

Squirrel, Pika Tips

Did you know you can...?

Versions * Baselines* ePToF * HR ions* HR families * IE for ET

Squirrel 1.21C, Pika 1.61C

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AMS Users Meeting, St. Louis, MO

September 10, 2018

Use Igor 6,7 or 8?

No plans in the near future (6 months) to require users to use newer Igor versions.

Igor 7 is a major upgrade and is recommended.

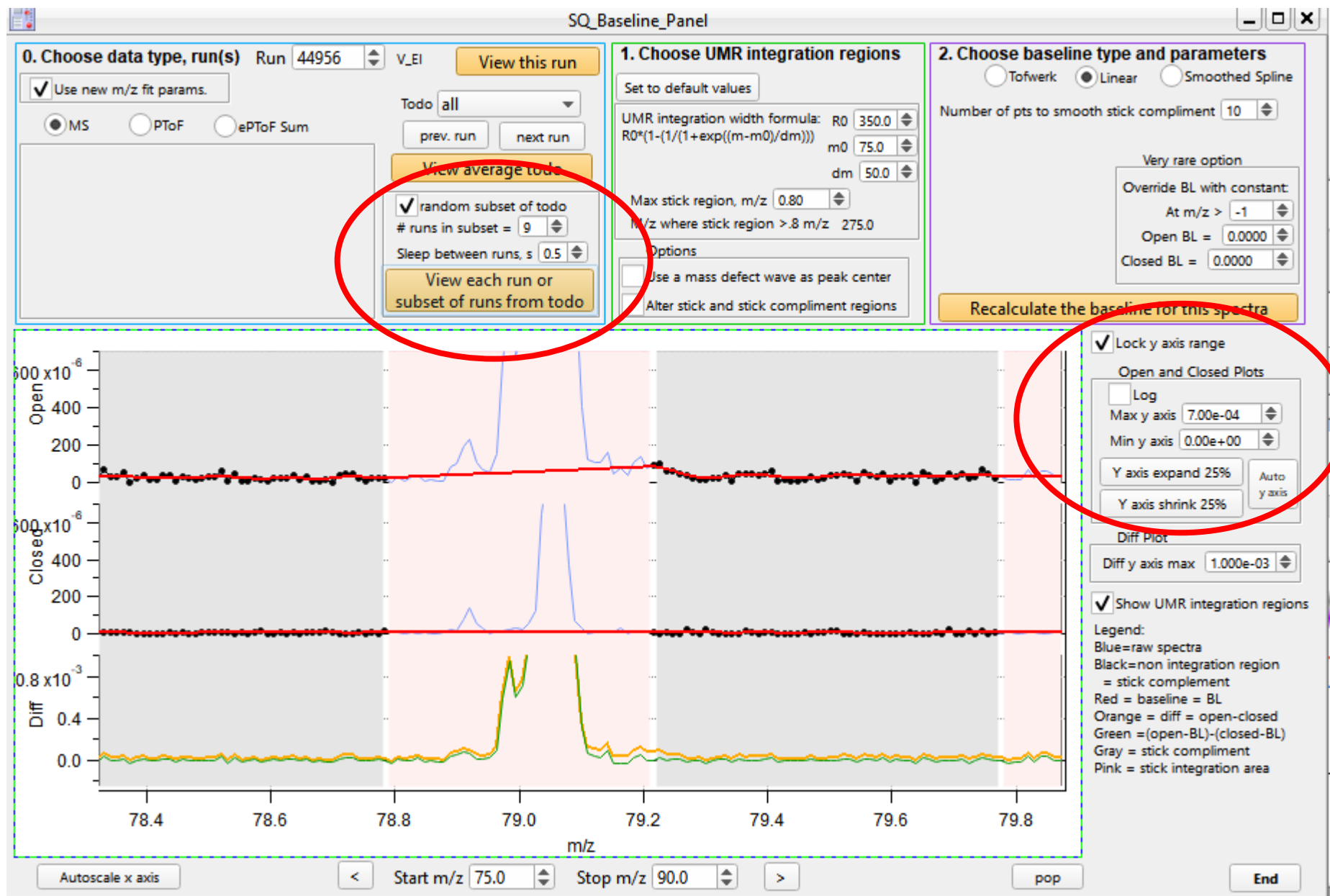
Can easily update between Squirrel, Pika versions?

