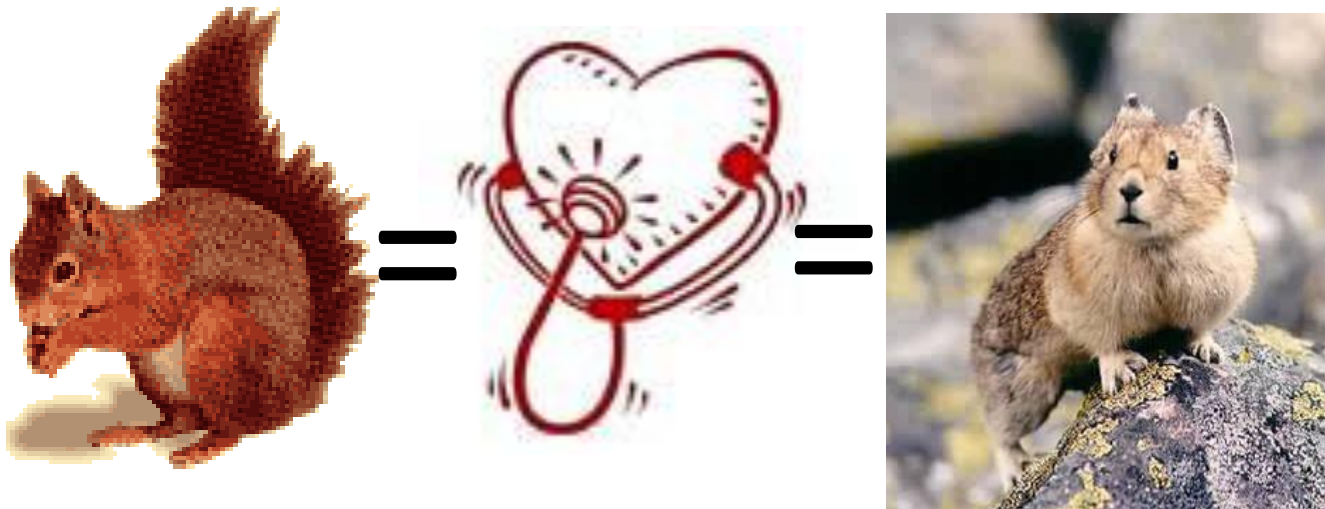


Data Analysis Updates for AMS-ToF (Squirrel 1.53 & Pika 1.12)



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AMS Users Meeting, 9 - Sept - 2013



Squirrel 1.53 Updates and Bug Fixes

No major changes

Increased speed, more functionality

- Added option for .h5 file extensions in DAQ5
- EPToF functionality added
- Fast mode overhauled, now > 4 x faster
- Revamped the look of the airbeam correction interface
- Added option for frag_air to be zero for PToF data
- New pX and dyymmddhhmmss options in todo wave creation

SQ 1.53 pX and dyymmddhhmmss, dyymmdd options for todos, part 1

ToDo Wave Creation

Run Interval

Name

RunIndexTable

8/31/2009 15:00:00

Point	t_series	rn_series
99	8/31/2009 14:55:00	44946
100	8/31/2009 15:00:00	44947
101	8/31/2009 15:05:01	44948
102	8/31/2009 15:10:01	44949

pX syntax

The letter p followed by a number

Indicates point number, i.e. row in run series wave.

The code translates pX to a run number then replaces the pX with the run number and proceeds with the creation of todo wave

Usage such as
p100-p120,
mytodo and not p3004
etc are all allowed

ToDoWavesTable

44847

Point	oneRun
0	44947
1	
2	

SQ 1.53 pX and dyymmddhhmmss , dyymmdd options for todos, part 2

ToDo Wave Creation

Run Interval

Name

d090831150000 = 2009, Oct 31, 15:00:00

dyymmddhhmmss syntax

dyymmdd syntax

Indicates date (and optionally) time

The code translates dyymmddhhmmss to a run number then replaces the dyymmddhhmmss with the run number and proceeds with the creation of todo wave

The code translates dyymmdd to a run number interval then replaces the dyymmdd with the run number interval and proceeds with the creation of todo wave

