Pika 1.05 Release Info

A smattering of general comments & technical details

Donna Sueper

June 6, 2009

Biggest changes in Pika 1.05

* The new default option is to use the raw spectra where the baselines, as calculated by the squirrel-baseline parameters, have been removed.
    Pika version 1.04 and previous found a constant baseline for each integer m/z, each run (more on this later).

* There is a more detailed interface for peak width/shapes. A method to identify a set of peak width/shape parameters for each run is now in place. The use of the more intuitive 'peak' shape is used throughout (instead of the "u" curve).

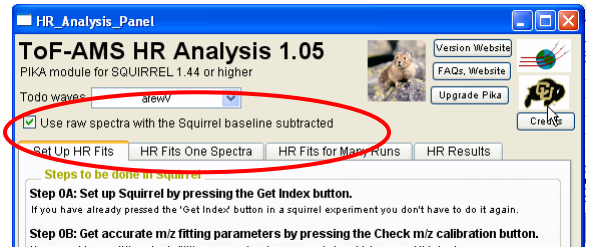
* Some uncertainty values are now automatically calculated to help diagnose issues.

* New features allow users to create average HR or unit mass spectra and time series and in NO_3-eq. ug/m3 units, with/without an airbeam correction.

* New family distinctions between $C_wO_xH_yN_z$ HR fragments for when x = 1 and x >=2. Specifically, CHO1 and CHOgt1, CHO1N and CHOgt1N.

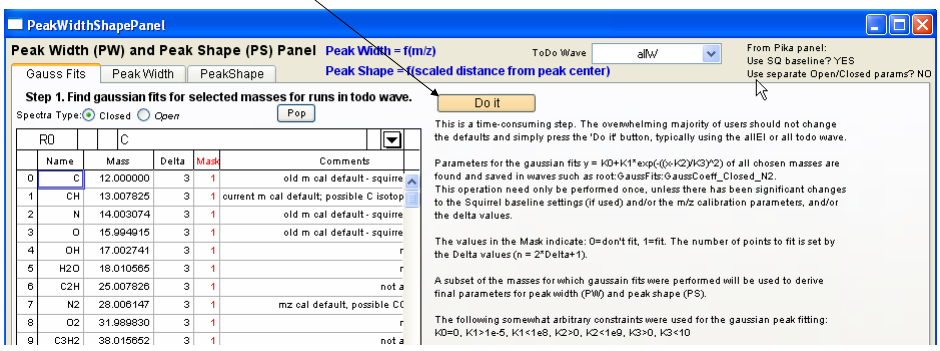
New Pika Panel - raw spectra

The decision to use raw spectra with squirrel baselines removed should be done first, so that the peak shape analysis and pika fits are performed on the same spectra.



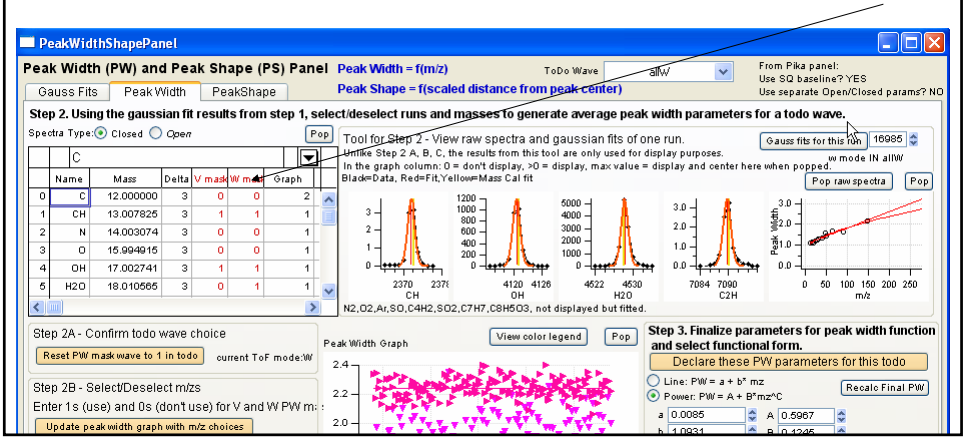
New Peak Width/Shape Panel - gauss fits

* The first step is the fitting to gaussian peaks of raw spectra. This time-consuming task is done first, and needn't be done again. The 4 parameters in y = K0 + K1*exp(-(x-K2)/K3)^2) for each run and 25 HR fragments are saved in a data folder called GaussFits.