Use the updater UpdateSQPKVersion.ipf – easy and fast

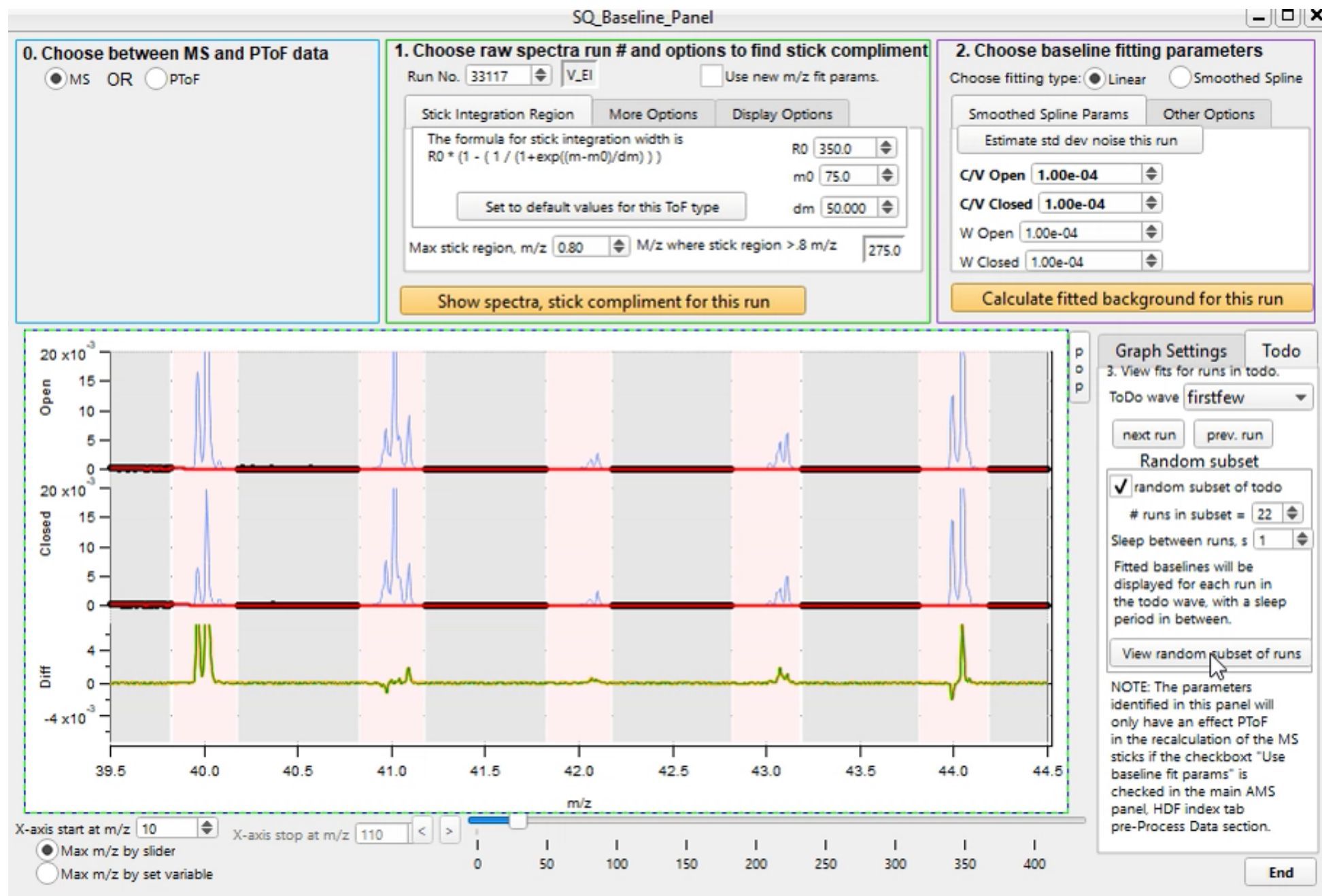
<http://cires1.colorado.edu/jimenez-group/ToFAMSResources/ToFSoftware/>

Baseline random run viewing

Most useful for
diagnosing the
consistency of baselines,
UMR integration regions,
etc