Usage such as
d130831-d130903
mytodo and not d130831
etc are all allowed

RunIndexTable		
8/31/2009 14:55:00.7		
Point	t_series	m_series
98	8/31/2009 14:50:00.9	44945
99	8/31/2009 14:55:00.7	44946
100	8/31/2009 15:00:00.5	44947
101	8/31/2009 15:05:01.3	44948
102	8/31/2009 15:10:01.0	44949
103	8/31/2009 15:15:00.9	44950
104	8/31/2009 15:20:00.6	44951
105	8/31/2009 15:25:00.4	44952
106	8/31/2009 15:30:01.1	44953
107	8/31/2009 15:35:00.7	44954
108	8/31/2009 15:40:00.5	44955
109	8/31/2009 15:45:00.3	44956
110	8/31/2009 15:50:00.9	44957
111	8/31/2009 15:55:00.7	44958
112	8/31/2009 16:00:00.4	44959

// The todo wave named ThreePmHour was created ... and contains 13 runs.



Pika 1.12 Updates and Bug Fixes

No major changes

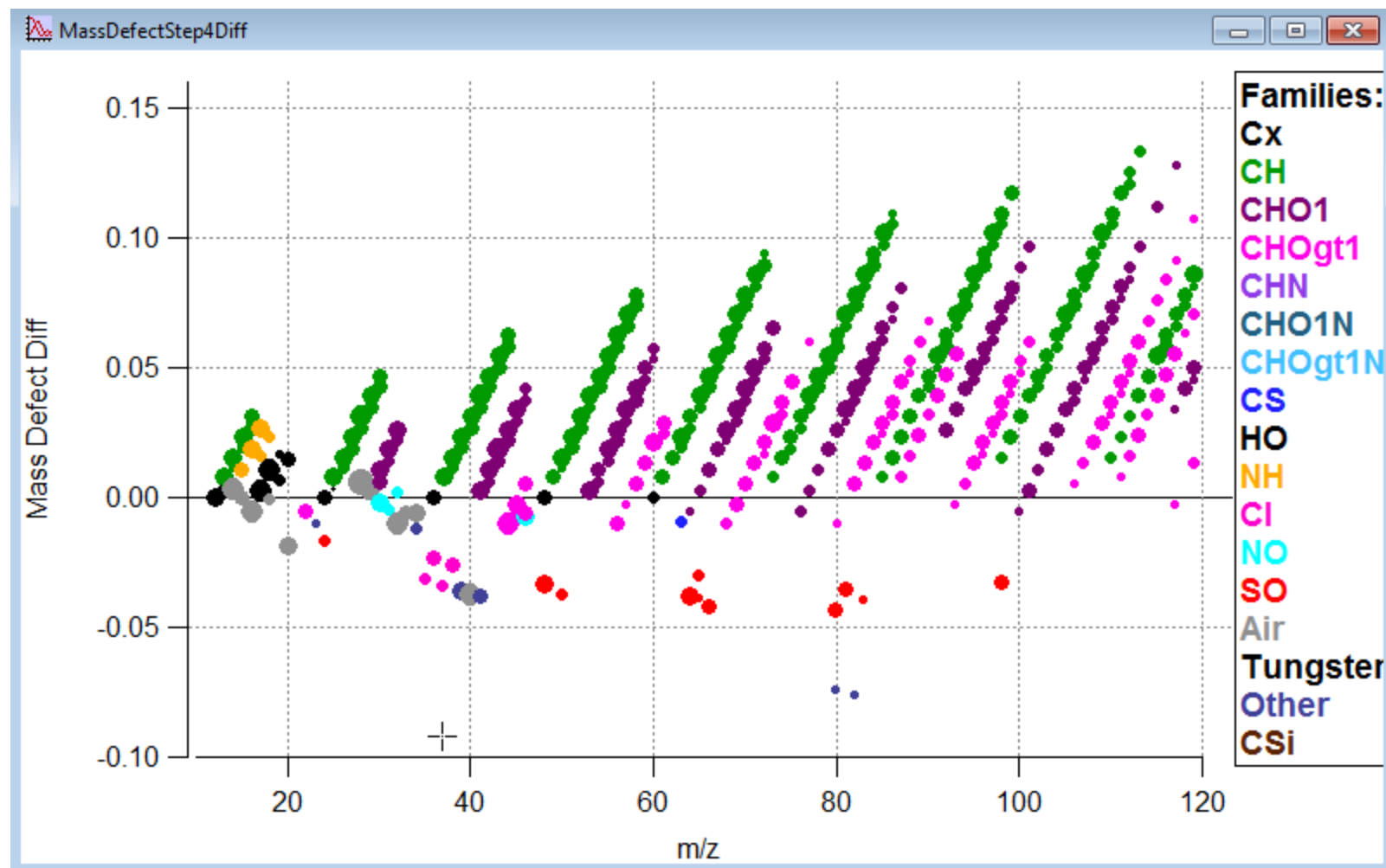
Increased speed, more functionality

- Linear Least Squares HR algorithm, > 10 x faster
- New warning system for when chosen HR ions are > max mz
- New look for tags in HR_peakHeights_gr
- Black carbon adjustments for SPAMS
- Optional removal of isotopes for export to PMF
- Mass defect plots!
- Overhauled HR ion calculator

Pika 1.12 Mass defect plots

Colored by family

Sized by $\sqrt{\log(\text{peak height})}$



Pika 1.12 New HR ion calculator – for a single HR ion

HR Ion Mass Calculator

HR Ion Mass & Isotopic Calculator and HR Ion Query Tool v1.05

HR Ion Mass & Isotope Calculator Verify Values in 'all' Waves Query Chemical Formula Matches Compare Two Sets of HR Ion Waves

Enter the chemical formula for the HR ion to investigate.

One HR Ion Mass

HR ion (i.e. j13CH)

Mass

Iso. abundance

Iso. Parent

Exists? Yes Chosen to fit? Yes

☒ Choose to fit?

Isotopic Children of HR Ion Mass