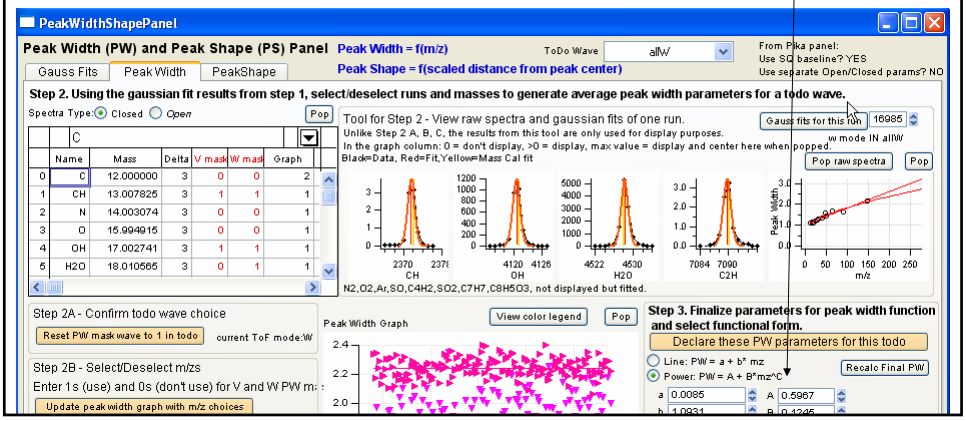
New Peak Width/Shape Panel – peak width

In the second step the user chooses which todo wave and which masses to use to generate peak width parameters. There are lots of tools to examine/add/remove masses, runs.

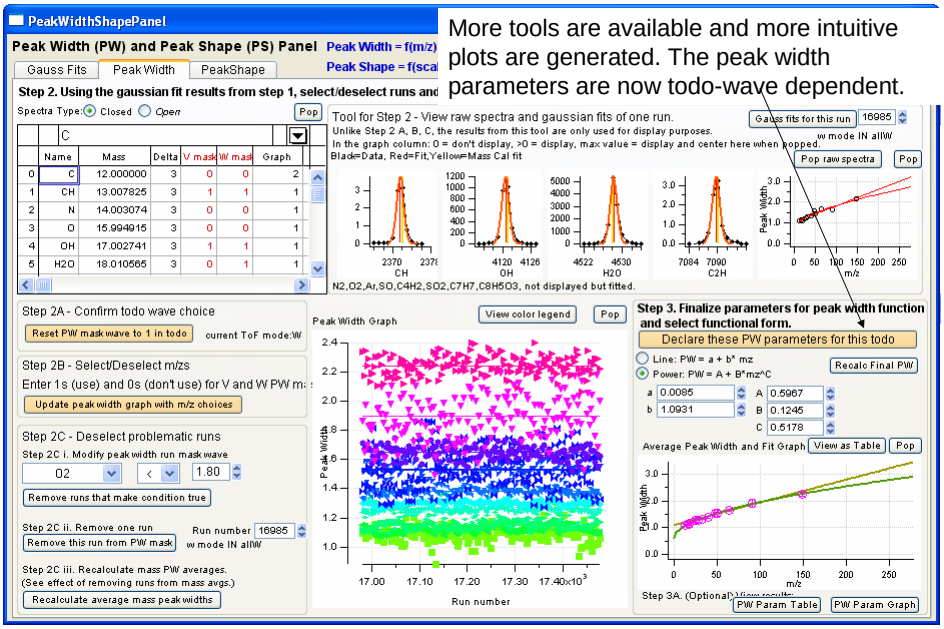


New Peak Width/Shape Panel – peak width

In the third step the user generates final parameters (slope, intercept) for V and W modes. The user now has the option to generate a fit using the power law function type.

