

Aerodyne
Research, Inc.

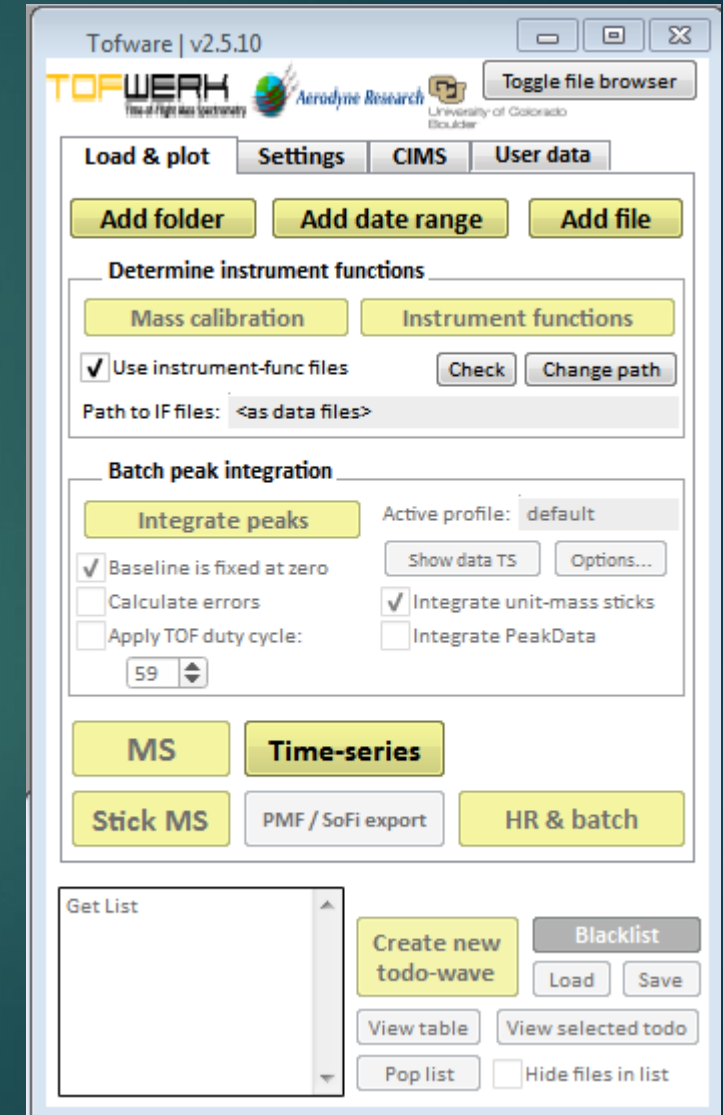
TOFWERK
Time-of-Flight Mass Spectrometry

Tofware

HARALD STARK

MIKE CUBISON

- ▶ Analysis software for multiple Aerodyne/Tofwerk instruments
 - ▶ CIMS (FIGAERO support)
 - ▶ IMS
 - ▶ PTR-MS
 - ▶ GC-TOF
 - ▶ Not AMS (except event trigger)
- ▶ Functionality
 - ▶ Data preaveraging
 - ▶ Data indexing (=pointing towards any sized dataset)
 - ▶ m/z calibration
 - ▶ Instrument function definition
 - ▶ Unit-mass-resolution (UMR) processing and display
 - ▶ High-resolution (HR) analysis
 - ▶ Peak identification
 - ▶ Multi-peak fitting
 - ▶ Display (time-series, spectra, chemical information)

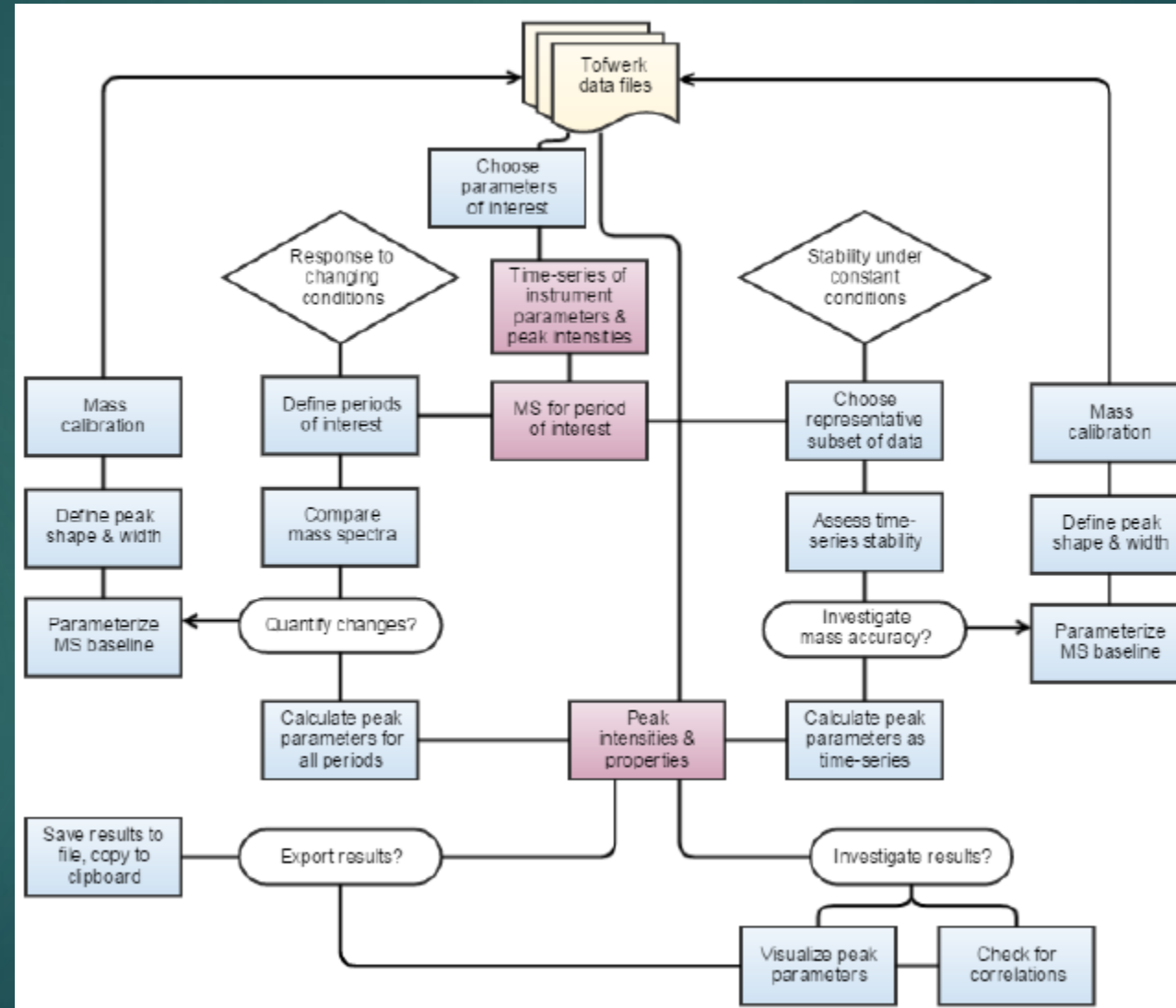


Tofware facts and faces

- ▶ Anyone with an Aerodyne (Tofwerk) instrument can use it
- ▶ Distributed via google site (what can we use in China?)
- ▶ Free initial training for all new users (5+ hours)
- ▶ Training videos (planned)
- ▶ User manual
- ▶ Continuous free user support
- ▶ Frequent (~6 months) updates
- ▶ Current version: 2.5.10
- ▶ Newest versions require igor 7
- ▶ Windows and Mac
- ▶ Developers/support: Mike Cubison (Tofwerk), Harald Stark (Aerodyne)

