Squirrel, Pika Tips

Did you know you can…?

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

Squirrel 1.21C, Pika 1.61C

Donna Sueper

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 user newer Igor versions.

Igor 7 is a major upgrade and is recommended.

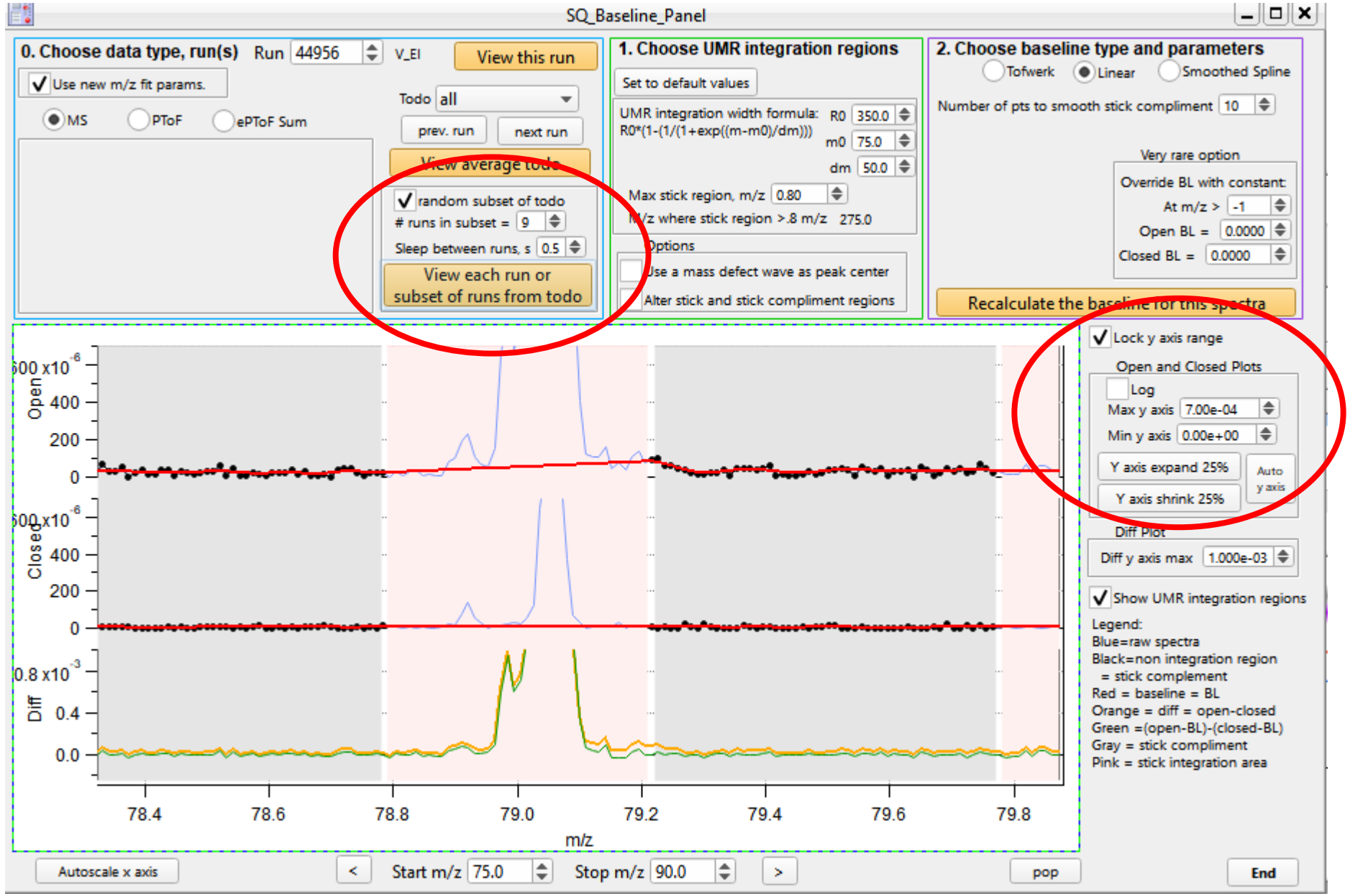
Can easily update between Squirrel, Pika versions?

Use the updater UpdateSQPKVersion.ipf – easy and fast

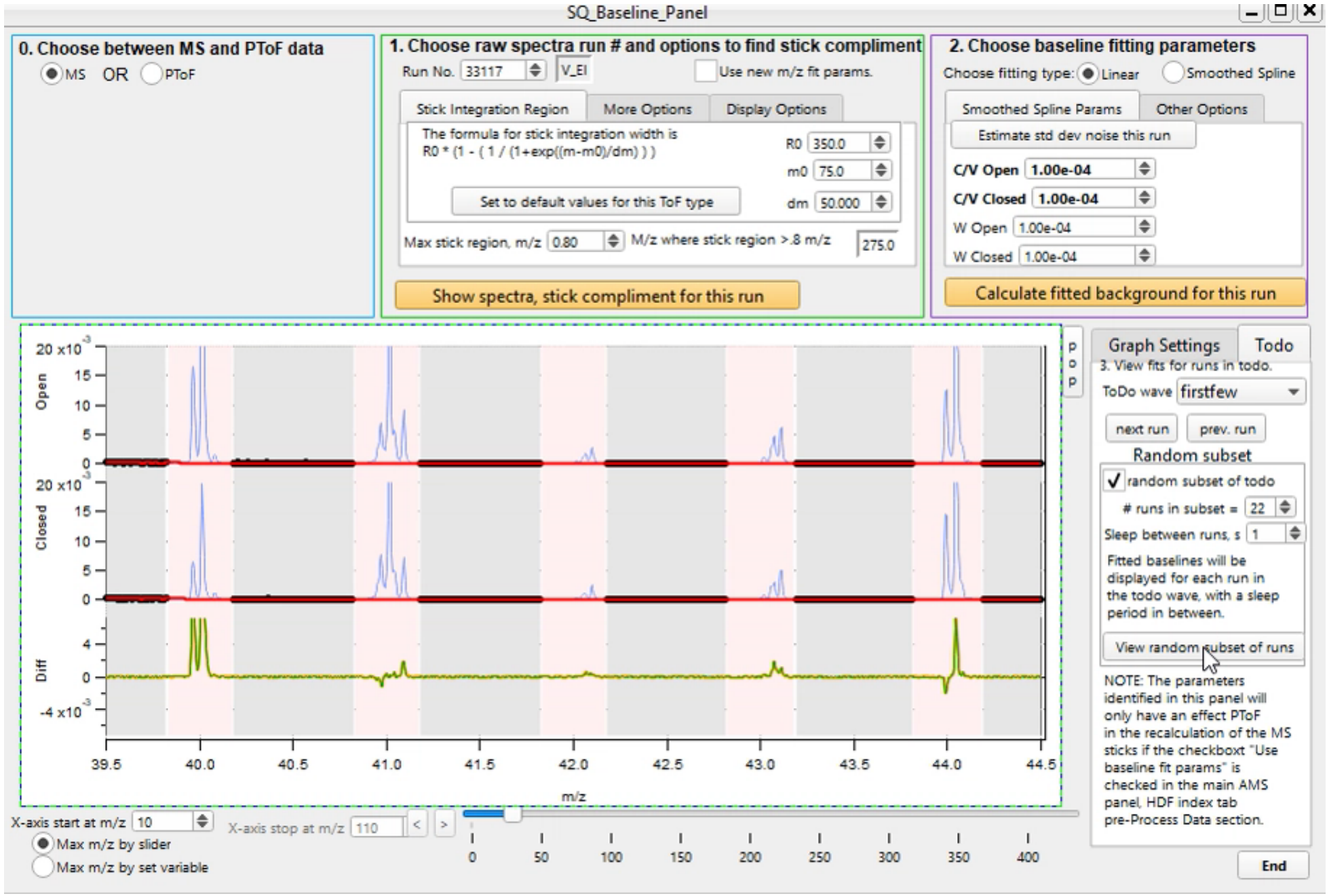
http://cires1.colorado.edu/jimenez-group/ToFAMSResources/ToFSoftware/