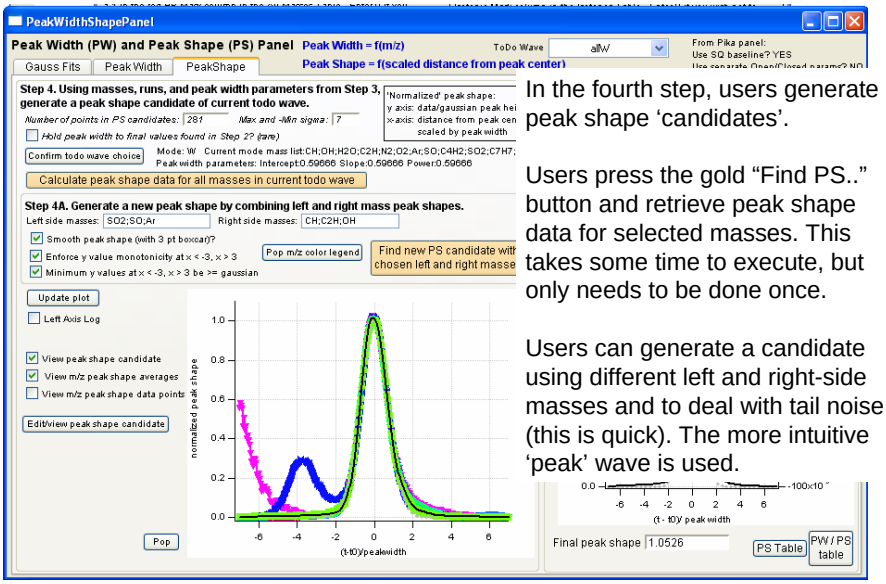


New Peak Width/Shape Panel – peak width



More tools are available and more intuitive plots are generated. The peak width parameters are now todo-wave dependent.

New Peak Width/Shape Panel – peak shape

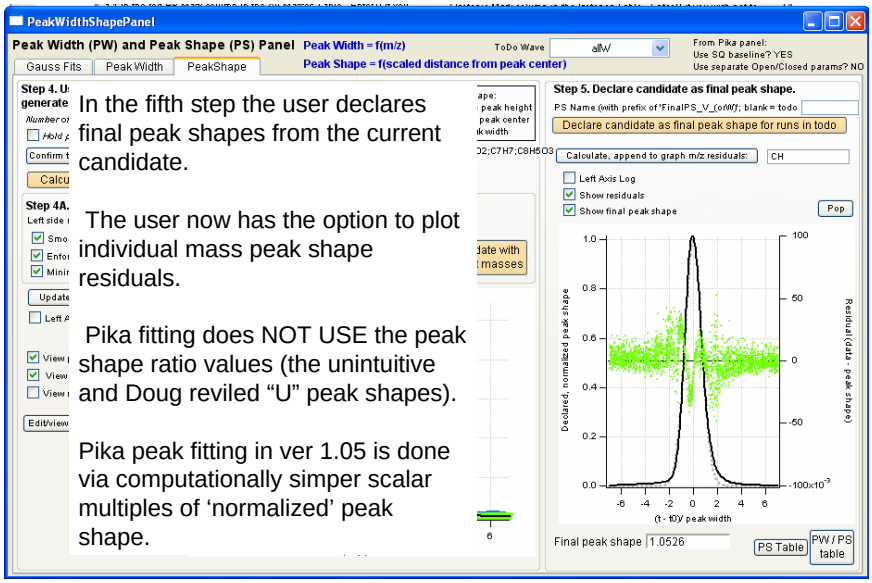


In the fourth step, users generate peak shape ‘candidates’.

Users press the gold “Find PS..” button and retrieve peak shape data for selected masses. This takes some time to execute, but only needs to be done once.

Users can generate a candidate using different left and right-side masses and to deal with tail noise (this is quick). The more intuitive ‘peak’ wave is used.