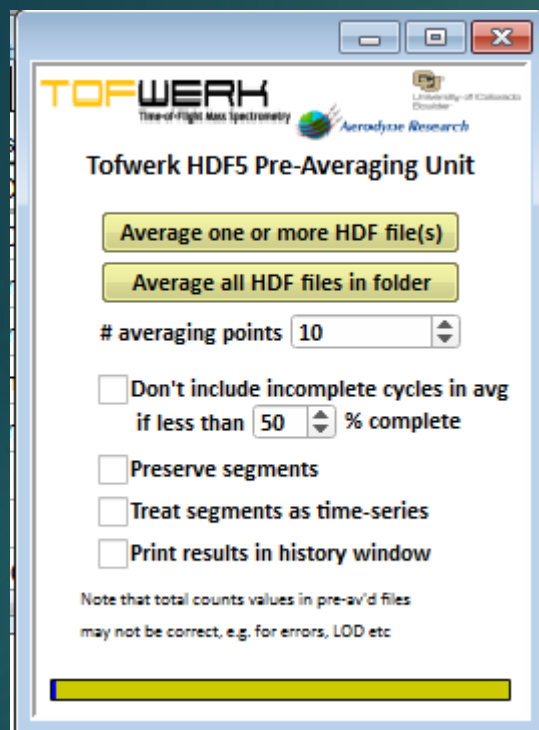


General workflow

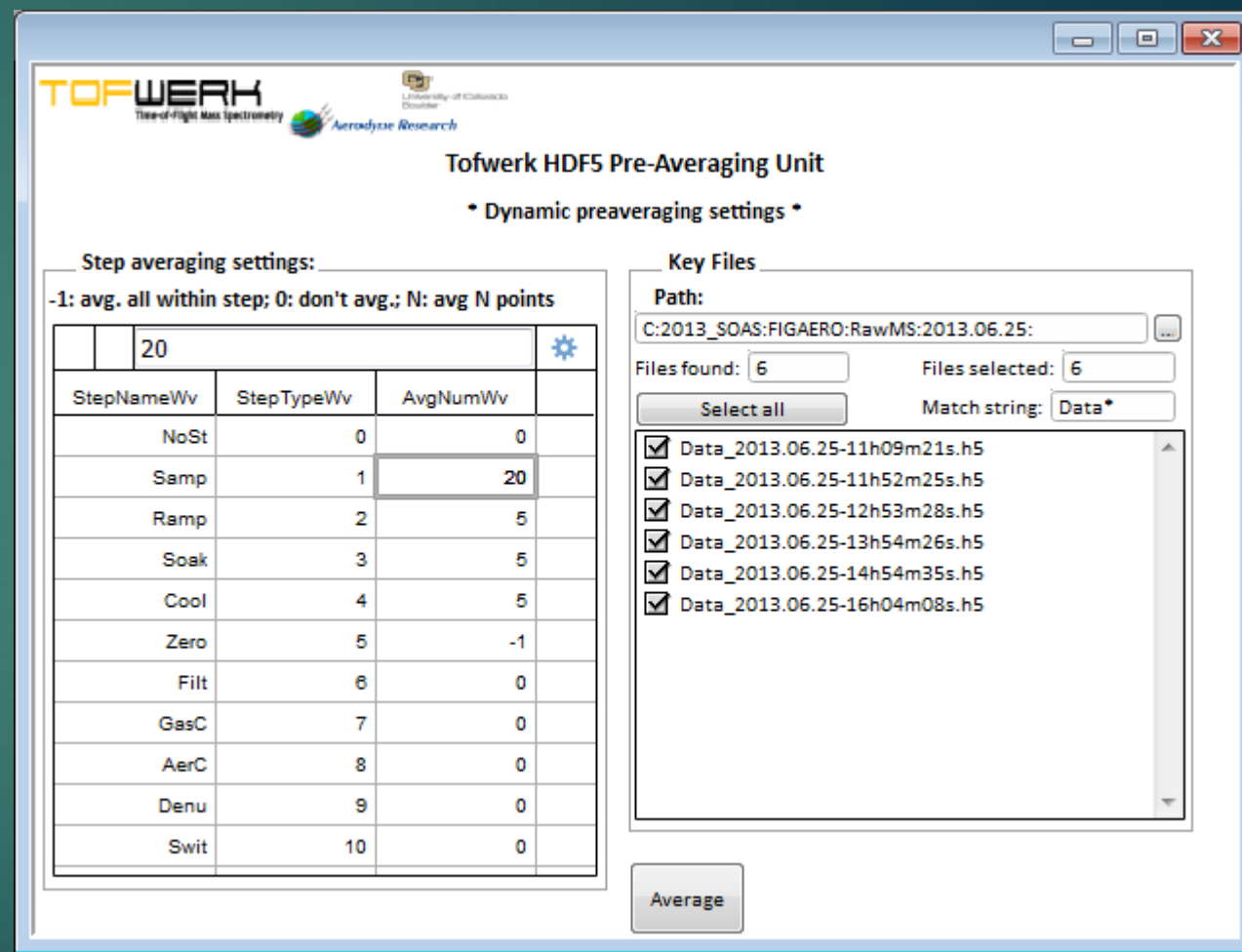


Demo: preaveraging data

Tofware v2.5.10



Future feature in Tofware v2.6.0



Demo: adding data to Tofware

6

The screenshot displays the Tofware v2.5.10 software interface. The main window is divided into several panels. On the left, the 'Load & plot' panel includes buttons for 'Add folder', 'Add date range', and 'Add file'. Below these are sections for 'Determine instrument functions' (with 'Mass calibration' and 'Instrument functions' buttons) and 'Batch peak integration' (with 'Integrate peaks' button). The bottom left shows a 'Get List' of HDF files and a 'Create new todo-wave' button. The top right panel, 'Tofware | File Browser', contains a table of data files. The bottom right panel, 'Tofware | Notebook', shows a log of dataset additions. A 'Select one or more Tofwerk data file(s)' dialog box is open in the foreground, showing a file selection interface with a list of files and a 'File name' field.

Tofware | v2.5.10

TOFWERK Time of Flight Mass Spectrometry Aerodyne Research University of Colorado Boulder

Toggle file browser

Load & plot Settings CIMS User data

Add folder Add date range Add file

Determine instrument functions

Mass calibration Instrument functions

☒ Use instrument-func files

Path to IF files: <as data files>

Batch peak integration

Integrate peaks Active profile: default

☒ Baseline is fixed at zero

☐ Calculate errors ☒ Integrate unit-mass sticks

☐ Apply TOF duty cycle: 59 ☐ Integrate PeakData

MS Time-series

Stick MS PMF / SoFi export HR & batch

Get List

all

HDF_fileID_0

HDF_fileID_1

HDF_fileID_2

HDF_fileID_3

Create new todo-wave

Blacklist

Load Save

View table View selected todo

Pop list ☐ Hide files in list

Tofware | File Browser

Sum MS Show location Acquisition log All acq. logs Browse & plot data All timestamps ☐ Show file info