Baseline random run viewing

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



Baseline random run viewing example



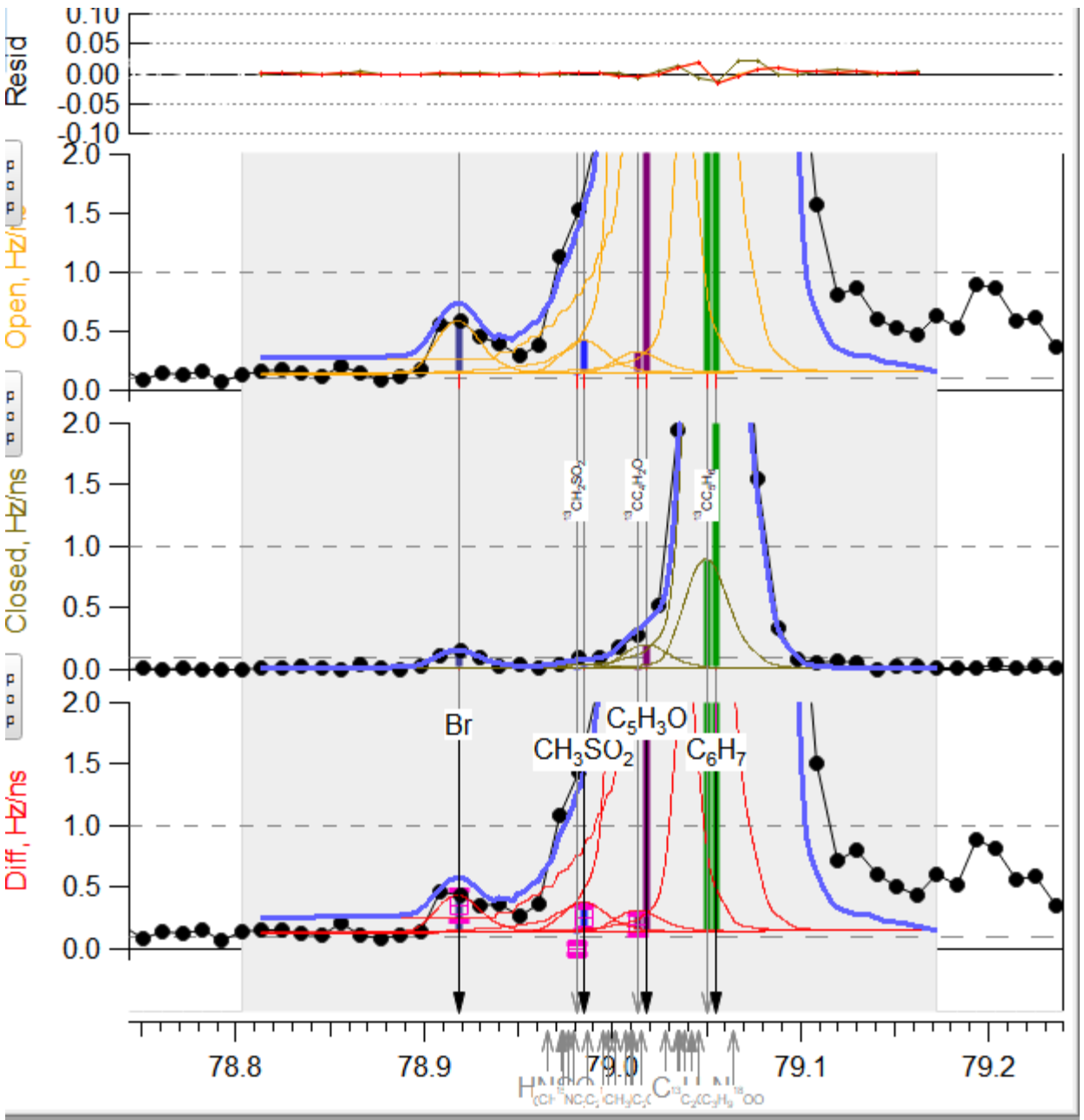
New baseline algorithm