Isotopic children of HR ion whose relative abundance to parent is >

☒ Child exists in 'all' wave

☒ Child is fit

☐ Child is not fit

☐ Child does not exist in 'all' wave

Point	HR Ion	Mass	Iso. abundance	Iso. parent
0				

☒ Choose to fit?

FYI only - Table of Elements and Isotopes (NOT editable unless advanced user)

Point	ElementIonName	ElementIonMass	ElementIsotopAb	ElementIsotopPe	ElementIsotopPe
0	H	1.00782503		j2H	1;
1	j2H	2.01410178	0.00011501		

Pika 1.12 New HR ion calculator – for comparing sets of HR ions

HR Ion Mass Calculator

HR Ion Mass & Isotopic Calculator and HR Ion Query Tool v1.05

HR Ion Mass & Isotope Calculator Verify Values in 'all' Waves Query Chemical Formula Matches Compare Two Sets of HR Ion Waves

Step 1A. Choose data folders which contain set of 8 waves for HR ion wave comparison

A

Data Folder for set "A" of waves

pts in ExactMass_all etc. waves | NaN

HR ions fit (mask_stick_integration) | NaN

B

Data Folder for set "B" of waves

pts in ExactMass_all etc. waves | NaN

HR ions fit (mask_stick_integration) | NaN

For reference: List of 8 HR ion 'all' waves and description

Poi	HRIonAllWaveNames	
0	ExactMassWave_All	The exact mass
1	ExactMassText_All	The text 'name'
2	ExactMassTag_All	The igor-code t
3	ExactMassComments_All	A text wave exi

Step 1 B. Choose how to resolve mask_stick_integration conflicts

Results from Step 2 comparison of HR ion waves

in A or B | NaN # in A and B | NaN # in A not B | NaN # in B not A | NaN

Point	ExactMassWave	ExactmassText	Mask_Stick_Integ	ExactMassCom
0				

Optional additional display below

Point				
0				

What's next for Squirrel and Pika?



+ **TOFWERK** =
Time-of-Flight Mass Spectrometry

