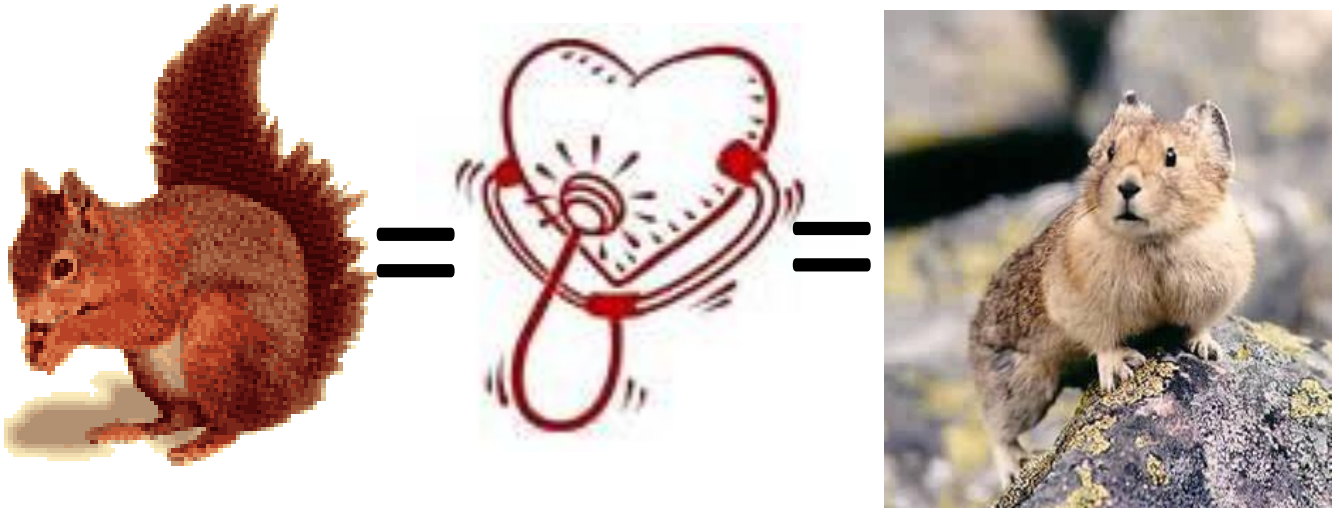
Data Analysis Updates for AMS-ToF (Squirrel 1.53 & Pika 1.12)