Baseline random run viewing example

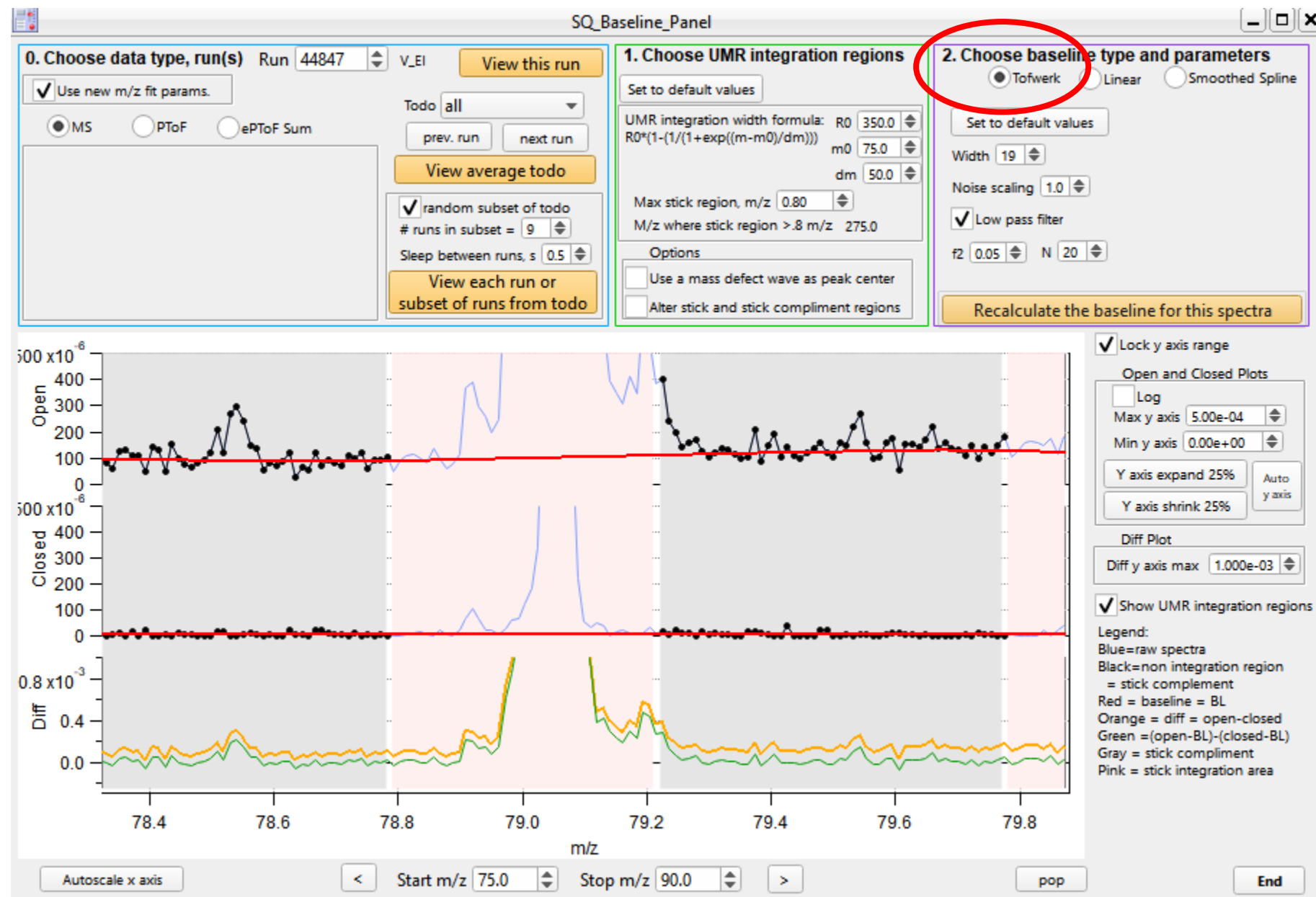


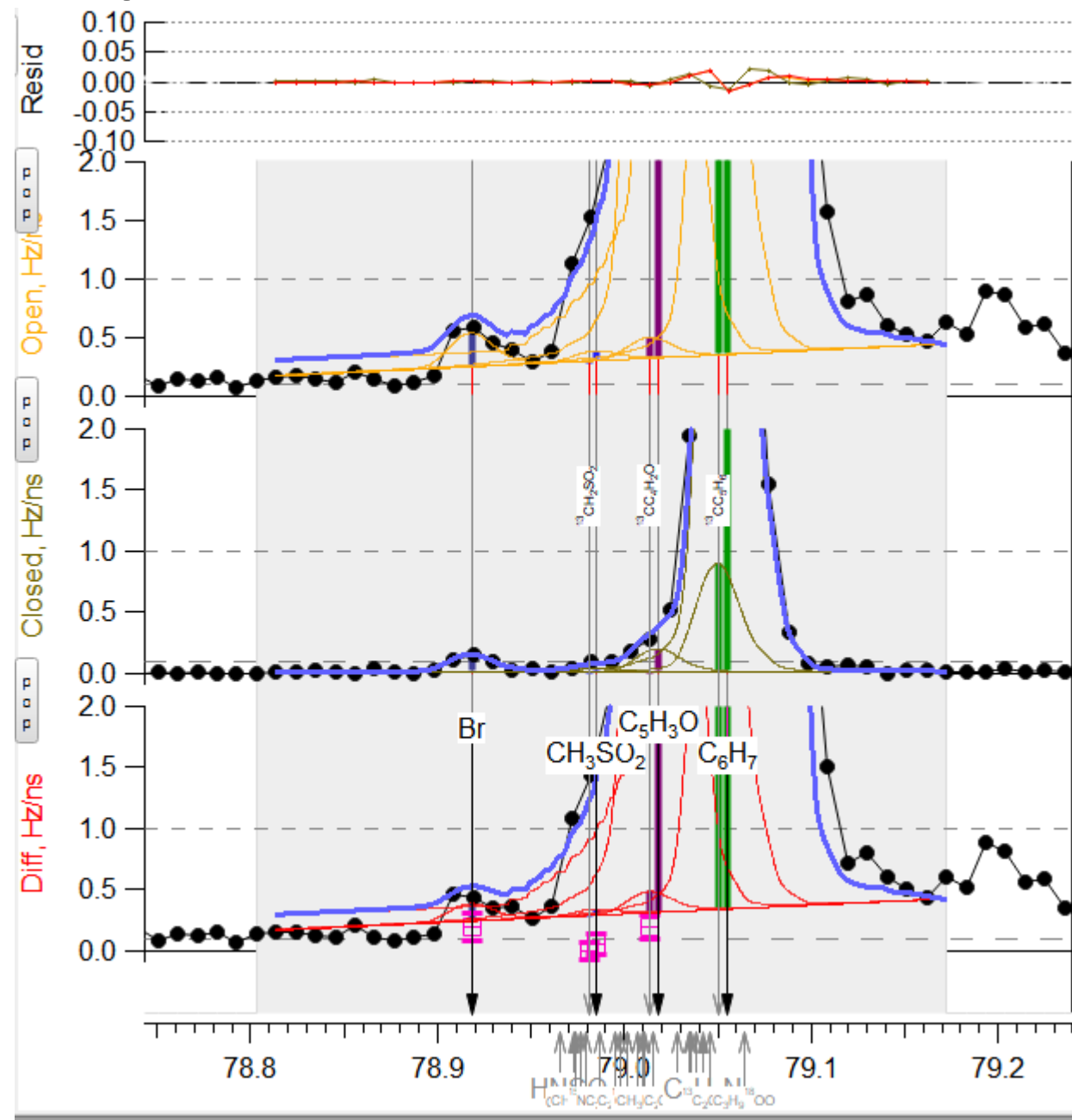
New baseline algorithm

Most useful for very small signals and for HR analysis

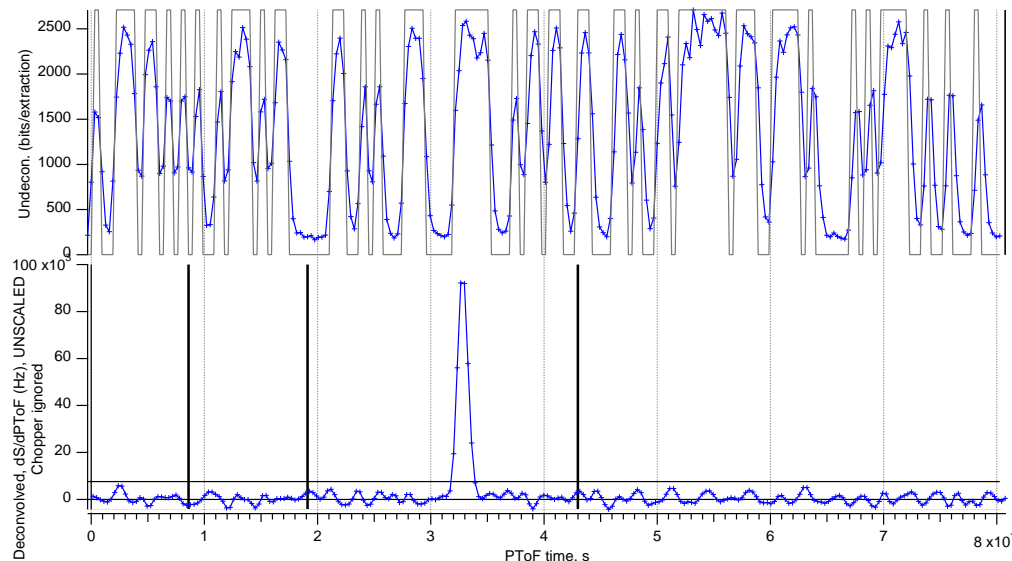
Independent of UMR integration regions

Tofwerk proprietary (code details are hidden ☹)