ID	Date&Time	#MS	Filename	Folder on disk	Comments
0	2013-06-25 16:09:21	2130	Data_2013.06.25-11h09m21s.h5	C:2013_SOAS:FIGAERO:RawMS:2013.C	
1	2013-06-25 16:52:25	2130	Data_2013.06.25-11h52m25s.h5	C:2013_SOAS:FIGAERO:RawMS:2013.C	
2	2013-06-25 17:53:28	2250	Data_2013.06.25-12h53m28s.h5	C:2013_SOAS:FIGAERO:RawMS:2013.C	
3	2013-06-25 18:54:26	2270	Data_2013.06.25-13h54m26s.h5	C:2013_SOAS:FIGAERO:RawMS:2013.C	
4	2013-06-25 19:54:35	2130	Data_2013.06.25-14h54m35s.h5	C:2013_SOAS:FIGAERO:RawMS:2013.C	
5	2013-06-25 21:04:08	2520	Data_2013.06.25-16h04m08s.h5	C:2013_SOAS:FIGAERO:RawMS:2013.C	

Tofware | Notebook

Added new dataset: /flowRead/TwData

Added new dataset: /flowSet/TwData

Added new dataset: /flowTime/TwData

Added new dataset: /heatRead/TwData

Added new dataset: /heatSet/TwData

Added new dataset: /heatTime/TwData

Added new dataset: /rht/TwData

Added new dataset: /valveState/TwData

Added new dataset: /valveTime/TwData

Add new dataset (from _p file): /Peaks/error

Add new dataset (from _p file): /Peaks/signal

Add new dataset (from _p file): /Sticks/amus

Add new dataset (from _p file): /Sticks/signal

Success: 1343 new writes were ad

Select one or more Tofwerk data file(s)

<< 2013_SOAS >> FIGAERO > RawMS > 2013.06.25

Search 2013.06.25

Organize New folder

Name	Date modified	Type
Data_2013.06.25-16h04m08s_p.h5	12/23/2015 16:30	HDF5
Data_2013.06.25-14h54m35s_p.h5	12/23/2015 16:28	HDF5
Data_2013.06.25-11h09m21s_p.h5	12/23/2015 16:27	HDF5
Data_2013.06.25-13h54m26s_p.h5	12/23/2015 16:27	HDF5
Data_2013.06.25-12h53m28s_p.h5	12/23/2015 16:25	HDF5
Data_2013.06.25-11h52m25s_p.h5	12/23/2015 16:23	HDF5
Data_2013.06.25-16h04m08s_IF.h5	12/22/2015 15:49	HDF5
Data_2013.06.25-14h54m35s_IF.h5	12/22/2015 15:49	HDF5
Data_2013.06.25-13h54m26s_IF.h5	12/22/2015 15:48	HDF5
Data_2013.06.25-12h53m28s_IF.h5	12/22/2015 15:48	HDF5

File name:

TofDAQ files (*.hdf *.h5)

Open Cancel

Demo: displaying instrument parameters

7

Tofware | v2.5.10

TOFWERK Time-of-Flight Mass Spectrometry Aerodyne Research University of Colorado Boulder

Toggle file browser

Load & plot Settings CIMS User data

Get lists for active todo Plot time-series Table

/TPS2 ☒ Show all bufs ☒ UTC time

- Turbo Motor Temp monitor [C]
- Fore pressure monitor [mbar]
- IMR pressure monitor [mbar]
- SSQ pressure monitor [mbar]
- BSQ pressure monitor [mbar]
- PB pressure monitor [mbar]
- TOF pressure monitor [mbar]
- TOF temp monitor [C]**
- Ambient pressure monitor [mbar]**
- IMR heater temp monitor [C]
- IMR body temp monitor [C]
- INTERLOCK monitor []
- IONMODE target [-]
- OPERATIONMODE target []
- EXT24V target []
- TPS body temp monitor [C]
- TPS air temp monitor [C]

Get List

- all**
- HDF_fileID_0
- HDF_fileID_1
- HDF_fileID_2
- HDF_fileID_3
- HDF_fileID_4

