



Squirrel/Pika Features

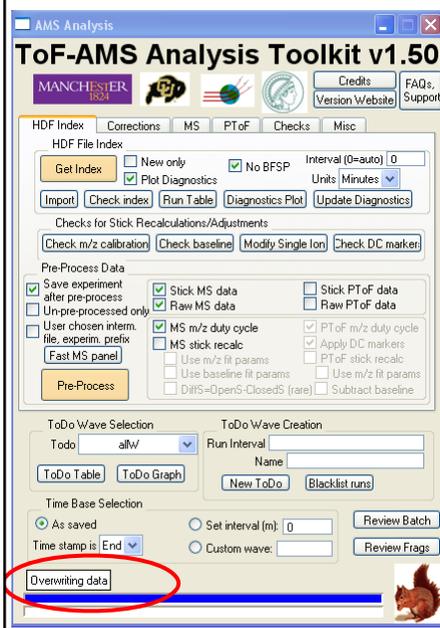
Dos and Don'ts

2010 AMS User's Meeting, Hyytiala

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Squirrel - What you should not do



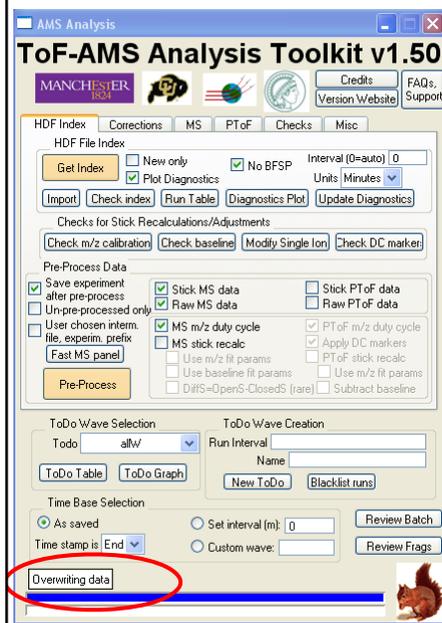
Abort while writing to intermediate HDF files!

Anecdotal evidence indicates that when you abort while writing to an intermediate file, you can corrupt the intermediate file.

Subsequent calls to retrieve data in file will return an error "File xxx not opened - aborting from squirrel_fetch".

Difficult to reconstruct intermediate file once corrupted.

Squirrel - What you should not do



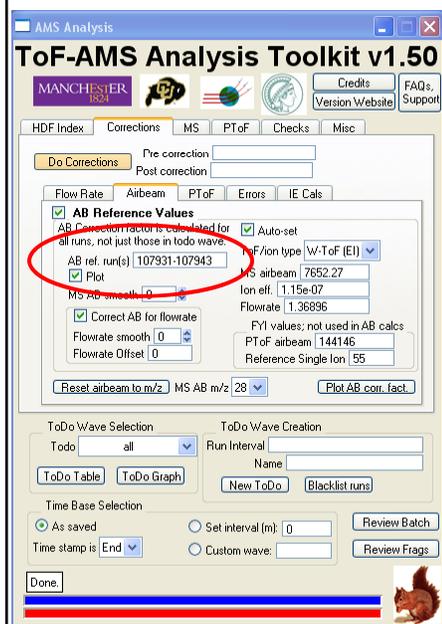
Blacklist a run when there is a chance it contains real information

Runs that seem like outliers may contain diagnostic information.

It is difficult, but not impossible to unblacklist.

Instead generate todo waves that 'quarantine' offending runs. (generate todowaves such as 'mystery' and quarantine them via 'allV and not mystery' todo wave creation entries.)

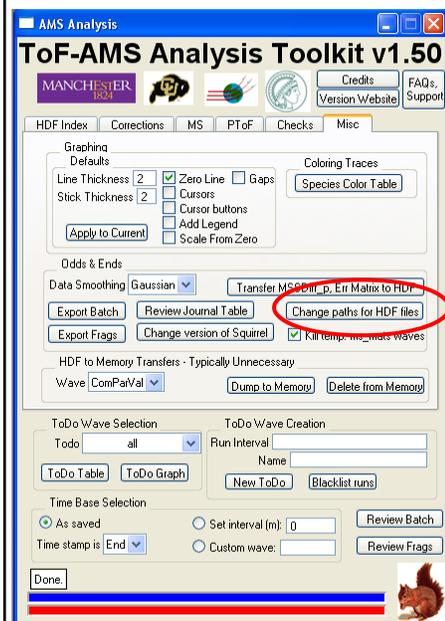
Squirrel - What you should not do



Select a period containing V and W runs for the airbeam reference period.

If you have V and W mode data in your experiment, the AB correction code will not work correctly unless you choose a reference period containing both V and W mode runs.