ePToF can generate 'regular' MS-like data

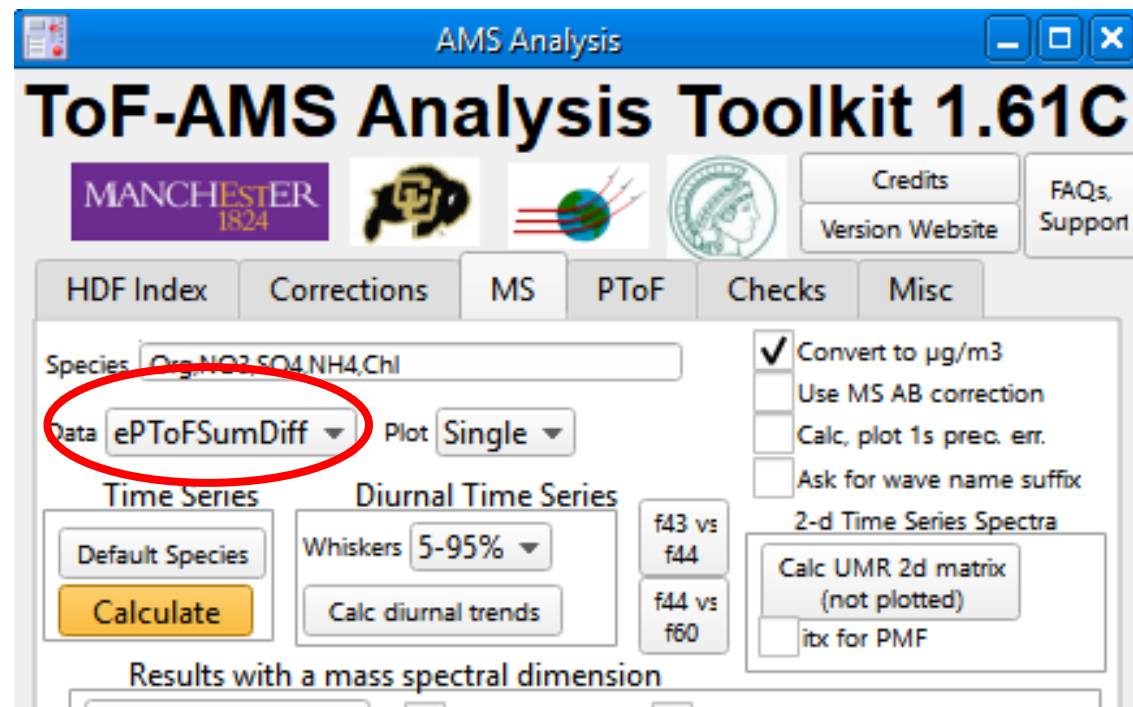
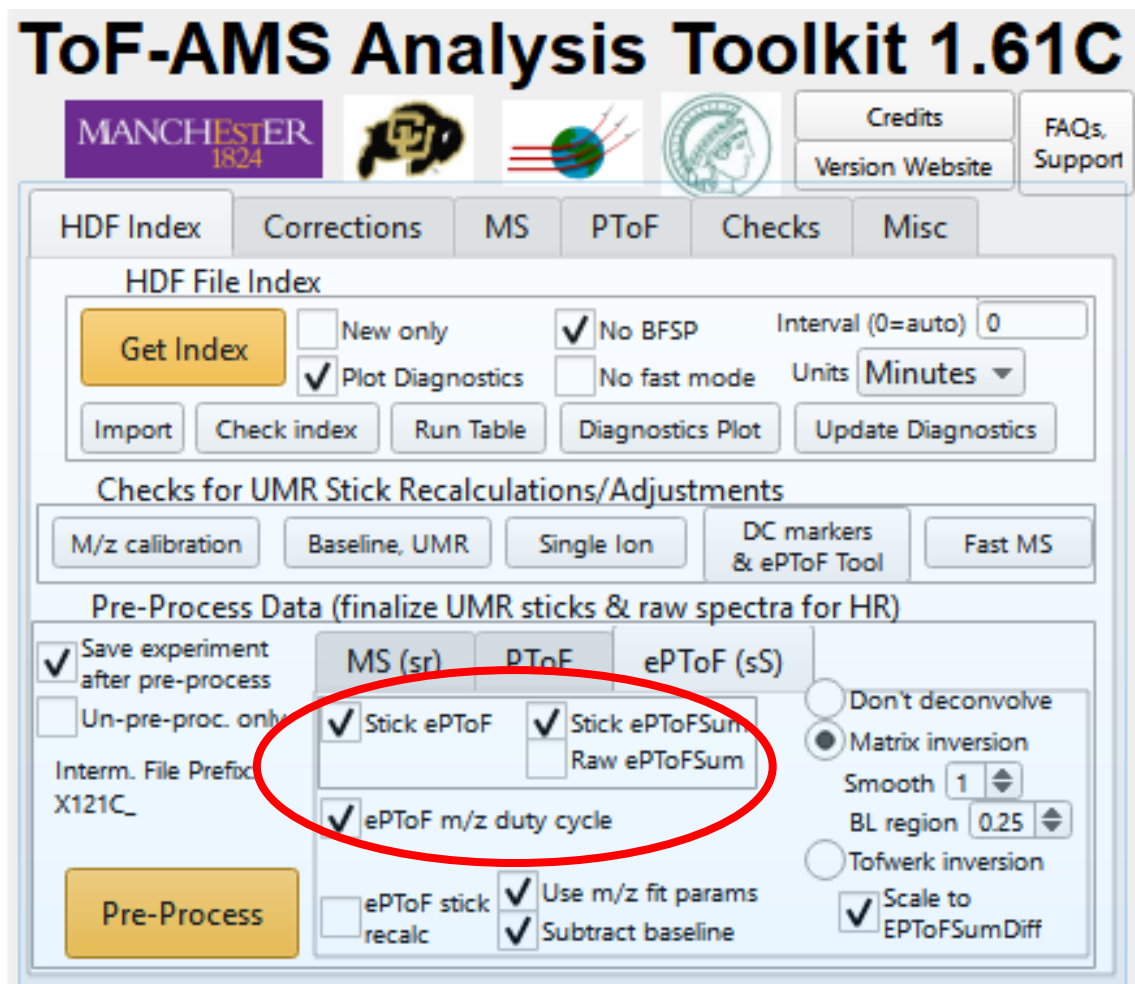