Donna Sueper

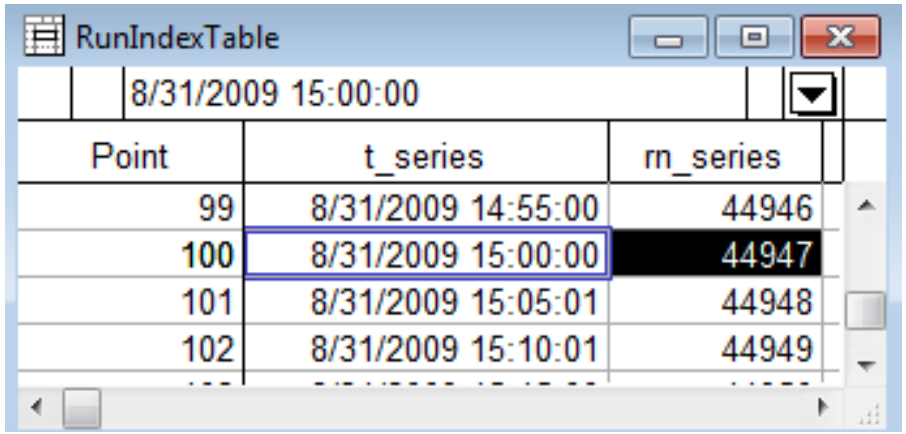
AMS Users Meeting, 9 - Sept - 2013

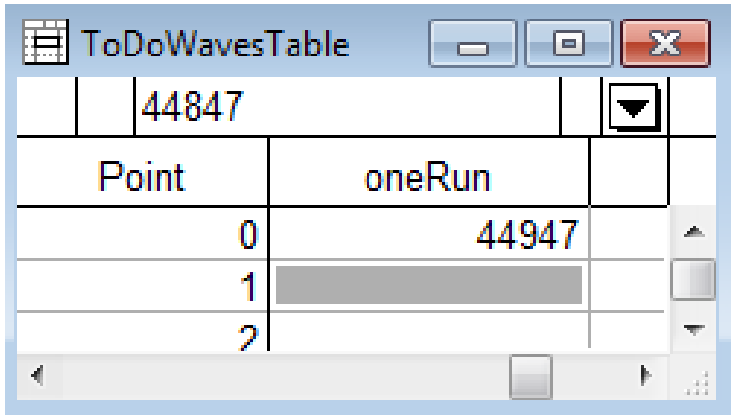
Squirrel 1.53 Updates and Bug Fixes

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





pX syntax

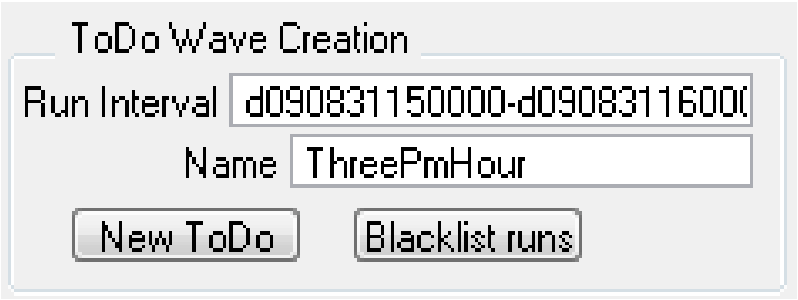
The letter p followed by a number

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

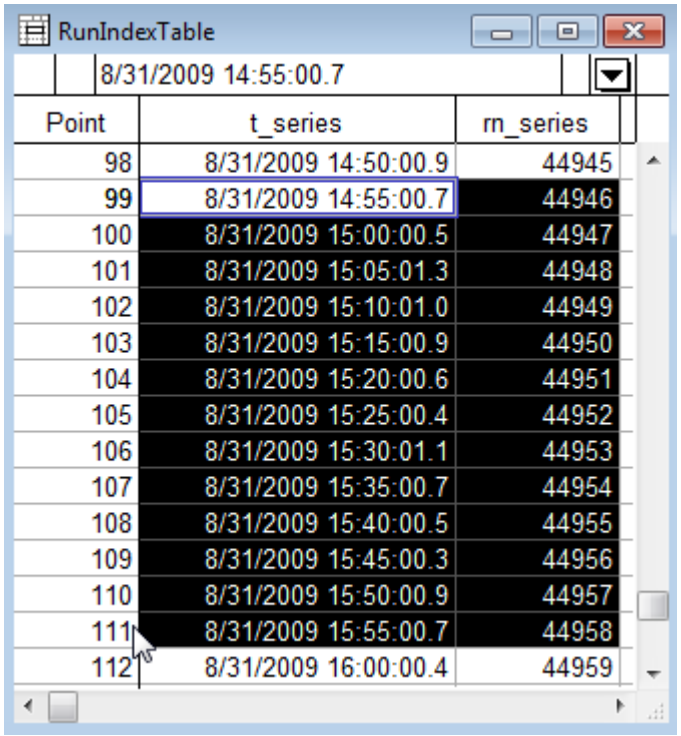
The code translates pX to a run number then replaces the pX with the run number and proceeds with the creation of todo wave

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

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



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



Point	t_series	rn_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.