Create new todo-wave Blacklist

Load Save

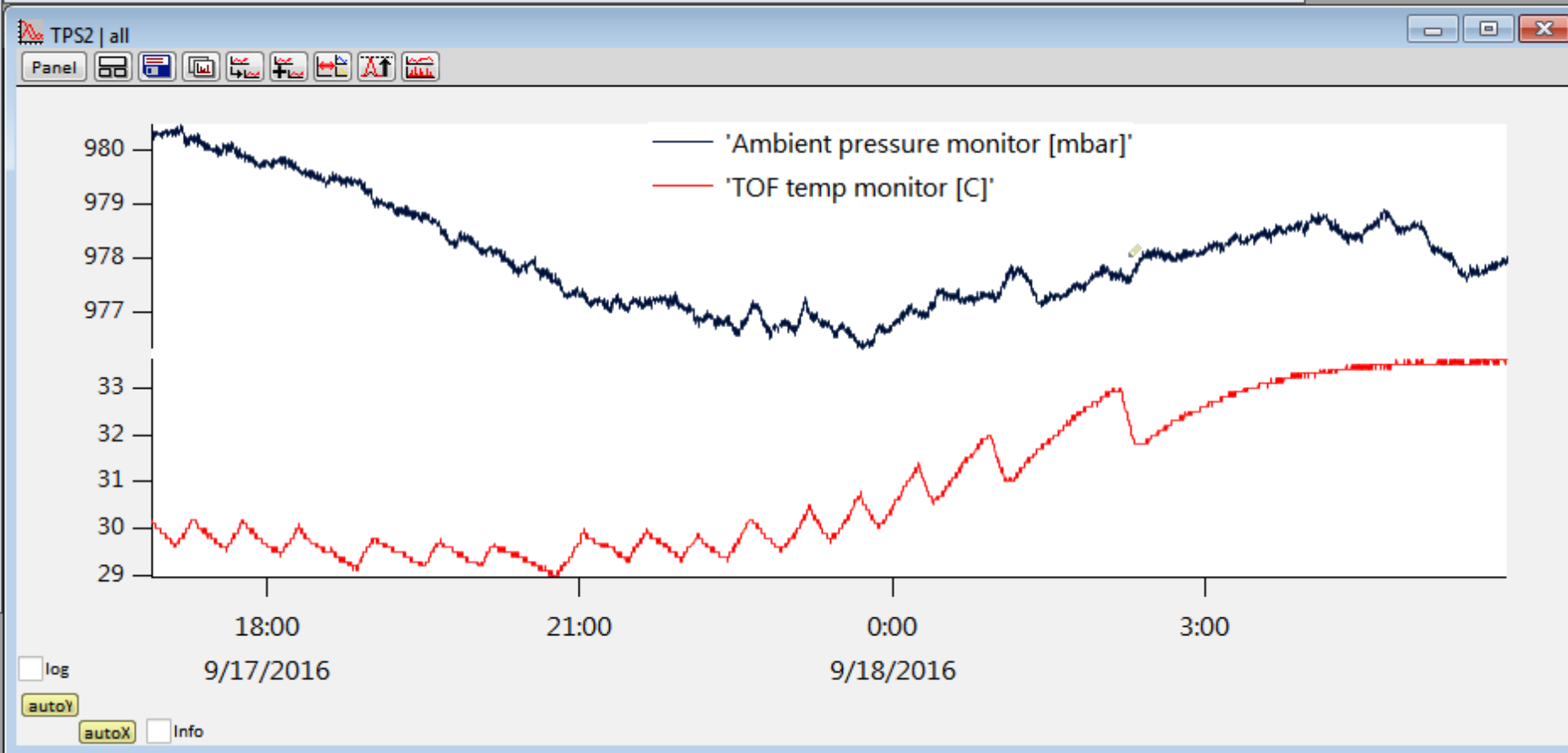
View table View selected todo

Pop list ☐ Hide files in list

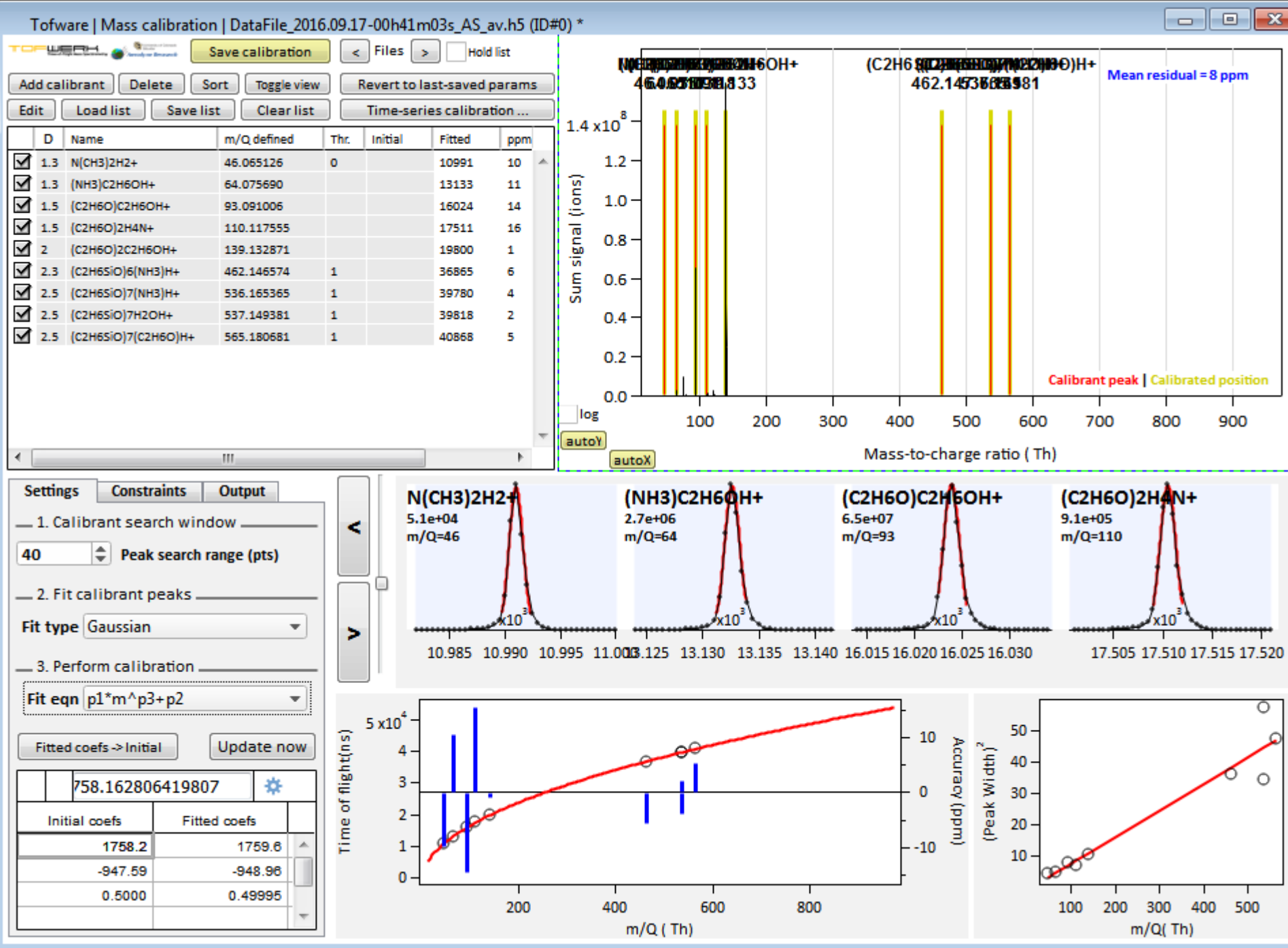
Tofware | File Browser

Sum MS Show location Acquisition log All acq. logs Browse & plot data All timestamps ☐ Show file info

ID	Date&Time	#MS	Filename	Folder on disk	Comments
0	2016-09-17 16:53:58	360	Data_n_2016.09.17_11h53m58s.h5	C:2016_SGP_Campaign:CU_LTOF:Cam	
1	2016-09-17 17:53:59	360	Data_n_2016.09.17_12h53m59s.h5	C:2016_SGP_Campaign:CU_LTOF:Cam	
2	2016-09-17 18:54:00	360	Data_n_2016.09.17_13h54m00s.h5	C:2016_SGP_Campaign:CU_LTOF:Cam	
3	2016-09-17 19:54:01	360	Data_n_2016.09.17_14h54m01s.h5	C:2016_SGP_Campaign:CU_LTOF:Cam	
4	2016-09-17 20:54:02	360	Data_n_2016.09.17_15h54m02s.h5	C:2016_SGP_Campaign:CU_LTOF:Cam	
5	2016-09-17 21:54:03	360	Data_n_2016.09.17_16h54m03s.h5	C:2016_SGP_Campaign:CU_LTOF:Cam	
6	2016-09-17 22:54:04	360	Data_n_2016.09.17_17h54m04s.h5	C:2016_SGP_Campaign:CU_LTOF:Cam	

