folder
0	2016-03-25 15:51:44	4320	20160325_16_51_44.h5	C:\User
1	2016-03-26 15:52:35	4320	20160326_16_52_35.h5	C:\User
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3	2016-03-28 15:54:23	4320	20160328_17_54_23.h5	C:\User
4	2016-03-29 15:55:14	4320	20160329_17_55_14.h5	C:\User
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6	2016-04-01 15:57:48	4320	20160401_17_57_48.h5	C:\User
7	2016-04-02 15:58:39	4320	20160402_17_58_39.h5	C:\User
8	2016-04-03 15:59:36	4320	20160403_17_59_36.h5	C:\User
9	2016-04-04 16:00:27	4320	20160404_18_00_27.h5	C:\User
10	2016-04-05 16:01:21	4320	20160405_18_01_21.h5	C:\User

Good2

☒ Averaged stick MS

☐ Time-series \* stick MS

☐ Show browser

☐ Box & whisker plot

Org,NO3,SO4,Chl,NH4,H2O ? Clear

1 Rolling average (1 = no effect)

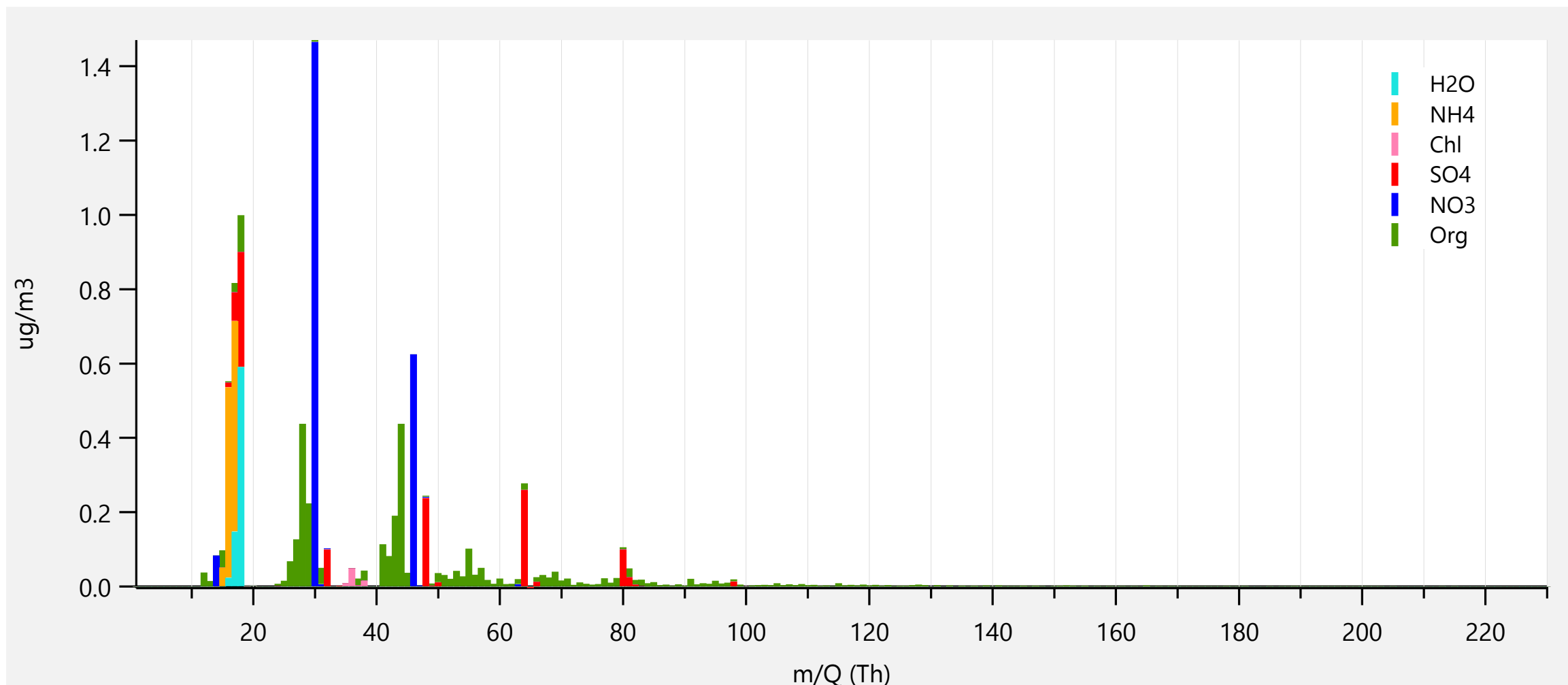
Show species panel ☒ Calculate frag. patterns