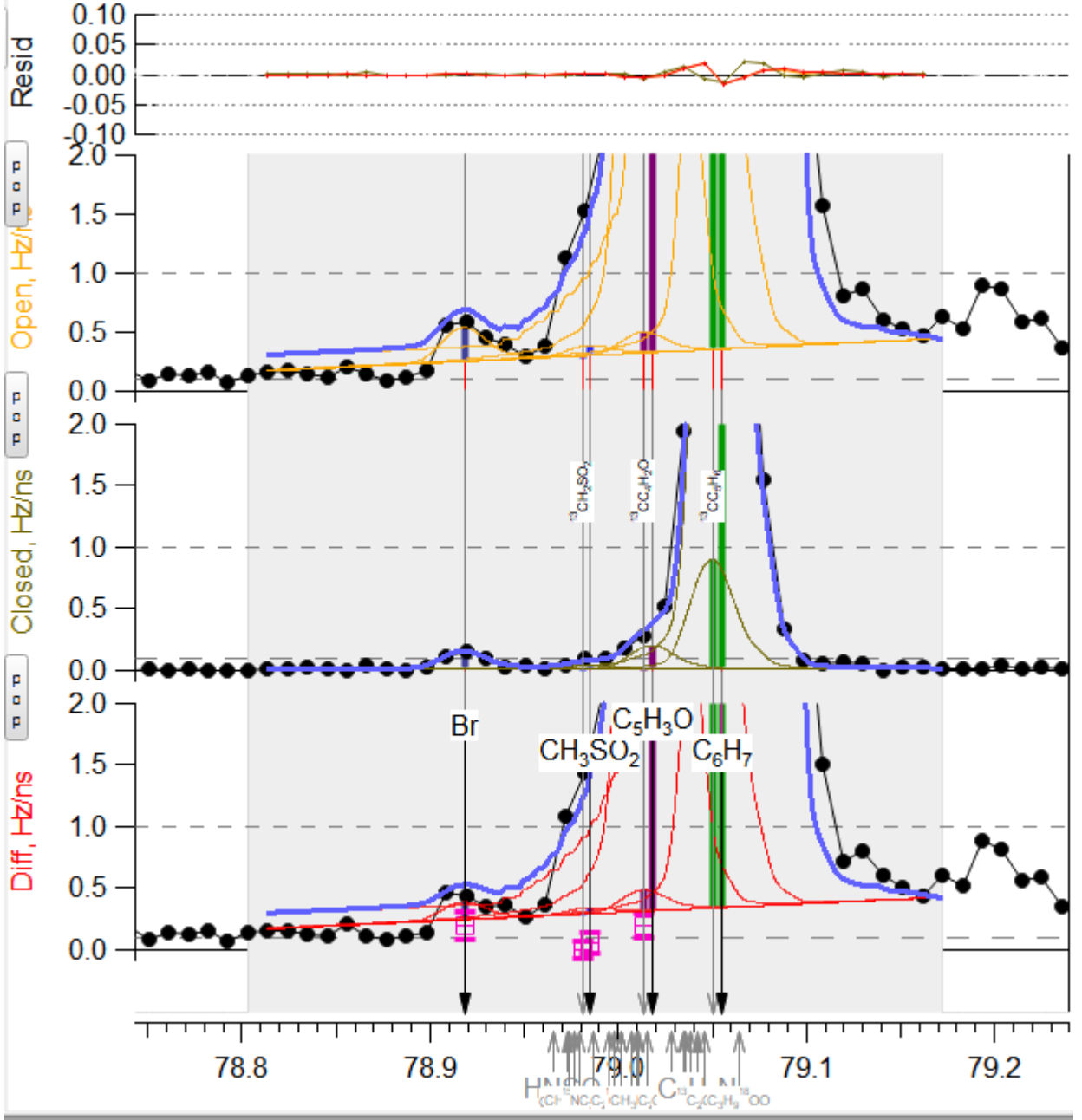
Most useful for very small signals and for HR analysis

Independent of UMR integration regions

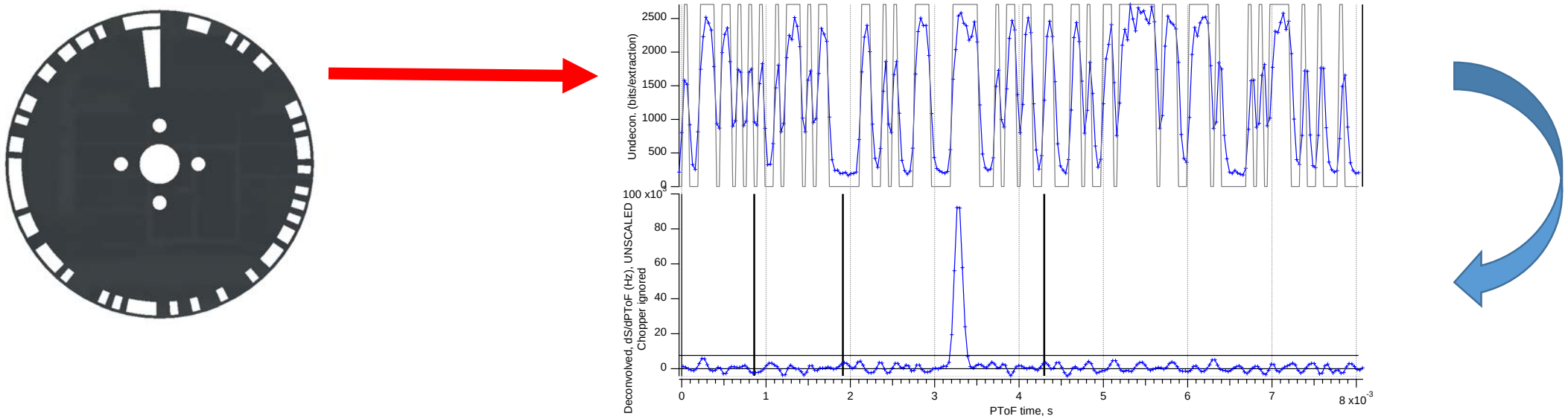
Tofwerk proprietary (code details are hidden ☹)