Squirrel - What you should do

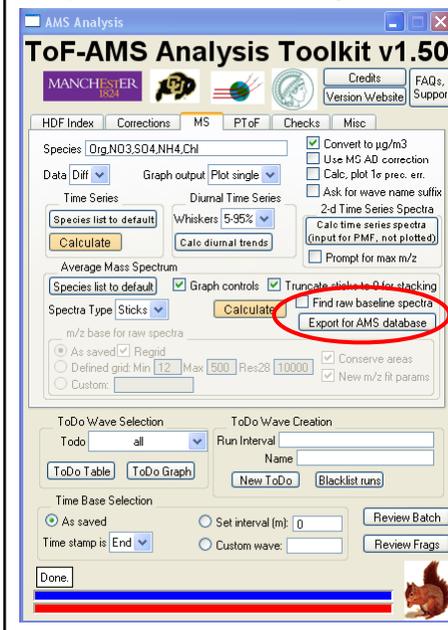


Use the “Change paths..” button when files have moved.

Depending on the operation, squirrel may need to access the DAQ files and/or the intermediate files.

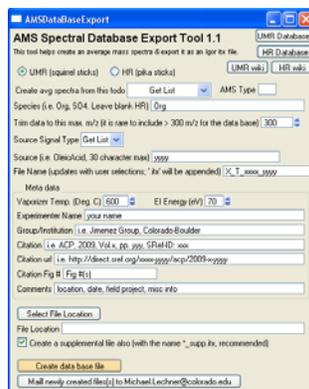
Squirrel will generate a prompt when it can no longer find a file, but this can be tedious.

Squirrel - What you should do



Export your data to the AMS data base.

Once your marvelous paper has been published, consider



AMS spectral data base, cont.

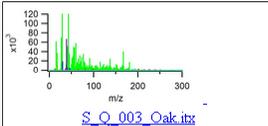
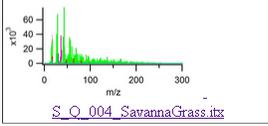
http://cires.colorado.edu/jimenez-group/AMSSd/

AMS Spectral Database (Unit Mass Resolution)

This page is a compilation of published spectra obtained with the [Aerodyne Aerosol Mass Spectrometer](#). See also the recently-created [Database of High-Resolution AMS Spectra](#)

Spectra are divided into several categories with respective ID labels:

- [source](#) (S_*_xxxx)
- [ambient](#) (A_*_xxxx)

S_Q_003	Biomass Burning: Oak	Johannes Schneider MPI Chemistry	Q-AMS 007	70 eV	440	Schneider, J. et al. Int. J. Mass Spec. 2006 258, 37-49	Fig 4b, pg. 42	Species spectra processed with standard frag table	
S_Q_004	Biomass Burning: Savanna Grass	N. Hock/S. Weimer MPI Chemistry	Q-AMS 007	70 eV	490	Schneider, J. et al. Int. J. Mass Spec. 2006 258, 37-49	Fig 4e, pg. 42	Species spectra processed with standard frag table	

Squirrel - What you should do

■ SQ_MzCalibration_Panel

Power Fit: ion time of flight = intercept + slope*(mass^power)

Step 1. Choose m/z fitting settings by editing values in the table and checkboxes.

Spec Type: 0 = Don't Use
 1 = Diff 2 = Closed 3 = Open 4 = PT of
 Delta: 1 = 2 Delta 1 Power

Plot: 0 = Don't Show 1 = Show
 MS PT of

Power param = 0.500000
 Use previous run's params
 TO fit peaks (Power)

Peak search factor: 1

Set to defaults

PT	Name	Mass	Spec Typ	Delta	Graph
0	C+	12	2	2	1
1	N+	14.0031	2	2	1
2	O+	15.9949	2	2	1
3	H2O+	18.0106	0	2	1
4	N2+	28.0061	0	2	1

Try some new features

Panels are densely packed with features.

New features are a result of user requests.

Squirrel/Pika - What you should do

Alert me to problems

Try to replicate the problem

If problem persists, try on a single run/other todo waves.

Upgrade your squirrel ipfs. (Everyone should try to be on Igor 6.1x)

Send screen shots, and fire me an email sueper@colorado.edu

Suggest features/donate code

Free, community-shared and community-used code is the best kind.

Squirrel/Pika – Play time!

Using the downloaded UsersMtg2010 igor experiment,

- ✓ Use the “Change paths..” button when files have moved.
- ✓ Create a file (UMR or HR) for submission to the AMS spectral data base.
- ✓ Try new (or new to you) features.

About this experiment:

Almost all defaults were used -> results NOT optimized!

For the HR part of the experiment:

The allV and allW todo waves were fit with different sets of HR ions.

Default set of HR ions fit, with the exception of the allW todo wave where one more HR ion was fit.

W mode quantification data suspect (W mode AN calibration or estimated)?

Pika play time

Compare HROrg for V, W, Org for V, W

Add/remove HR ions to fit for one spectra, todo waves. Save list of masses and import them.

Create a new family, HRspecies

Modify HR frag table (add new HR ions and change the coefficients)