Independent of deconvolution, we can collapse the PToF dimension

$$\begin{aligned} \text{ePToFSum} &\sim \frac{1}{2} * \text{open} + \frac{1}{2} * \text{closed} \\ &= \frac{1}{2} * (\text{diff} + \text{closed}) + \frac{1}{2} * \text{closed} \\ &= \frac{1}{2} * \text{diff} + \text{closed} \end{aligned}$$

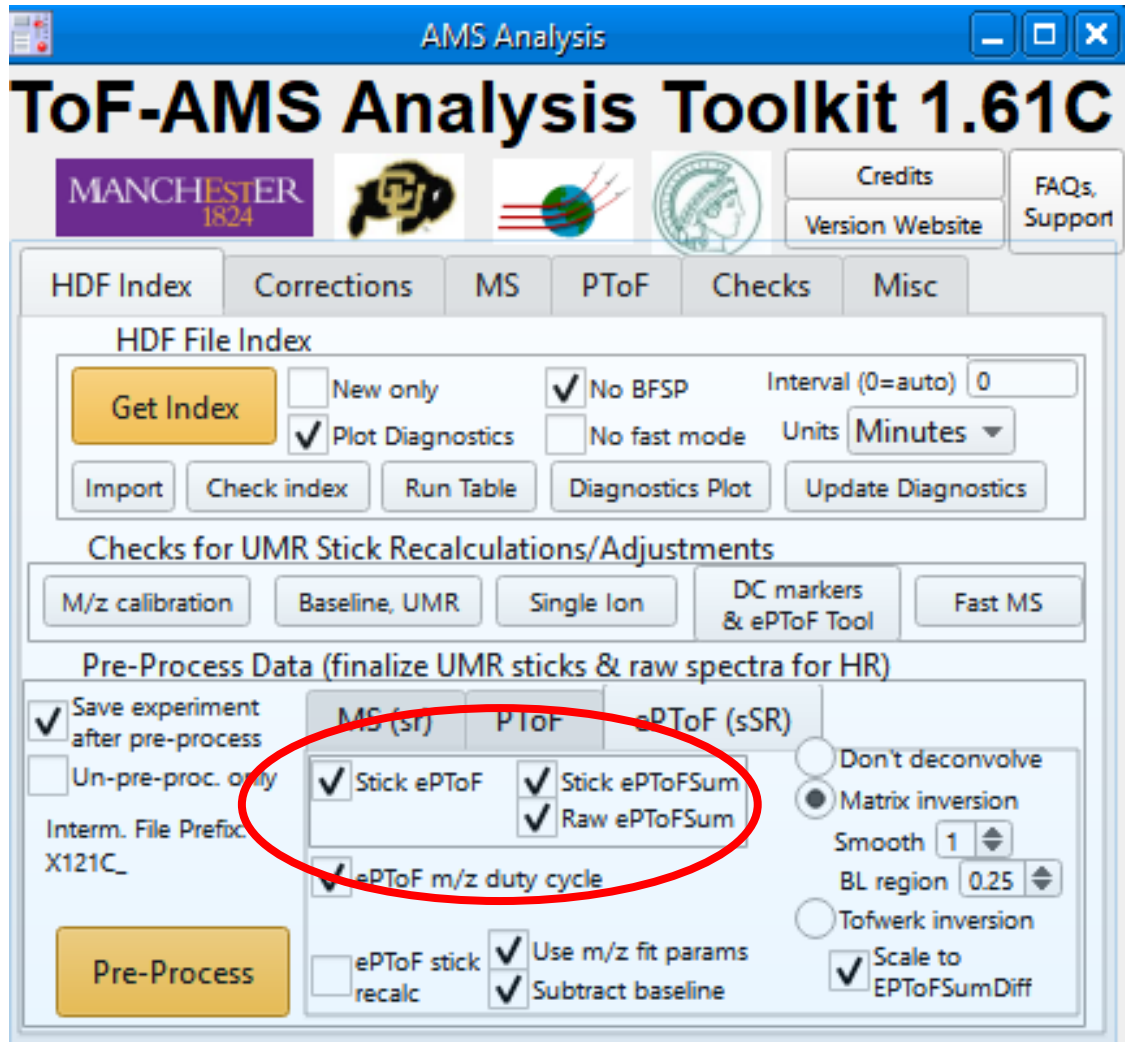
$$\begin{aligned} \text{epToFSumDiff} &= 2 * (\frac{1}{2} * \text{diff} + \text{closed} - \text{closed}) \\ &\sim \text{MS Diff, } (\sim 5\%) \text{ not exact because of slowly vaporizing ions} \end{aligned}$$

ePToF can generate 'regular' MS-like stick data



See Williams talk earlier this meeting for comparison of ePToFSumDiff with Diff

ePToF can generate 'regular' MS-like raw & HR data



Unintegrated, 'raw' PToF spectra

- saved in *_p.h5 files
- not saved by default.
- files are large ~ 20x larger, per run, than *_m.h5 files

We can collapse the spectra, to obtain
'raw' ePToFSum and 'raw' ePToFSumDiff

- one can do HR fitting etc, on this raw spectra – it works!

Can we do HR ePToF (not collapsing in the PToF dimension)?

Painful!

We need to perform HR fits on undeconvolved (low signal issues, time consuming)

THEN deconvolve HR matrices.