New baseline algorithm example





ePToF can generate ‘regular’ MS-like data



Independent of deconvolution, we can collapse the PToF dimension

ePToFSum ~ ½ *open + ½* closed

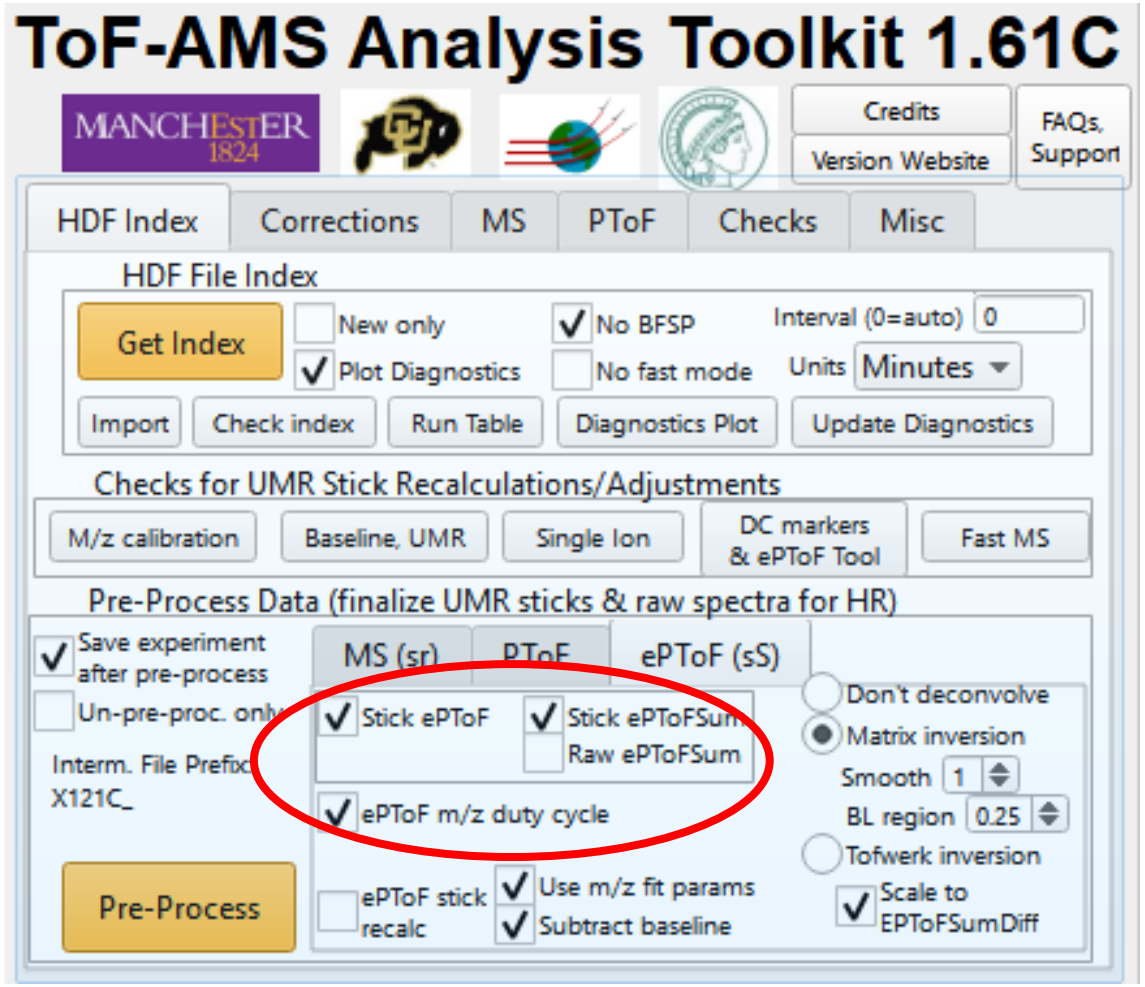
= ½ *(diff+closed) + ½ *closed

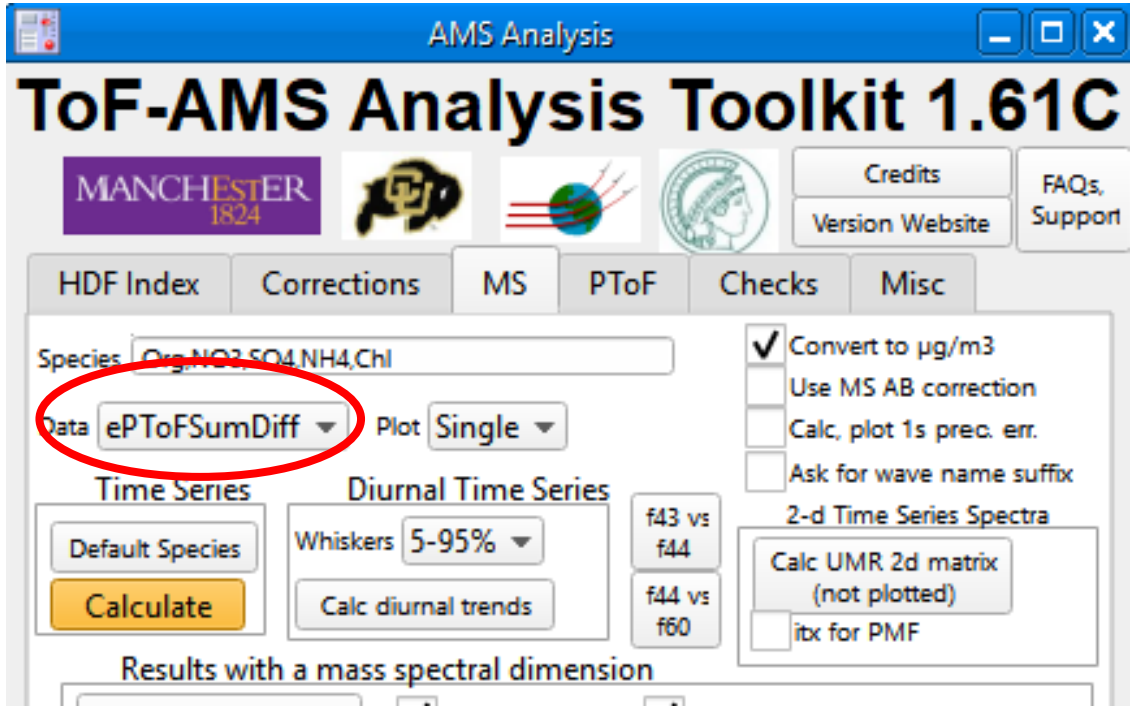
= ½ *diff + closed

epToFSumDiff = 2* (1/2*diff + closed – closed)