Species

- all (TIC)
- Org
- NO3
- SO4
- Chl
- NH4
- H2O



Sum of sticks for a species = average of time series.



NOTE: RIE is applied to MS in Tofware (unlike in AMS analysis).

# Very useful table: Tofware/Advanced/Table of file attributes

## Information from workspace profile

Tofware   File attribute table					
C0 Label	TofwareFlag				
Attribute	20160325_16_51_44	20160326_16_52_35	20160327_17_53_26	20160328_17_54_23	20160329_17_55_20
HDF5 File Creation Time	3/25/2016 16:51:44	3/26/2016 16:52:35	3/27/2016 17:53:26	3/28/2016 17:54:23	3/29/2016 17:55:20
Configuration File	C:\Tofwerk\TofDaq_1.99r334_SF	C:\Tofwerk\TofDaq_1.99r334_SF	C:\Tofwerk\TofDaq_1.99r334_SF	C:\Tofwerk\TofDaq_1.99r334_SF	C:\Tofwerk\TofDaq_1.99r334_SF
CurrentRun	1	2	3	4	5
NbrRuns	999	999	999	999	999
NbrSamples	15872	15872	15872	15872	15872
NbrRawSamples	15872	15872	15872	15872	15872
NbrPeaks	230	230	230	230	230
NbrWaveforms	50000	50000	50000	50000	50000
NbrSegments	1	1	1	1	1
NbrBlocks	1	1	1	1	1
NbrMemories	20	20	20	20	20
NbrBufs	30	30	30	30	30
NbrCubes	1	1	1	1	1
IonMode	positive	positive	positive	positive	positive
Configuration File Contents	[TOFParameter]BlockPeriod=100	[TOFParameter]BlockPeriod=100	[TOFParameter]BlockPeriod=100	[TOFParameter]BlockPeriod=100	[TOFParameter]BlockPeriod=100
NbrWrites	144	144	144	144	144
ACSMACSMmode	1	1	1	1	1
ACSMswitchBuf	0	0	0	0	0
ACSMstartBuf_C	0	0	0	0	0
ACSMstopBuf_C	0	0	0	0	0
ACSMstartBuf_O	0	0	0	0	0
ACSMstopBuf_O	0	0	0	0	0
ACSMugConv_ionspg	150	150	150	150	150
ACSMABref	355000	355000	355000	355000	355000
ACSMflowRef	1.3301	1.3301	1.3301	1.3301	1.3301
ACSMFlowM	1.0152	1.0152	1.0152	1.0152	1.0152
ACSMFlowC	-0.4059	-0.4059	-0.4059	-0.4059	-0.4059
ACSMCoulombs	0.1254054152	0.1266145834	0.1279255448	0.1292724339	0.1306193230

# Names of useful ancillary data:

- PRESSA2 monitor [mbar] = Lens pressure (used to calculate flow rate)
- PressA3\_V monitor [V] = Analog input 3 on BNC panel
- PressA4\_V monitor [V] = Analog input 4 on BNC panel
- PressA5\_V monitor [V] = Analog input 5 on BNC panel
- PressA6\_V monitor [V] = Analog input 6 on BNC panel
- A monitor [V] = Detector Voltage
- T1Text monitor [C] = Vaporizer T