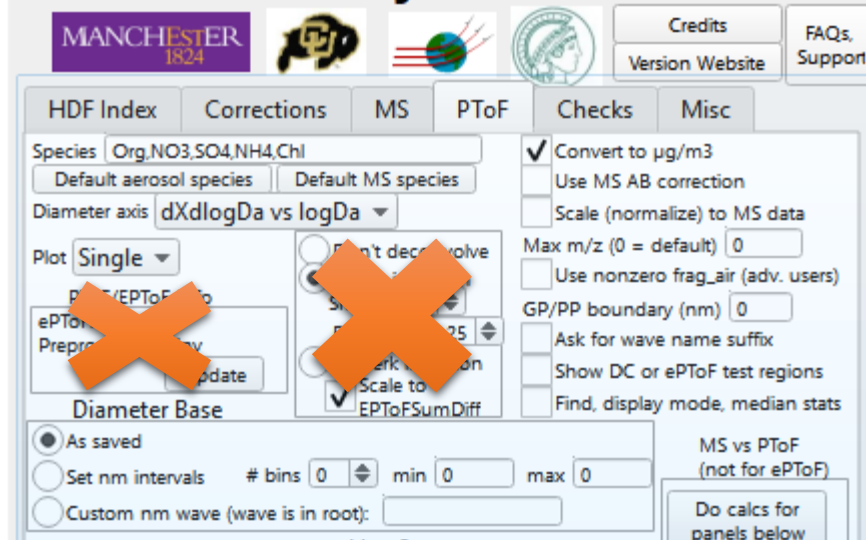
Will not be coded in the foreseeable future

ePToF Deconvolution

Next major release, Squirrel 1.62

- will have all the Tofwerk deconvolution options hidden
- mostly due to problems of getting NH₄ ions at m/z 15,16,17
- matrix inversion works well, is linear

ToF-AMS Analysis Toolkit 1.61C



MANCHESTER 1824

Credits Version Website FAQs, Support

HDF Index Corrections MS PToF Checks Misc

Species Org.NO₃,SO₄,NH₄,Cl

Default aerosol species Default MS species

Diameter axis dXdlogDa vs logDa

Plot Single

Don't deconvolve

Simple matrix inversion

Scale to EPToFSumDiff

Convert to µg/m³

Use MS AB correction

Scale (normalize) to MS data

Max m/z (0 = default) 0

Use nonzero frag_air (adv. users)

GP/PP boundary (nm) 0

Ask for wave name suffix

Show DC or ePToF test regions

Find, display mode, median stats

MS vs PToF (not for ePToF)

Do calcs for panels below

PToF and ePToF Preview and Parameter Setting Tool

Important! Values indicated in this panel will be used for preprocessing PToF & ePToF data. If data is already preprocessed data will be overwritten. For ePToF data you can choose to deconvolve each run at the preprocess stage by selecting a deconvolution method. This is necessary if you will be applying time-dependent correction waves later, e.g., for CE or CO₂ frags. Alternatively, you can choose 'Don't deconvolve' at the preprocess stage. Then, when you generate a PToF product for a todo, the runs will be averaged, then deconvolved in a method you can choose then. This results in better signal to noise. You can switch between approaches by changing the selection in Step 1 and pre-processing again.

Step 0. Select a run or todo.

☒ Run number 103147 ePToF

☐ Todo allePToFGrp00

Info for current run or todo

ePToF oversampling (nan for non ePToF) 4

PToF t0 (s) -5.5451e-05 Min m/z 4 # of PToF bins 508

PToF t step (s) 2.7680e-05 Max m/z 211 PToF duration (s) 1.606

DC marker settings for single slit PToF

Step 1. Select DC marker parameters for PToF

PToF DC marker calculations can be redone through the Corrections section.

☒ Use PToF bin # as units - if unchecked, µs units are used

Region 1 start 5 Region 2 start -15 ☐ Use Region 1 only for all m/zs not in Region 2 only.

Region 1 stop 15 Region 2 stop -5

Region 1 only m/zs

Region 2 only m/zs 14,15,16,17,18,20,28,29,32,34,40,44,

Step 1. Select ePToF deconvolution

☐ Don't deconvolve

☒ Simple matrix inversion

Low pass filter then smooth by this factor (<1 mean no filtering smoothing, applied to all m/z) 1

Baseline region (fraction of ending bins which should be noise) 0.25

☐ Tofwerk deconvolution (different smoothings for different m/zs)

☒ ePToFSumDiff Scaling (scaling will happen during preprocess & is not shown here)

Details of Tofwerk deconvolution of DAQ sticks, one run or todo

New HR ion convention, HR ions 'library'

The order of atoms within HR fragment names:

C H N S F Cl Br I O X

EXCEPT for 'traditional' ammonium ions, i.e. NH, NH₂, NH₃, NH₄
isotopic 'children' come before the 'parent', so j13CC2H7, NOT C2j13CH7

i.e. CH₃SO₂, not CH₃O₂S

Mostly intuitive, except for salts, i.e. ClK
Won't overwrite existing HR ion names

Library ExactMassWaves121C released

Same default list of HR ions fit as before except ~ 6 isotopes now included.
5979 in list (old list had ~ 3000)
Mass waves now double precision

ToF-AMS
software downloads

Upgrade SQUIRREL PIKA APES SPARROW IE Calibration

- DAQ web site
- Squirrel and PIKA Information Web Site
- AMS Analysis Web Site
- All Igor 6.x users are must upgrade to at least Igor 6.37. There is a known issue with MacOS High Sierra and Igor notebooks for Igor versions < 7.07. For Igor 6.37 and High Sierra users, one must kill all notebooks, which include the readme files, before saving an experiment.
- All the latest code as of June, 8 2018 has been tested on Igor 7.07 and Igor 8.0 and is compatible.
- All Igor 7.x users are strongly encouraged to upgrade to at least Igor 7.07

Upgrade Existing SQUIRREL, PIKA Experiments

Version	Date	Release Notes	File Type	File Type
v1.02	5-Sept-2018	Release Notes v1.02	1.02 Igor Update ipfs (single ipf that compiles independently)	Zipped Procedures, ReadMe files (zipped ipf & readme file)

Igor Data Analysis for HDF Files (SQUIRREL)

Version	Date	Release Notes	File Type
v1.21C	5-Sept-2018	Release Notes v1.81	1.81C Igor Template (experiment file for new analyses)
v1.81C	5-Sept-2018	Release Notes v1.81	1.81C Procedures, ReadMe files (zipped files for upgrading existing experiments)