~= MS Diff, (~ 5%) not exact because of slowly vaporizing ions

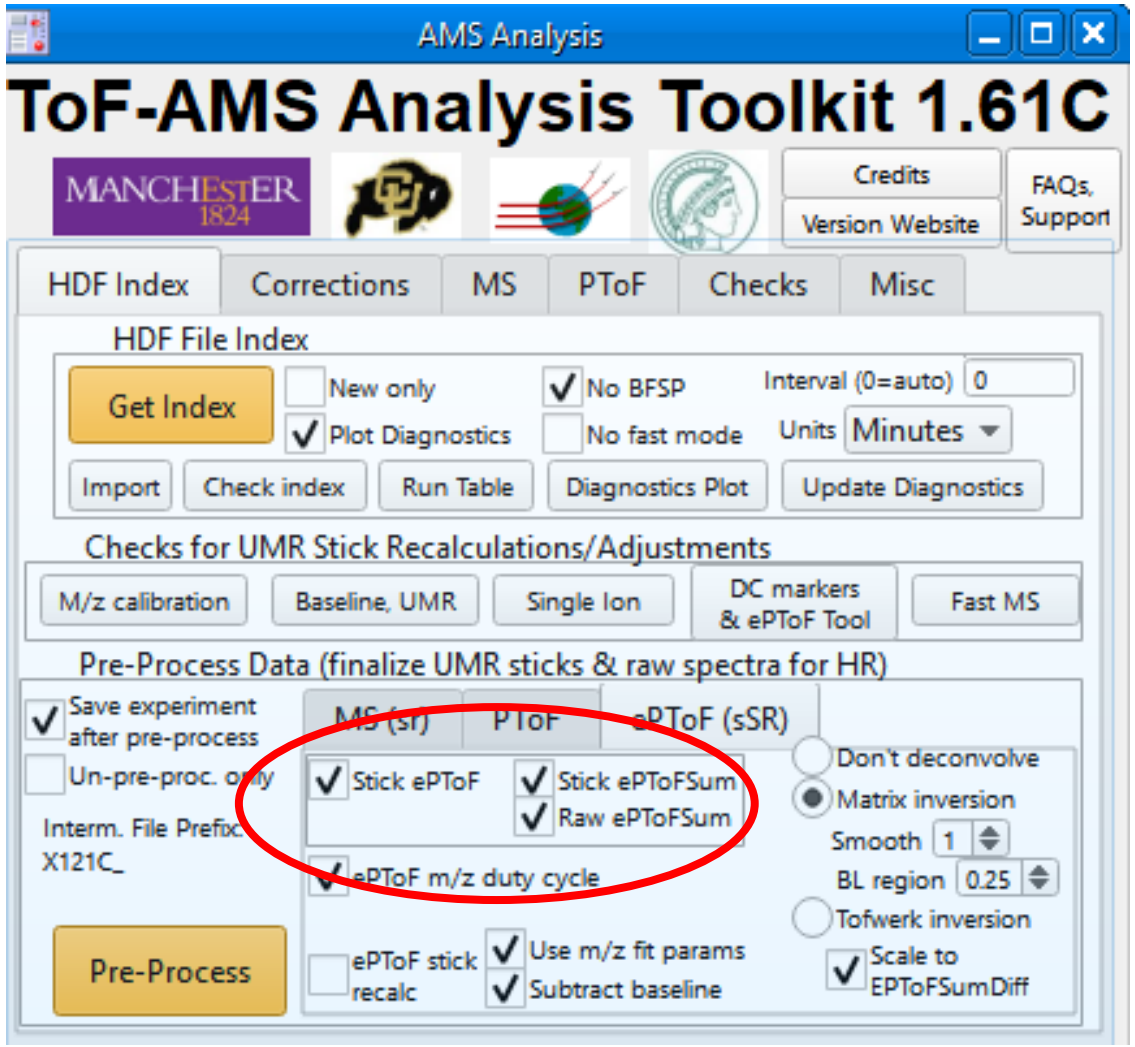
ePToF can generate ‘regular’ MS-like stick data





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!

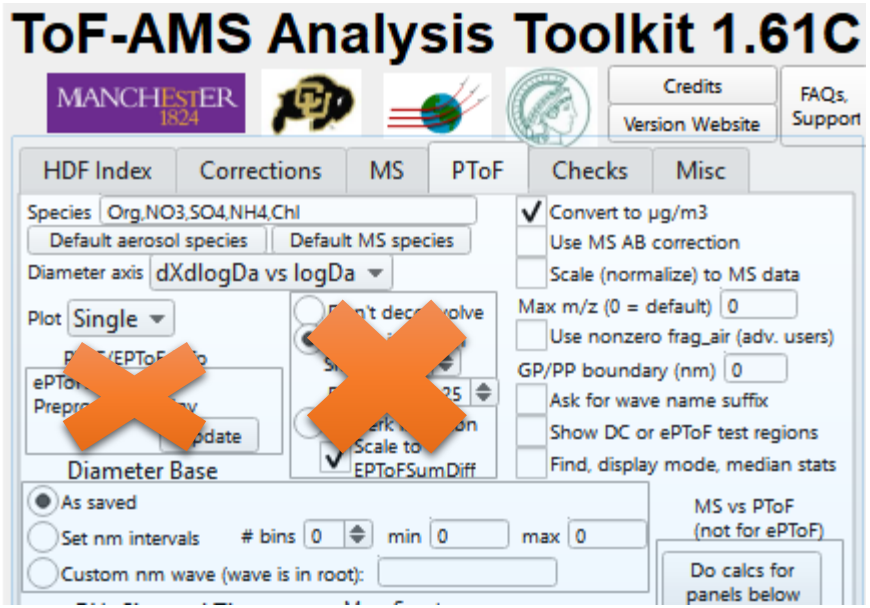
Can we do HR ePToF (not collapsing in the PToF dimension)?

