What is new in Squirrel since last year? Part 1

The MS tab was revamped for more consistency, clarity.

Error calculations & plotting fully implemented for MS data.

Added code specific for fast mode data. (Thanks Mike C!)
What is new in Squirrel since last year? Part 2

Some new features may help prevent out-of-memory errors.

* Allow user to put MSSDiff_p and error matrices into intermediate files instead of memory

* When generating 2-d time series spectra (i.e. Org matrix for input into PMF), Users can now choose a maximum m/z value instead of entire m/z range.

What is new in Squirrel since last year? Part 4

Changed the default variables the indicated stick integration region so that all ToF modes, C, V, and W, are now the same.

New (VERSION 1.48) all ToF Types:

- resolution_R0 = 350
- resolution_dm = 50
- resolution_m0 = 75

Version 1.47:

- C mode:
  - resolution_R0 = 380 (was 500 <1.47)
  - resolution_dm = 50.213
  - resolution_m0 = 75
- V/W mode:
  - resolution_R0 = 350
  - resolution_dm = 50.213
  - resolution_m0 = 75
What is new in Squirrel since last year? Part 3

Speeded up some calculations through the use of sparse matrix multiplication. (This introduced a bug with errors in version 1.47 and was fixed in 1.47D).

Various small bugs, mostly display issues, have been fixed.

Added ability to subtract baselines from raw PToF spectra.

What is new in Squirrel since last year? Part 4

Better web documentation!

http://cires.colorado.edu/jimenez-group/wiki/index.php/ToF-AMS_Analysis_Software
What are the most common Squirrel issues?

How do I move/upgrade an experiment?
Tools are in place for users to easily change hdf file locations (misc tab).

How do I know that my m/z calibration is good enough?
It depends on what you want to do. For UMR (Unit Mass Resolution) it is very very rare to get it ‘not good enough’.

How do I know that my baseline settings are good enough?
You can almost always make the stick integration region bigger than it needs to be without a big penalty.

Should I upgrade an experiment? YES!

What is the best way to get help with my problem data?
Make sure the problem is replicable. Isolate the issue. Check the wiki. Send me an email.

My data isn’t typical because of X; how do I change the frag table to account for this?
You need to think this through.

What is next for Squirrel?

Squirrel has matured!

Remaining issues:

• Non EI considerations
• PToF m/z calibration, errors
• CE algorithms
• 40/28 ratio correction (threshholding issues)
• Baseline parameters (stick integration region) be run-number specific
• More intuitive interface for frag checks & frag table modifications
• Perhaps some very minor frag table adjustments (based on Pika results?)
What is next for Squirrel?

More great collaboration with users!

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