Igor High Resolution Data Analysis for ToF HDFs (PIKA)

Version	Date	Release Notes	Installer
v1.21C (Pika 1.21C with 1.81C Squirrel)	5-Sept-2018	Release Notes v1.21	Pika 1.21C template experiment (for new analyses)
v1.21C (Pika 1.21C with 1.81C Squirrel)	5-Sept-2018	Release Notes v1.21	Pika 1.21C AND Squirrel 1.81C Procedures, ReadMe files (procedure files for upgrading)
v1.21C (Pika 1.21C with 1.81C Squirrel)	5-Sept-2018	Release Notes v1.21C	All HR ions, v1.21C zipped Igor files waves to reside in HR data folder (HR ion all waves for upgrading)

Pika families can be easily generated

The main idea is that instead of explicitly indicating every HR ion in a list, you can generate a large set of related ions more automatically.

HR Ion Mass Calculator

HR Ion Mass & Isotopic Calculator and HR Ion Query Tool v1.21C

HR Mass, Isotope Calculator Verify Values in 'all' Waves Query Chemical Formulas 2 Sets of HR Ion Waves Using familyWave_*

HR family table (editable) HR batch table (editable) All HR masses table View/update current HR family wave table (all families defined by a familyWave_*)

Select the HR family defined by root:HR:familyWave_ **APAH**

Create/overwrite a new family from a list of HR chemical formulas

List of base HR ions in family

Include other related HR ions in this family: ☒ Isotopes ☒ [M-H] ☒ [M-H2]

☒ Include this family in HROrg species?

Make a new or overwrite a family defined by the HR list above and named Optional list of RGB (RedGreenBlue) color for this family

Verify that familyWave_* ions are NOT in other families (only needed if they were modified 'by hand')

One click selection of fitting or not fitting all HR ions within a family

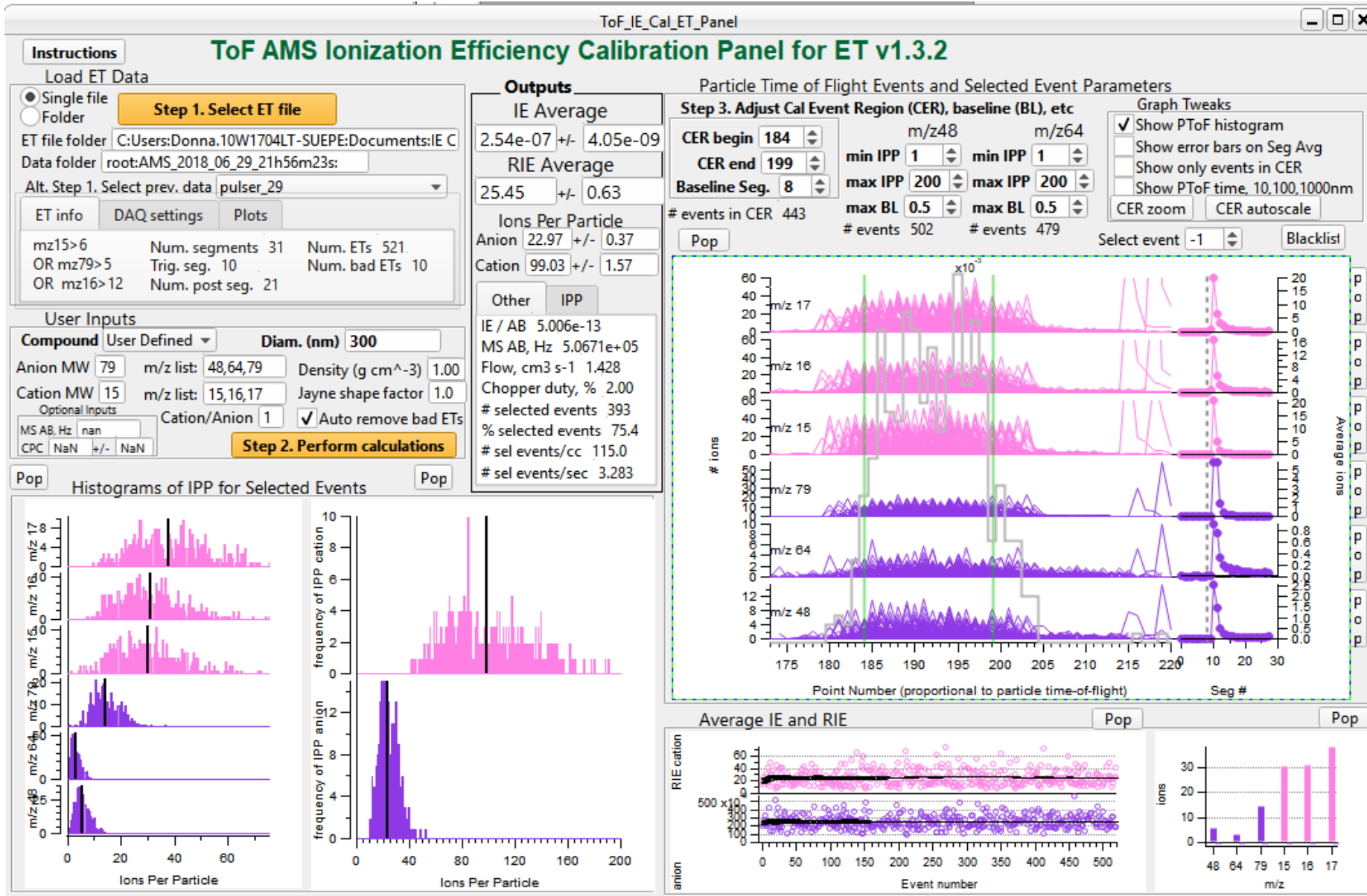
familyWave_APAH
C16H10N
j13CC15H10N
C16H11N
j13C2C14H10N
j13CC15H11N
j13C2C14H11N
C18H12N
j13CC17H12N
C18H13N
j13C2C16H12N
j13CC17H13N
j13C2C16H13N
C20H12N
j13CC19H12N
C20H13N
j13C2C18H12N
j13CC19H13N
j13C2C18H13N
C21H12N
j13CC20H12N
C21H13N
j13C2C19H12N
j13CC20H13N
j13C2C19H13N