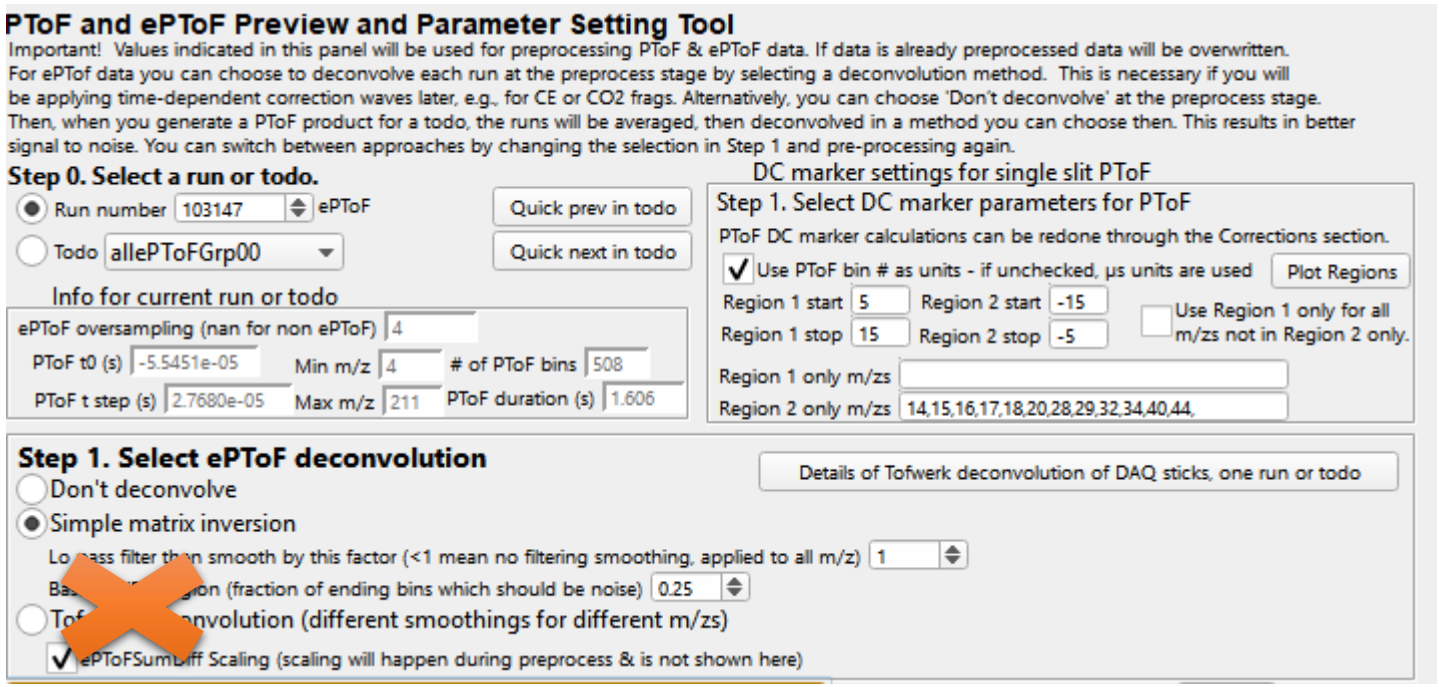
Painful!
We need to perform HR fits on undeconvolved (low signal issues, time consuming)
THEN deconvolve HR matricies.
Will not be coded in the forseeable future

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





New HR ion convention, HR ions ‘library’

The order or atoms within HR fragment names:

C H N S F Cl Br I O X

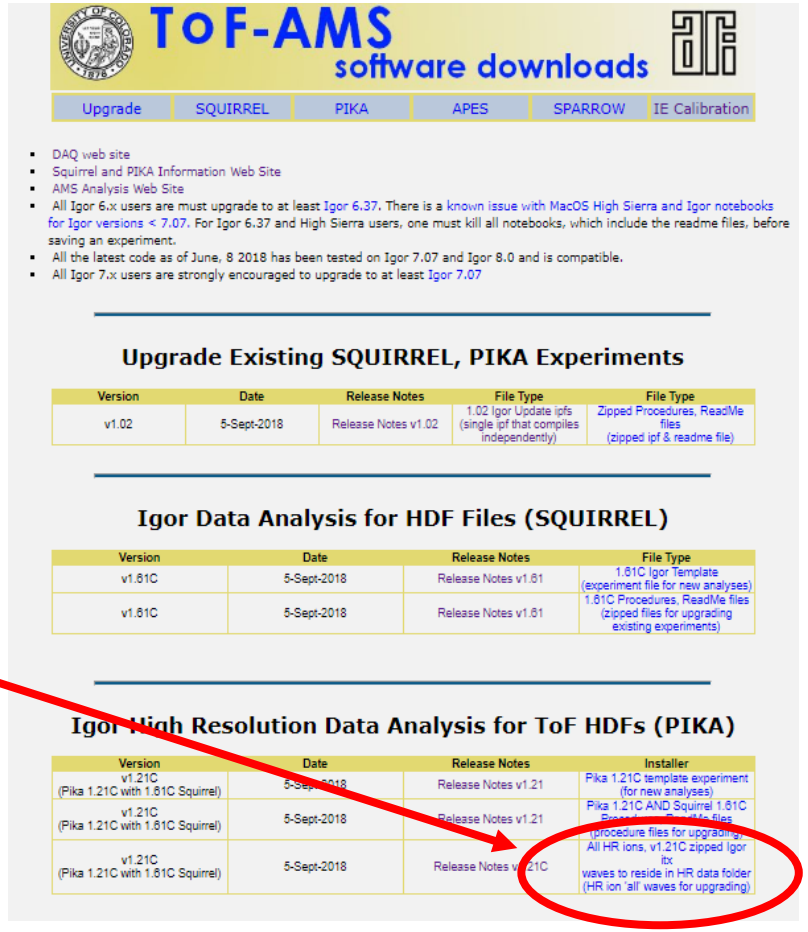
EXCEPT for ‘traditional’ ammonium ions, i.e. NH, NH2, NH3, NH4
isotopic ‘children’ come before the ‘parent’, so j13CC2H7, NOT C2j13CH7