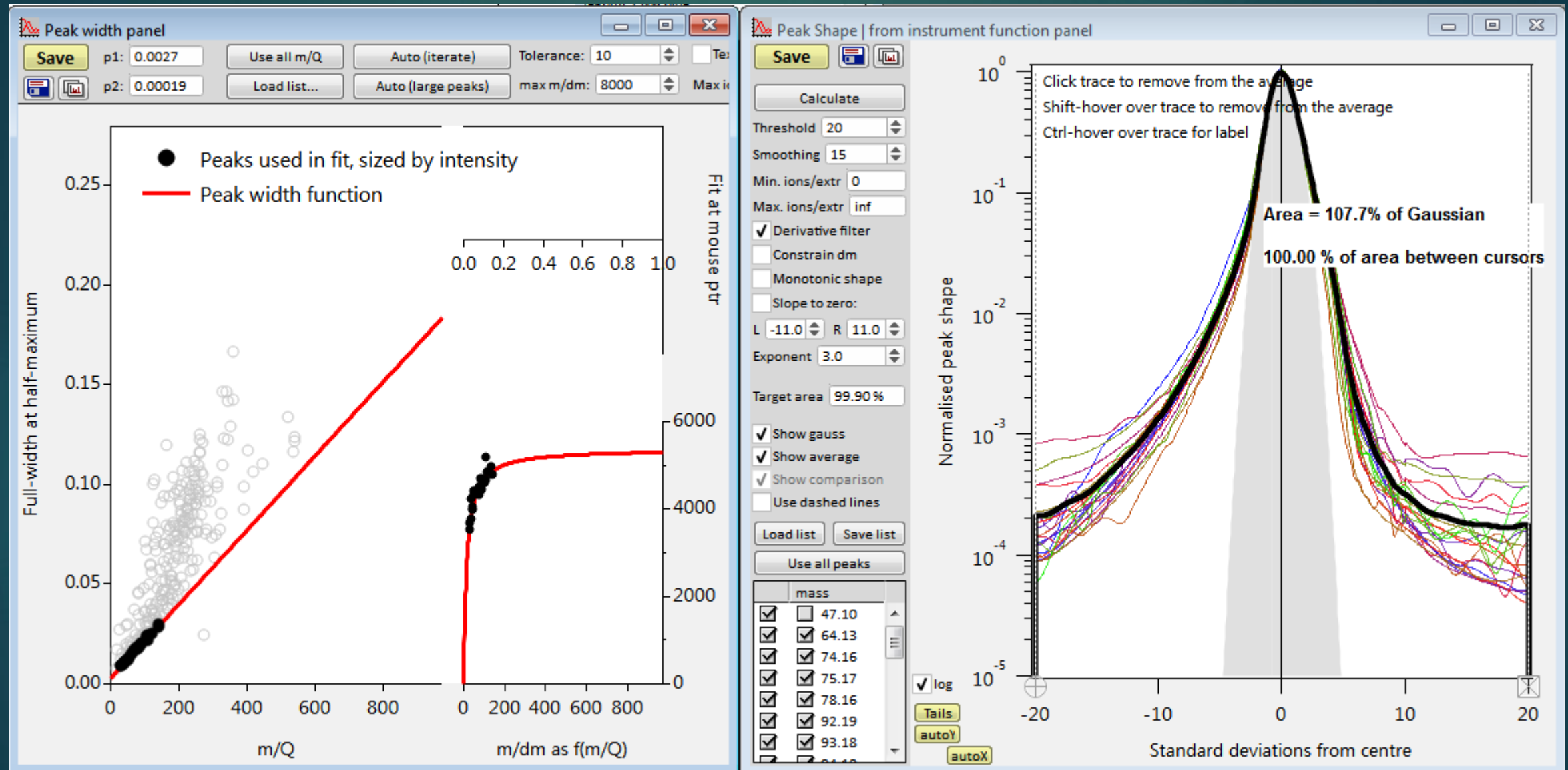


Demo: “mass” (m/z) calibration



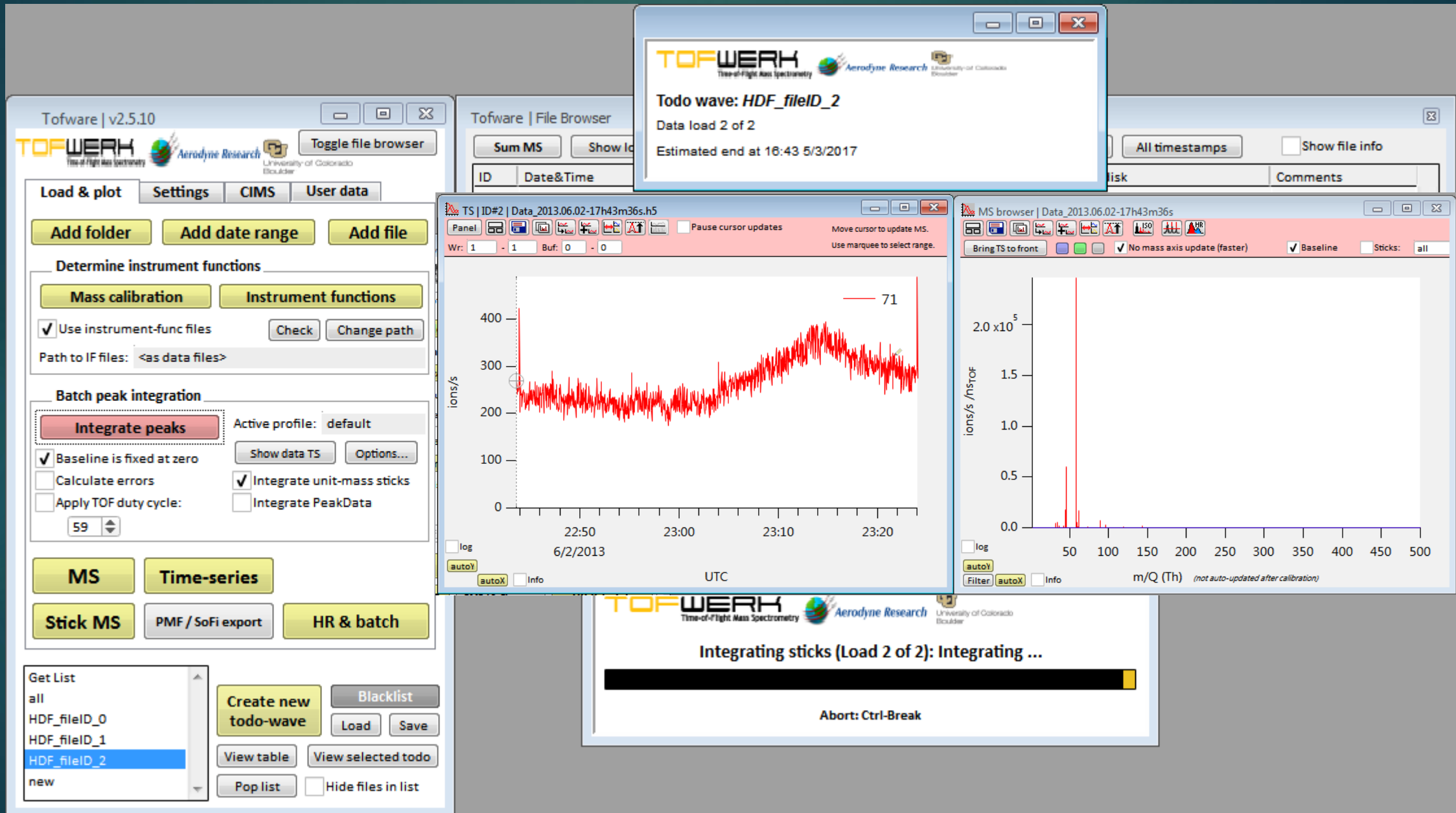
Demo: peak shape and peak width (not showing baselines)