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

Pika 1.12 Updates and Bug Fixes

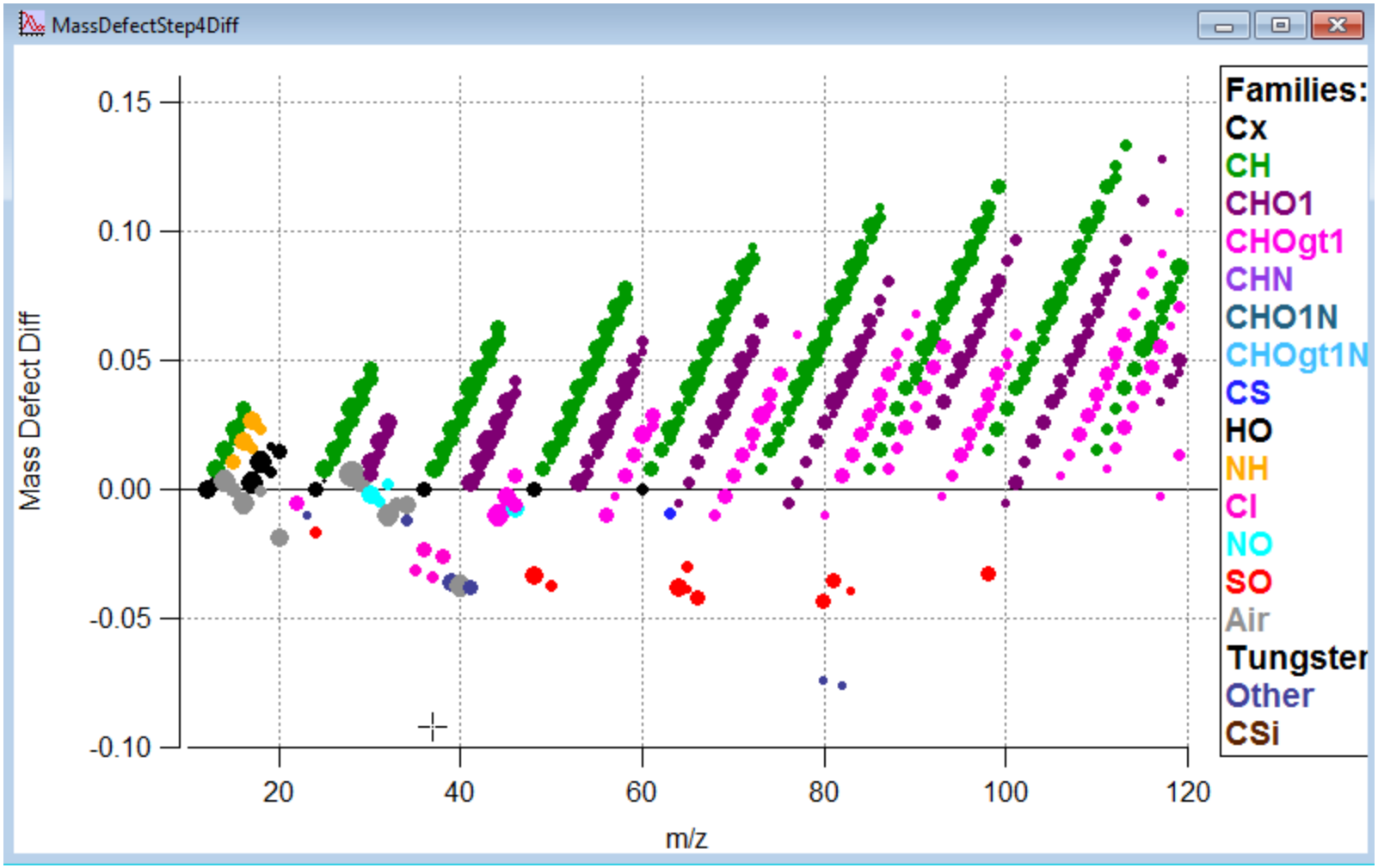
No major changes
Increased speed, more functionality