i.e. CH3SO2, not CH3O2S

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

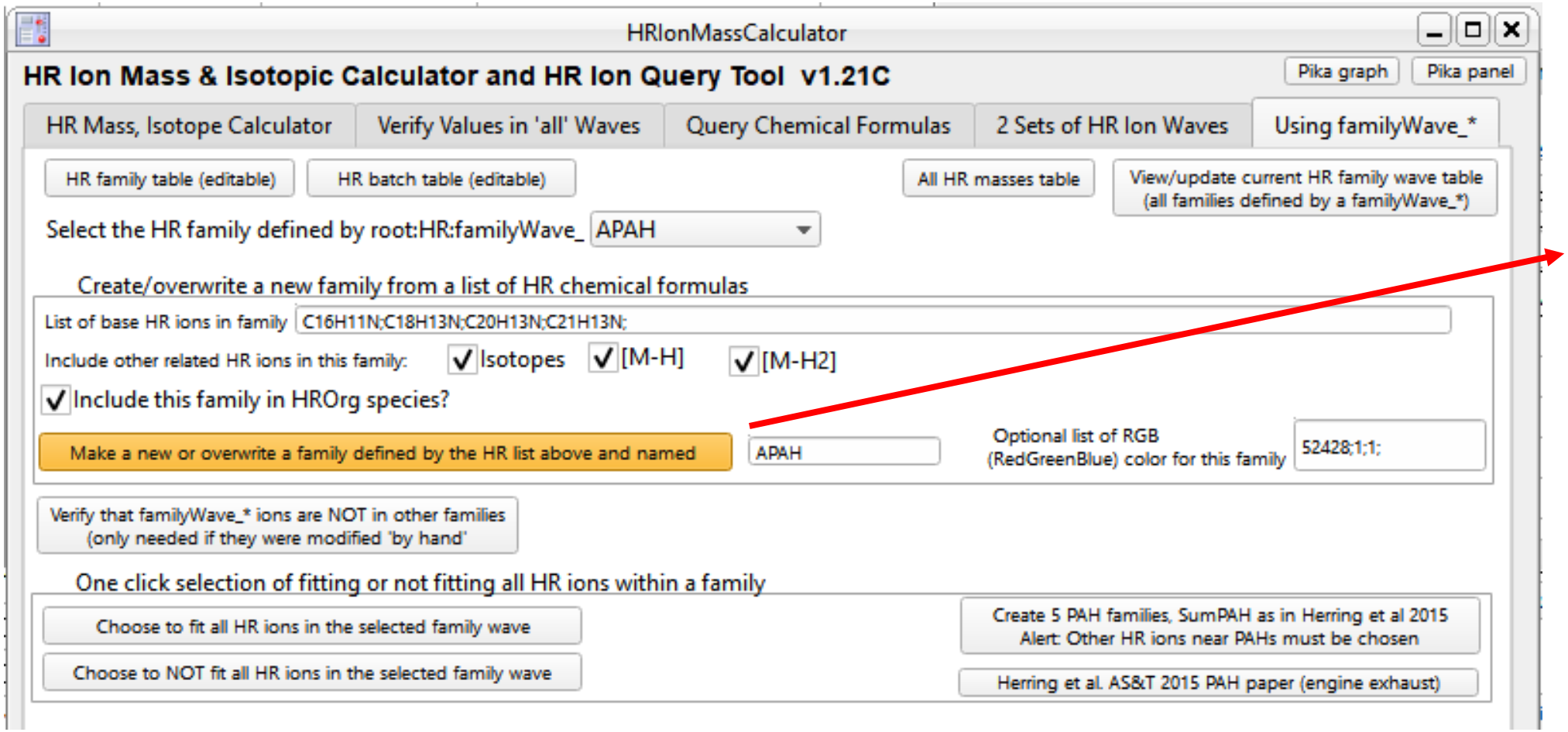
Library ExactMassWaves121C released

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



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.



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

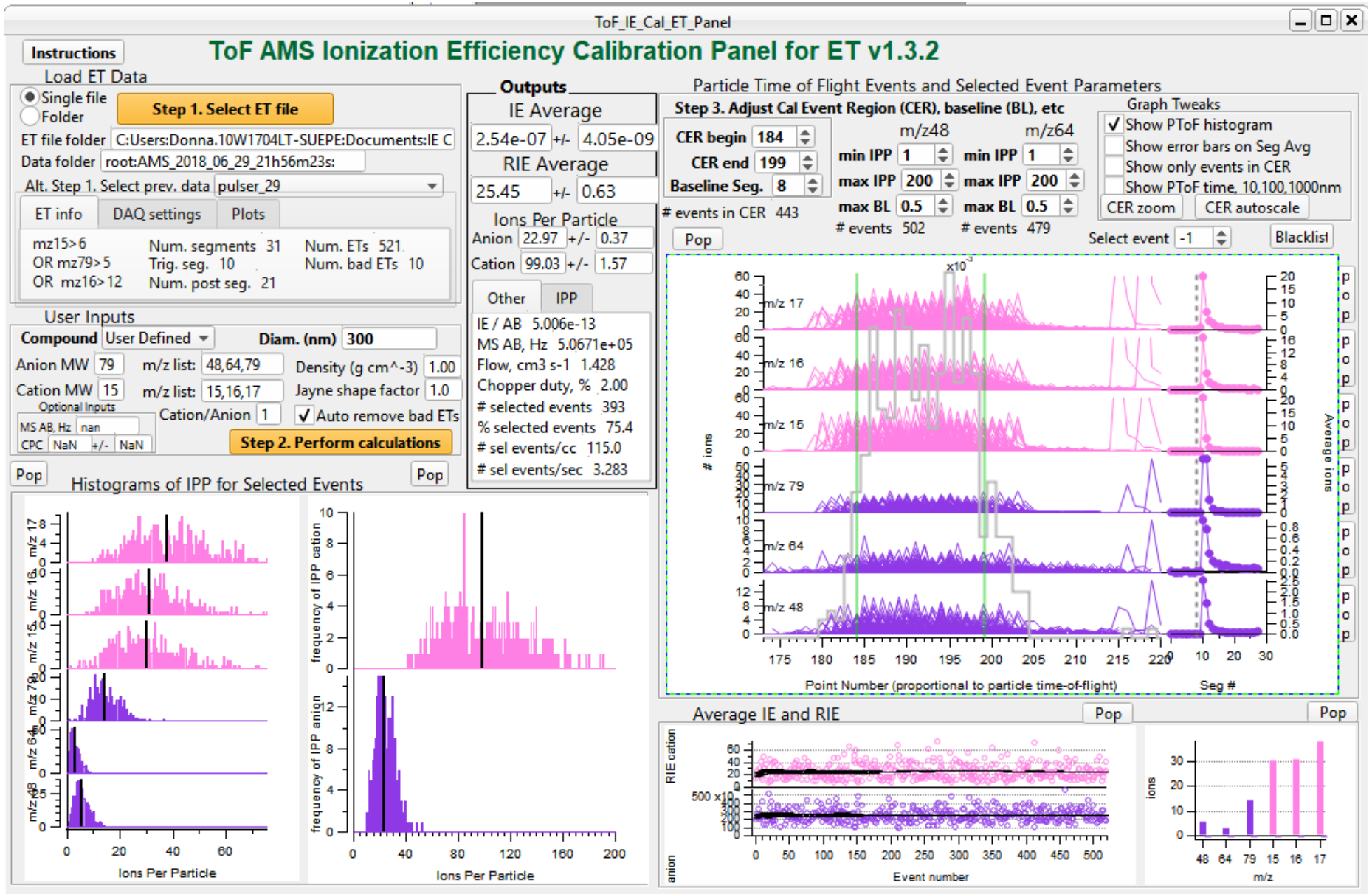
Point	HR_familyName	HR_familyListDefinition
0	Cx	default
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		
11	NO	default
12	SO	default
13	Air	default
14	Tungsten	j182Wplus2;j184Wplus2;j186Wplus2;W;WO
15	Other	default
16	CSi	default
17	APAH	familyWave_APAH
18		