Pika families can be easily generated

HR_FamilyTable

R18			
Point	HR_familyName	HR_familyListDefinition	
0	Cx	default	
1	HRBatchTable		
2	R5	familyCx;familyCH;familyCHO1;familyCHOgt1;familyCHN;familyCHO1N;familyCHOgt1N;familyCS;familyAPAH;	
3	Point	HR_specFrag_list	HR_specFamilyBase
4	1	HR_frag_Pwater	familyHO
5	2	HR_frag_ammonium	familyNH
6	3	HR_frag_nitrate	familyNO
7	4	HR_frag_sulphate	familySO
8	5	HR_frag_organic	familyCx;familyCH;familyCHO1;familyCHOgt1;familyCHN;familyCHO1N;familyCHOgt1N;familyCS;familyAPAH;
9	6	HR_frag_chloride	familyCl
10	7	HR_frag_organic[44]	
11	NO	default	
12	SO	default	
13	Air	default	
14	Tungsten	j182Wplus2;j184Wplus2;j186Wplus2;W;WO	
15	Other	default	
16	CSi	default	
17	APAH	familyWave_APAH	
18			

IE for ET cal code allows for any cal standard



MSA was used in this file to example.

Users can select the compound as 'User Defined' and list their own anions and cation m/z lists (which don't have to be in increasing m/z order).

The first 2 m/z ions in the anion list will be available in step 3.

IE for ET cal code allows for any cal standard

Instructions **ToF AMS Ionization E**

Load ET Data

☒ Single file ☐ Folder **Step 1. Select ET file**

ET file folder: C:\Users\Donna.10W1704LT-SUEPE\Documents\IE C

Data folder: root:AMS_2018_06_29_21h56m23s:

Alt. Step 1. Select prev. data: pulser_29

ET info DAQ settings Plots

ROI Details Flowrate, AB graph Segment Average Mass Spec

User Inputs

Compound: User Defined Diam. (nm): 300

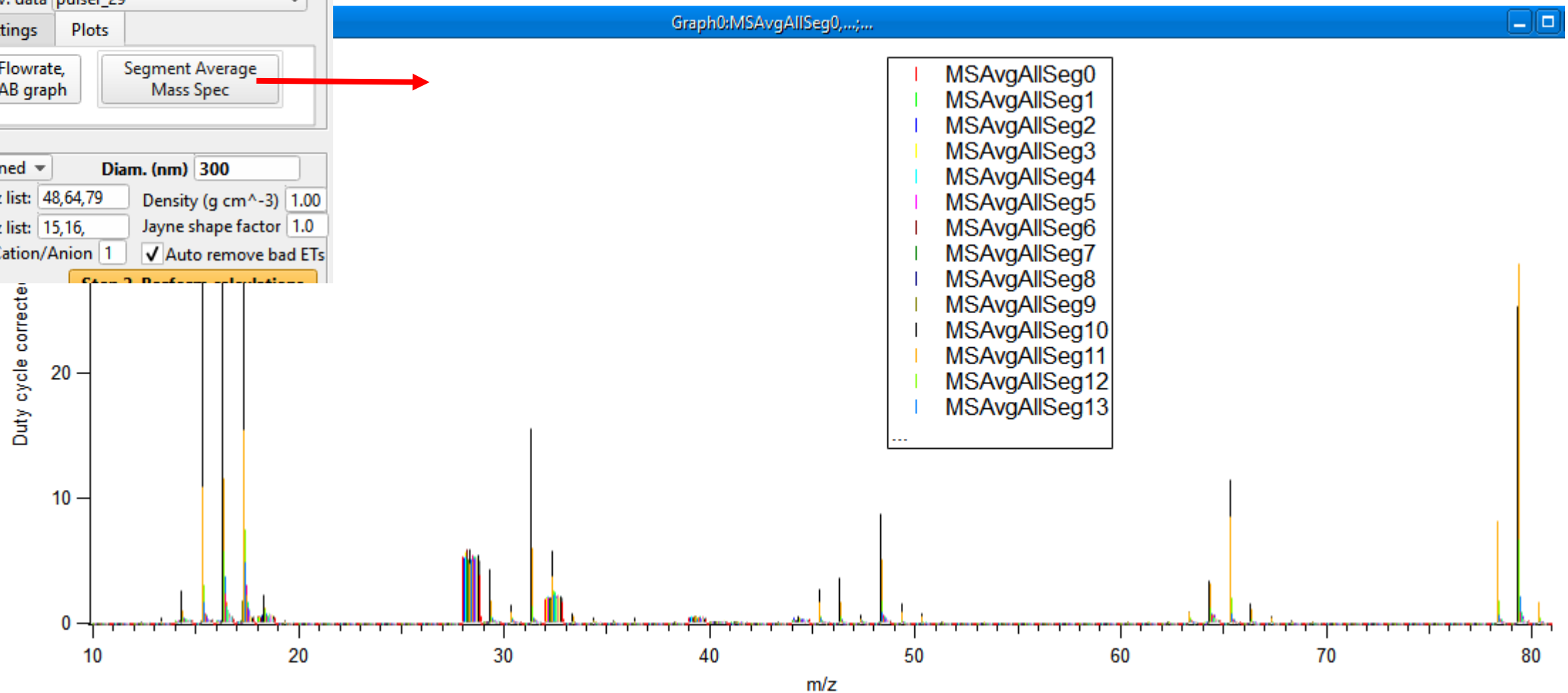
Anion MW: 79 m/z list: 48,64,79 Density (g cm⁻³): 1.00

Cation MW: 15 m/z list: 15,16 Jayne shape factor: 1.0

Optional Inputs

MS AB, Hz: nan Cation/Anion: 1 ☒ Auto remove bad ETs

Neat new graph showing the average mass spectra for each ET segment!
Mass spectra are slightly offset from each other in the m/z dimension



Thanks to all the users for feedback and suggestions!