

What version of Squirrel/Pika should I be using?

A brief summary and timeline for the different versions.

Donna Sueper
April 2010

Valentin's brief, earlier points:

(A) Species-specific correction waves

For all versions of Squirrel, Pika, a species-specific time correction factor is not applied to 2D matrices. Neither is the RIE or CE, but this is ok for PMF, as these are simple scaling factors. Species specific correction factors could be an issue when doing comparisons of time series waves (i.e. nitrate).

(B) m/z 189

Quad and Squirrel have an issue with Org = 0 at 189, will get back to you but it should not be a big deal.

(C) For PMF ~ max 300 m/z

For PMF it is often not useful to include $m/z > \sim 300$. Beyond 300 there are PAH vs Org frag table points that need to be thought through.

Squirrel- Unit Resolution – Part 1

Current Version 1.49A Apr 2010

In version 1.49, Org frag wave was changed to include PAHs. Previously PAHs were a disjoint set from Org. There is an OrgLessPAH frag wave one can use. PMF users should use Org, not OrgLessPAH.

Version 1.48D Nov2009 - IF YOU UPGRADED TO 1.47, YOU MUST UPGRADE TO 1.48D!

Bug fix for incorrect error matrix calculations.

Version 1.48 Oct 2009 (User's meeting release)

Added functionality, misc. bug fixes

Version 1.47 Aug 2009

An bug was introduced in the error calculation with the introduction of the sparse matrix technique for speeding up calculations.

Use of Igor version 6.x made mandatory.

Squirrel- Unit Resolution – Part 2

Version 1.46 Mar 2009

Fixed compatibility issues with Igor 6.05, fixed bugs.

Version 1.45 Feb 2009

Added functionality to stick integration regions & other panels.

Version 1.44 Sept 2008 - USERS MUST UPGRADE TO AT LEAST THIS!

Bug in Error Calcs fixed.

Bug in 1.43, Frag table not updated unless a time series calc was done, this is fixed.

Version 1.43 Feb 2008

Version 1.42 Sep 2007

Recommendation:

It is not too difficult to upgrade all the wave to 1.49A, so just do it!

Pika - High Resolution

Version 1.08CA March 2010
Bothersome bugs fixed.

Version 1.08 Feb 2010
New list of masses, default list to fit have been more thoroughly vetted. HO family renamed.

Version 1.07 Nov 2009
HR species defined, HR frag tables etc. Much nicer interface for results. APES integrated. New peak shape interface.

Recommendation:

If your experiments are at least 1.07, it is worthwhile to upgrade to 1.08CA.

If your experiments are 1.06, it is slightly more bothersome to upgrade. If the data is fully 'cooked', it may not be worthwhile to upgrade. To do PMF you have extract the HR sticks and error matrices "by hand".