- 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

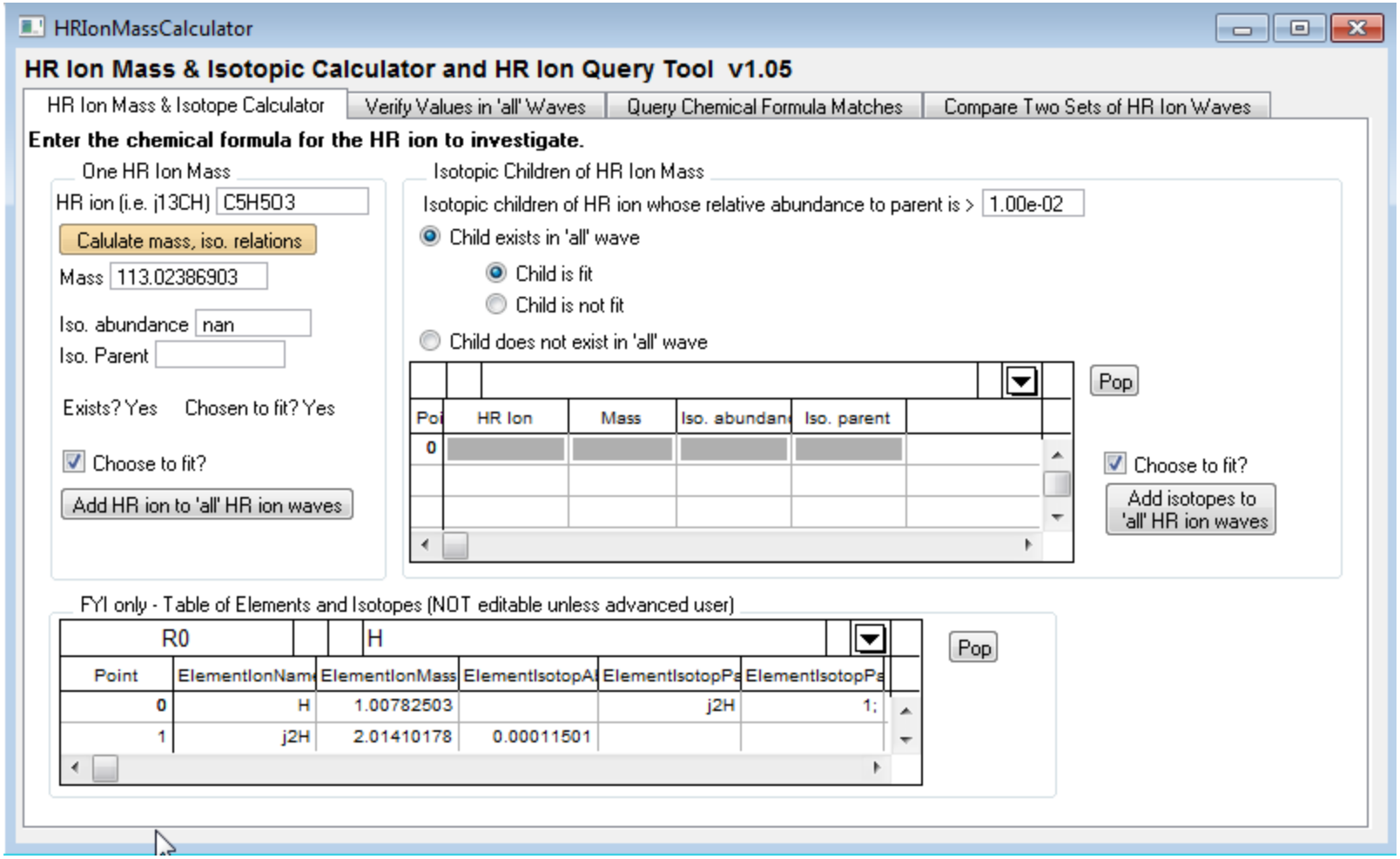
Pika 1.12 Mass defect plots

Colored by family

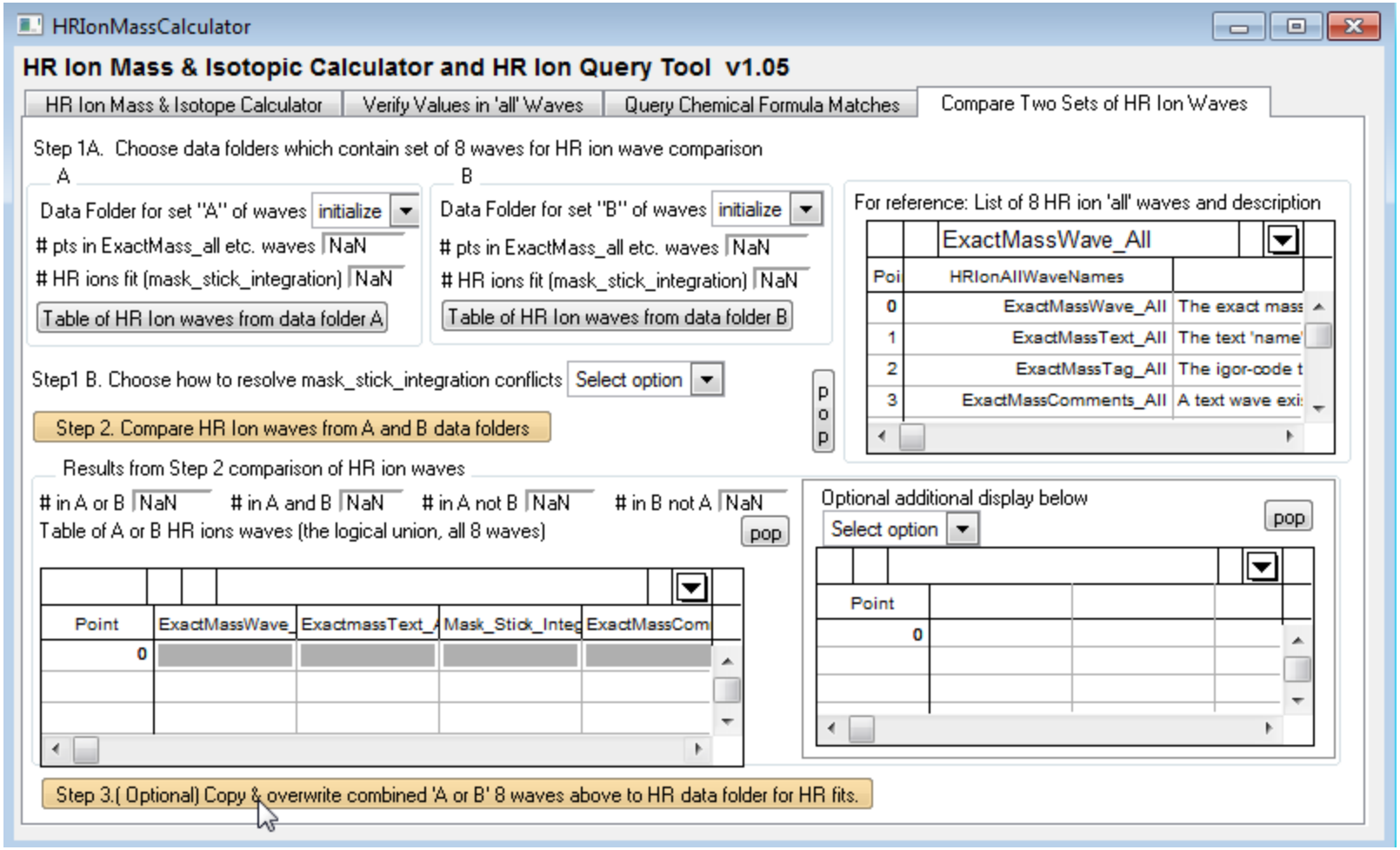
Sized by sqrt(log(peak height))



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



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



What's next for Squirrel and Pika?

+ TOFWERK Time-of-Flight Mass Spectrometry =