HRBatchTable

R5 familyCx;familyCH;familyCHO1;familyCHOgt1;familyCHN;familyCHO1N;familyCHOgt1N;familyCS;familyAPAH;

Point	HR_specFrag_list	HR_specFamilyBase	H
1	HR_frag_Pwater	familyHO	
2	HR_frag_ammonium	familyNH	
3	HR_frag_nitrate	familyNO	
4	HR_frag_sulphate	familySO	
5	HR_frag_organic	familyCx;familyCH;familyCHO1;familyCHOgt1;familyCHN;familyCHO1N;familyCHOgt1N;familyCS;familyAPAH;	
6	HR_frag_chloride	familyCl	
7	HR_frag_organic[44]		

IE for ET cal code allows for any cal standard

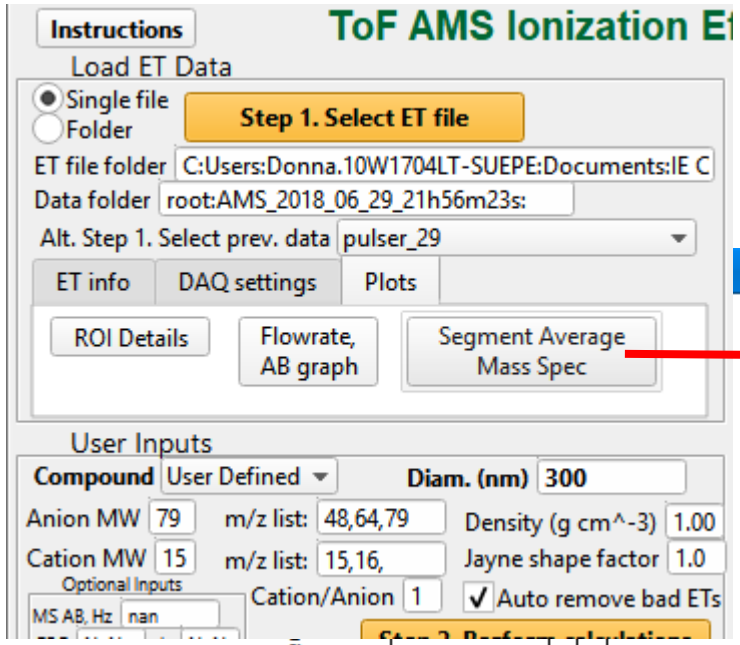


MSA was used in this file to example.

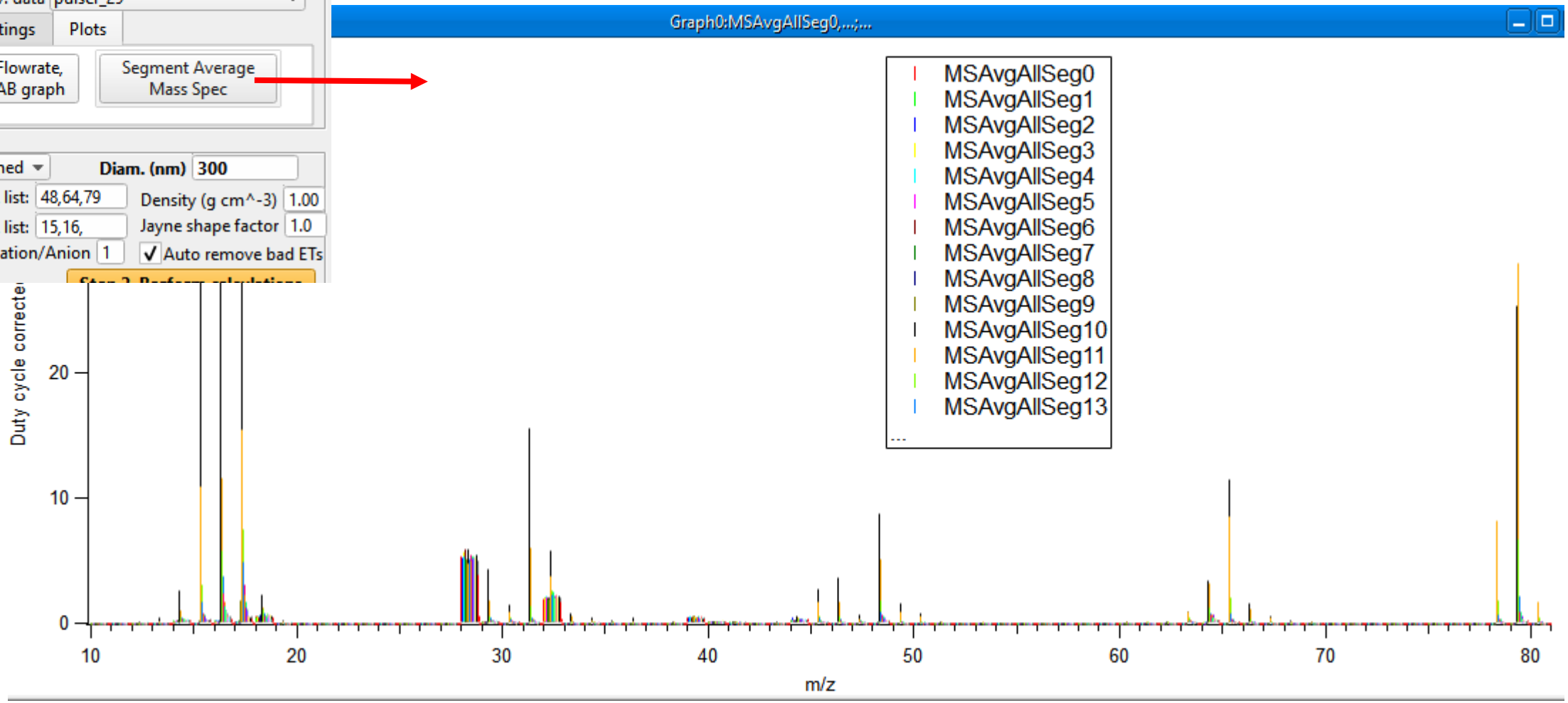
Users can select the compound as 'User Defined' and list their own anions and cation m/z lists (which don't have to be in increasing m/z order).

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



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!