9



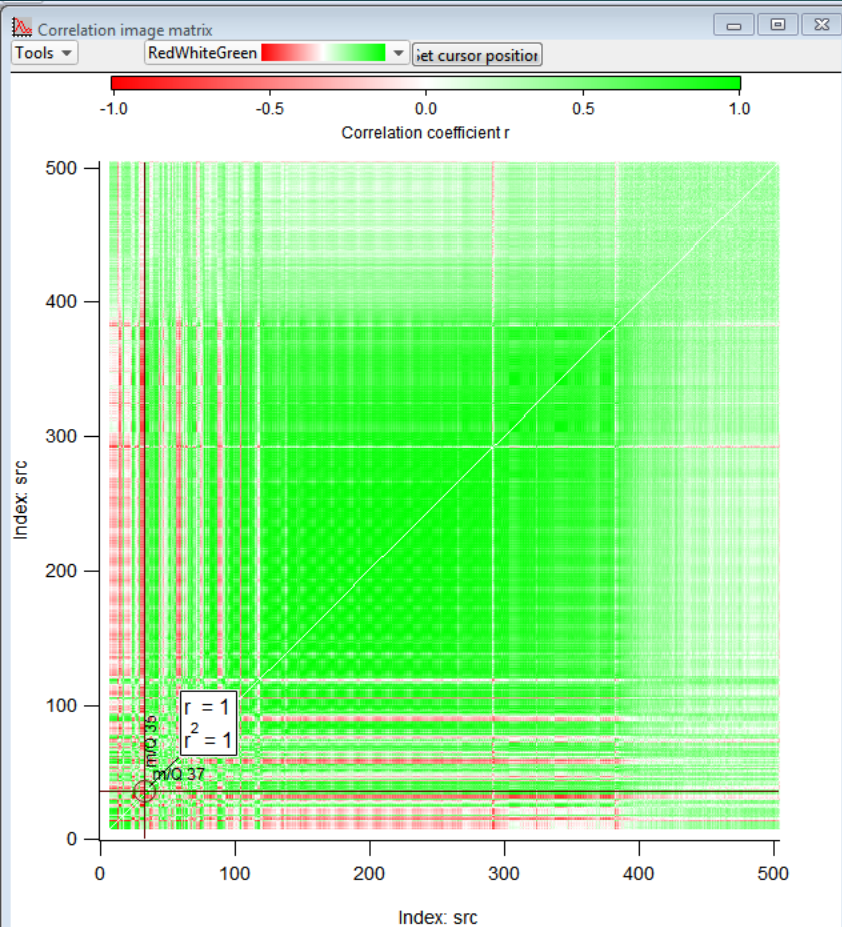
Demo: UMR data processing and display

10



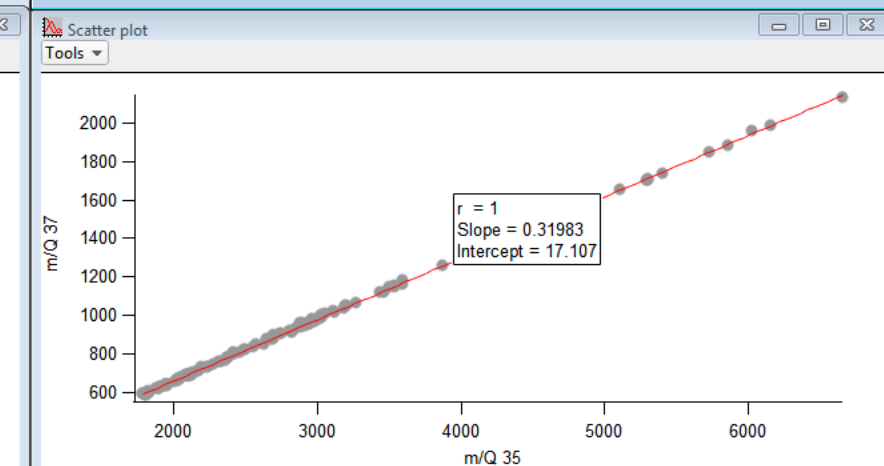
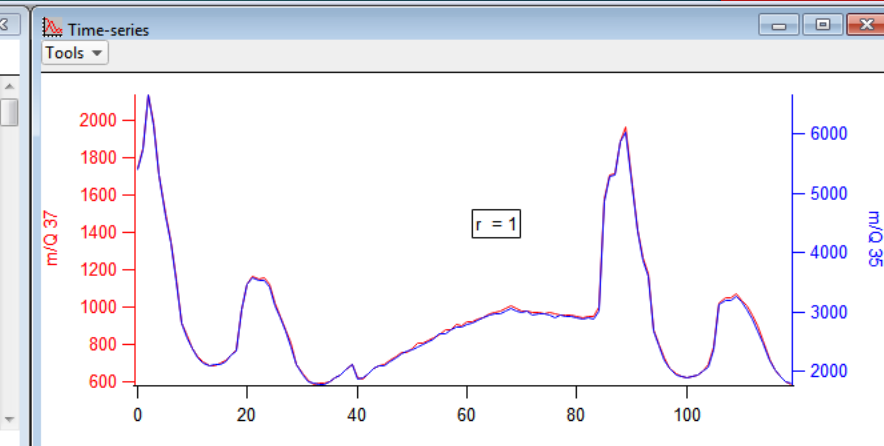
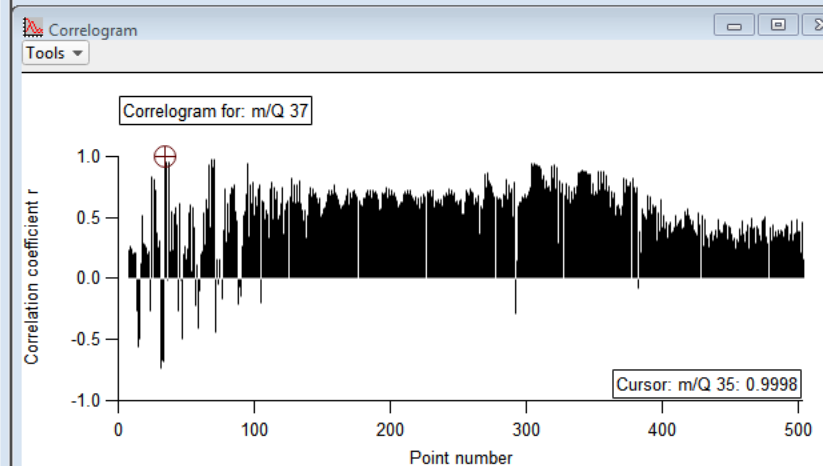
Demo: UMR analysis and export to PMF/SoFi

11



Best correlations

Peak 1	Peak 2	r
m/Q 35	m/Q 37	0.999801
m/Q 119	m/Q 120	0.998336
m/Q 82	m/Q 112	0.997902
m/Q 203	m/Q 217	0.997673
m/Q 201	m/Q 215	0.997525
m/Q 169	m/Q 183	0.99737
m/Q 153	m/Q 167	0.997302
m/Q 112	m/Q 139	0.997276
m/Q 305	m/Q 307	0.997141
m/Q 173	m/Q 187	0.996851
m/Q 185	m/Q 213	0.996833



MS Time-series

Stick MS PMF / SoFi export HR & batch

Get List

- all
- HDF_fileID_0
- HDF_fileID_1
- HDF_fileID_2

Create new todo-wave

Blacklist

Load Save

View table View selected todo

Data Browser

Current Data Folder: root:

Display

- ☒ Waves
- ☐ Variables
- ☐ Strings
- ☒ Info
- ☒ Plot

PMF_SoFi_export

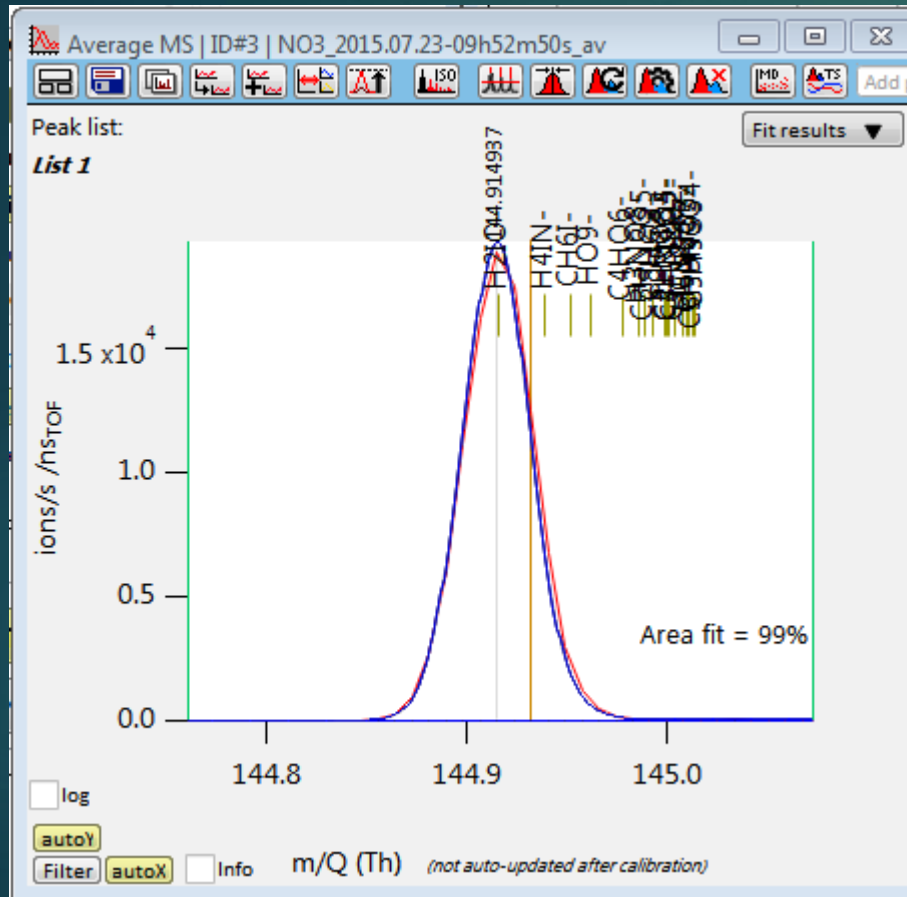
Up

Name

- PMF_SoFi_export
 - amus
 - MinErr
 - Mx_data

Demo: Raw spectra and HR peak assignment

12



Composition & isotopes

Find composition

m/Q: 144.914937 Search DBE

Range +/- 100 mTh Charge -1

Composition search list: Periodic table...

Name	mQ	Lo	Hi
C	12	0	20
H	1.00782503	0	50
O	15.99491462	0	10
I	126.90447300	0	1
N	14.00307400	0	20

Ctrl-click to assign peak: Toggle traces

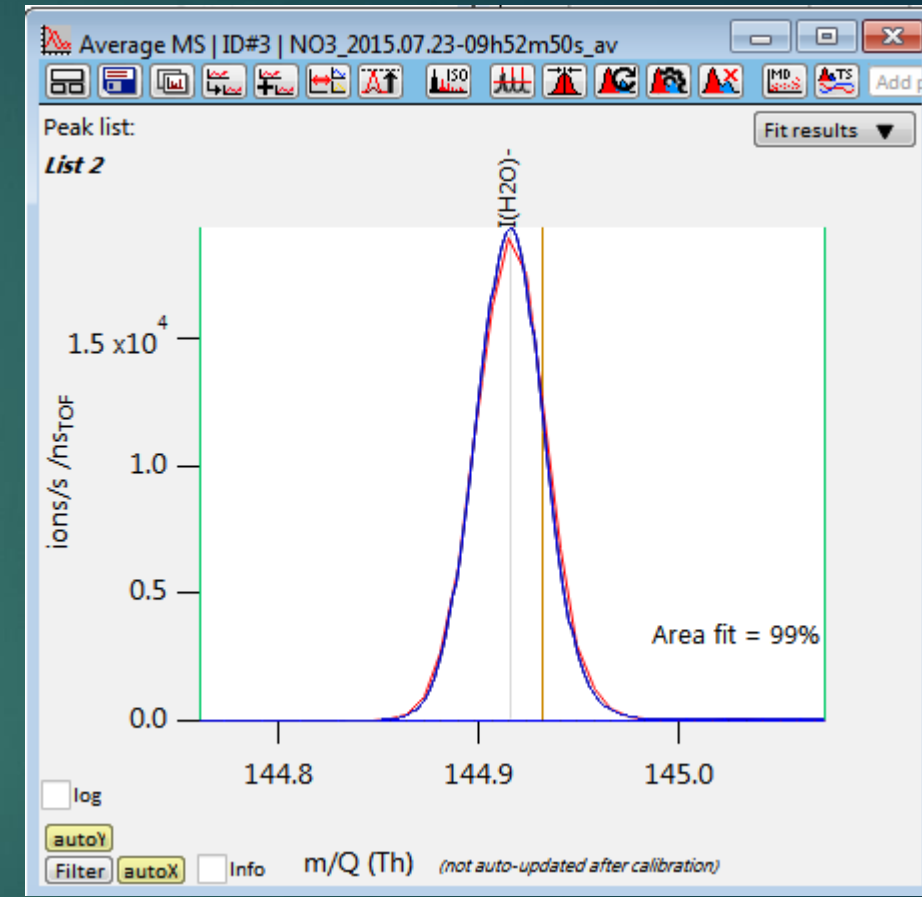
☒ Relative tol. ☐ Absolute Pop table

Sum formula	m/Q (Th)	ppm
H2IO-	144.915586	-4.48
H4IN-	144.939396	-169
CH6I-	144.951972	-255
HO9-	144.962605	-329
C4HO6-	144.977861	-434

Isotopes

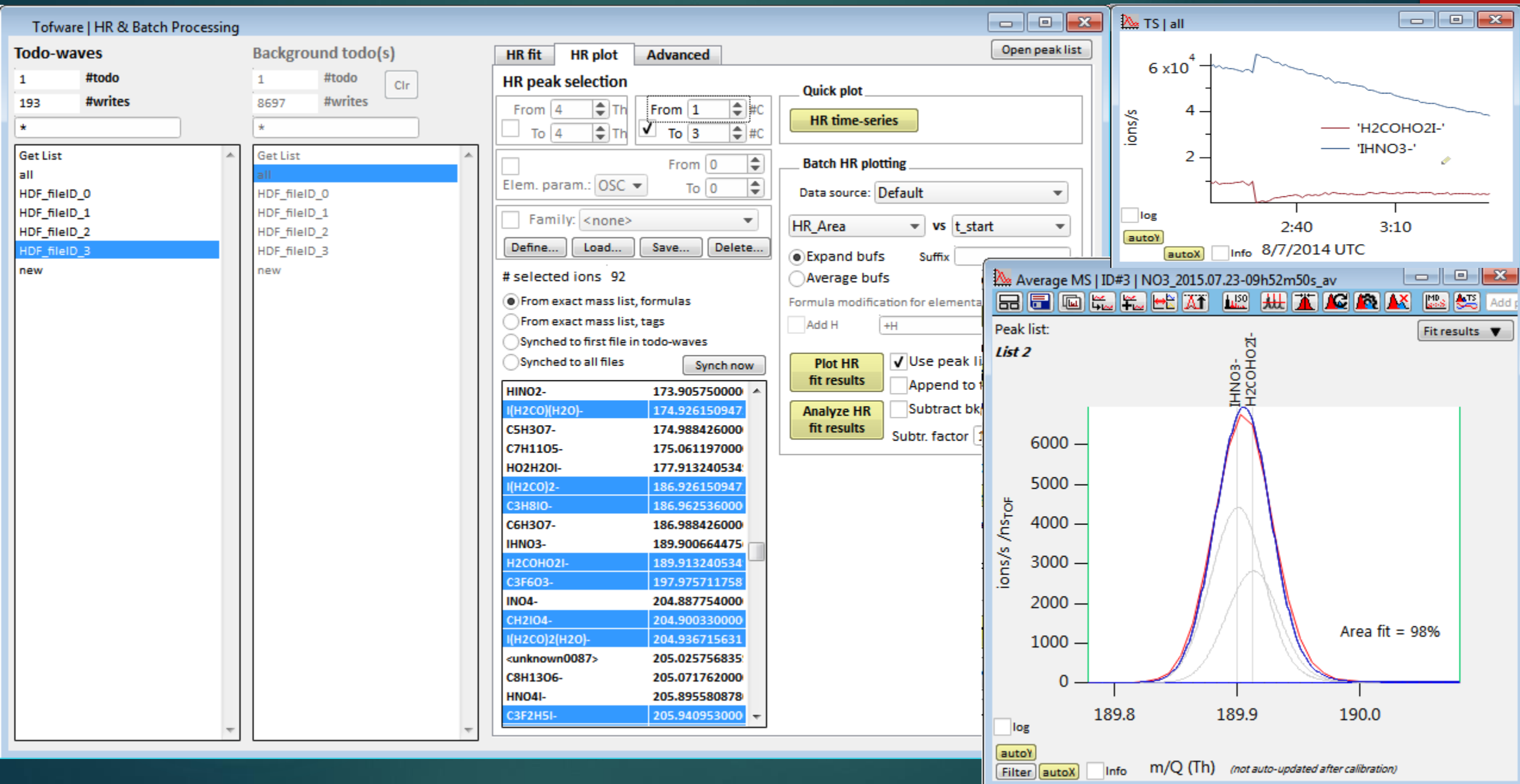
Formula: Click results table or type

Threshold 0.0001 Calculate



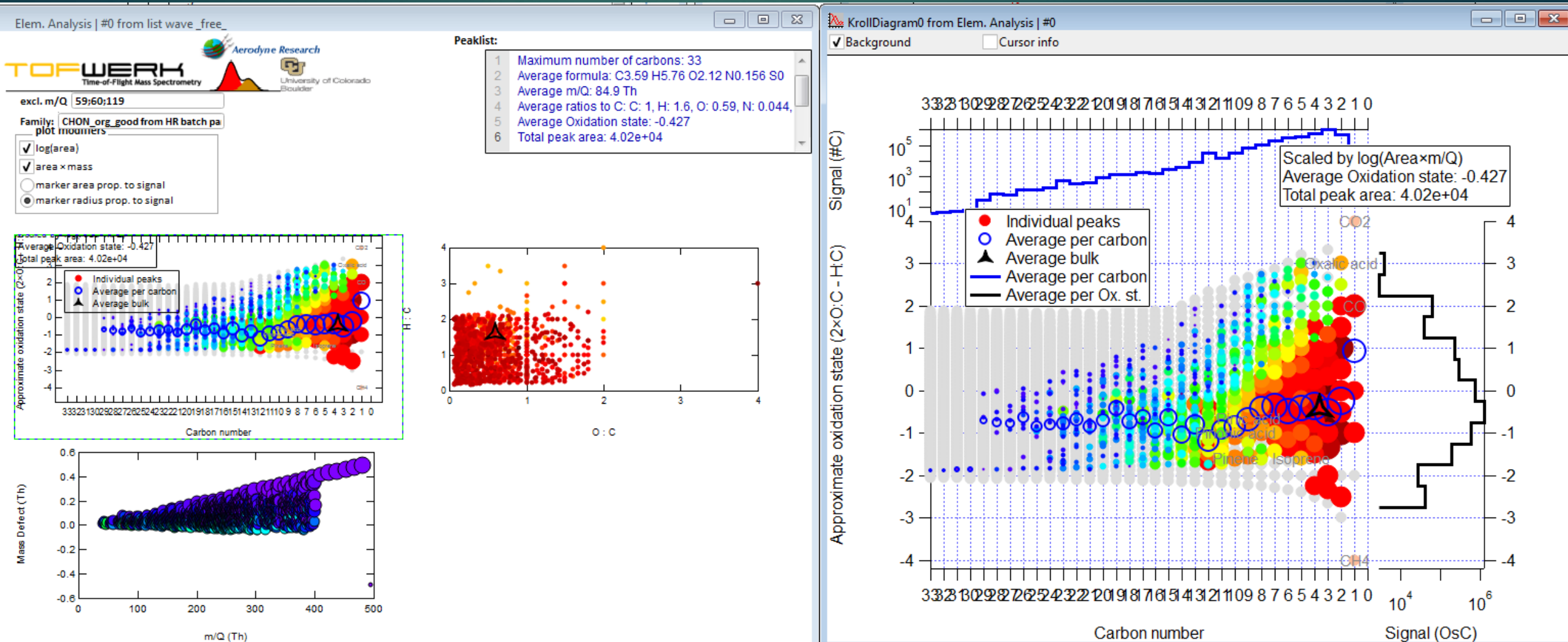
Demo: HR multi-peak fitting, batch processing

13



Demo: advanced analysis: chemical properties

14



Demo: further analysis: HR PMF export

15

HR fit

HR plot

Advanced

Open peak list

☒ Multithread ☒ Don't use last thread

Test sensitivity to mass calibration during HR fitting

Offset (+/- ppm)

Peak list setup table

☐ Sum todo(s) and graph

☐ Error bars (combined) on HR stick spectra

☐ Remove uncertain peaks on HR stick spectra when below $n \times \text{Sigma}$:

☒ Fast fitting (only whole files)

☐ Allow negative peak heights

Kroll Diagram settings

☐ Logarithmic marker sizes

☐ Scale marker sizes by mass

☐ Sum signals with same coordinates

PMF settings

f(Downweigh 1)

f(Downweigh 2)

t(avg.) (secs)

Thresh(Downweigh 1)

Thresh(Downweigh 2)

Make PMF input waves

☒ Take notes

☒ Save files

HR sticks | heat082505

Calc. correlation

R0		8/25/2011 08:14:30.329593				
		C2HO	C2H2O	C2H3O	CH2NO	
0	8/25/2011 08:14:30	375.827	842.611	1236.64	38.2692	
1	8/25/2011 08:14:45	327.253	1035.02	1248.58	160.974	
2	8/25/2011 08:15:00	343.527	934.917	1320.76	115.346	
3	8/25/2011 08:15:15	372.475	687.405	1542.27	111.741	
4	8/25/2011 08:15:30	417.231	927.546	1974.99	208.423	
5	8/25/2011 08:15:45	444.628	894.888	2445.84	176.796	
6	8/25/2011 08:16:00	562.072	953.858	3152.04	220.946	
7	8/25/2011 08:16:15	664.497	865.544	4068.81	218.628	
8	8/25/2011 08:16:30	847.343	735.202	4808.78	301.389	
9	8/25/2011 08:16:45	780.123	759.457	4685.7	266.19	
10	8/25/2011 08:17:00	812.331	668.143	4500.12	355.385	
11	8/25/2011 08:17:15	792.448	873.902	4994.2	342.029	
12	8/25/2011 08:17:30	884.159	865.944	5189.85	393.859	
13	8/25/2011 08:17:46	926.441	803.942	4949.77	432.973	
14	8/25/2011 08:18:01	808.6	637.234	4648.47	397.588	
15	8/25/2011 08:18:16	824.24	540.238	3777.97	318.954	
16	8/25/2011 08:18:31	795.906	356.28	3726.51	438.58	
17	8/25/2011 08:18:46	739.931	300.972	3669.93	311.474	
18	8/25/2011 08:19:01	703.69	248.62	3898.64	380.61	
19	8/25/2011 08:19:16	688.22	0	3667.8	419.305	
20	8/25/2011 08:19:31	758.332	29.2523	3722.67	441.314	
21	8/25/2011 08:19:46	776.195	0	4034.06	512.873	
22	8/25/2011 08:20:01	700.454	13.8047	3954.74	540.611	
23	8/25/2011 08:20:16	747.414	0	4099.83	495.472	
24	8/25/2011 08:20:31	749.42	0.963949	4130.9	519.976	
25	8/25/2011 08:20:46	731.743	0	4526.36	549.177	
26	8/25/2011 08:21:01	724.398	0	4427.65	443.539	
27	8/25/2011 08:21:16	821.127	0	4528.02	645.589	

- ▶ Many more features available, see manual, ask Harald
- ▶ Continued development, new features can be requested