New Peak Width/Shape Panel – peak shape



In the fifth step the user declares final peak shapes from the current candidate.

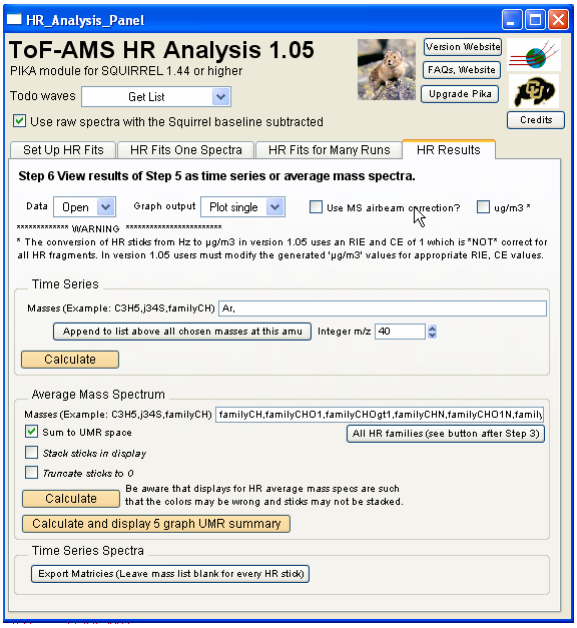
The user now has the option to plot individual mass peak shape residuals.

Pika fitting does NOT USE the peak shape ratio values (the unintuitive and Doug reviled “U” peak shapes).

Pika peak fitting in ver 1.05 is done via computationally simper scalar multiples of ‘normalized’ peak shape.

New Pika Panel - results

Users can now convert HR sticks to NO_3 eq. µg/m3 units, can generate HR average mass spectra.



Pika 1.05

Thing **not** yet incorporated, in order of importance:

* The HR frag table, batch table functionality.

* Fitting uncertainty values be plotted throughout. (Note: Fitting uncertainty is one component of several errors to sum for use in PMF)

* Better organization scheme for HR sticks. Likely scheme: organize HR sticks not by column number, but by column labels This is to prevent the necessity of redoing pika fits of all runs when a single HR fragment is added/removed from HR fragment chosen list).

* Regularly have available two sets of difference sticks – one found by pika fitting raw difference spectra (HRDiffStick), one found by the simple open – closed HR sticks (HROminusCStick).

* Mike C's tools,  tools

Pika 1.05

To use:
http://cires.colorado.edu/jimenez-group/ToFAMSResources/ToFSoftware/index.html#Analysis3

For new Pika experiments: download 1_05.pxt from the web site above.

For upgrading Pika experiments 3 issues:

(1) Igor Procedure Files (.ipfs)
- Download and import all PK_***1_05.ipfs
- Kill all old pika PK_**.ifps
- Kill and recreate the main Pika Panel.
- One does not have to update their squirrel ipfs from version 1.44 to the current 1.46, but it doesn't hurt.
- Uncheck 'Use squirrel baseline' (unless you want to redo Pika step 1)

(2) Chosen HR Mass fragments
- One does not have to update their all masses list, but it is encouraged. If no new HR fragments were identified in the old experiment, all HR mass choices (what masses to fit) and all HR fits can be retained.
- If not redoing the fits you still need to reselect them. Pika 1.05 creates new HR families and the HR family mask waves need initializing.

For upgrading Pika experiments 3 issues, cont.:

(3) Converting Peak Width and Peak Shape information

Open the new peak shape/width panel

From the command line run:
Pk_upgradePWPSfrom104(todowave, PWIntercept, PWSlope, PSwave)

where
- Todowave is the name of a todo wave (for example AllW)
- PW intercept is the numerical value (or global variable) for the PW intercept value for all runs in the chosen todo wave
- PW slope is the numerical value (or global variable) for the PW slope value for all runs in the chosen todo wave
- PS wave is the name of the todo wave that contains the Pika version 1.04 peak shape coeficients ('U'-shaped curve)

As an example:
Pk_upgradePWPSfrom104(allW, root:HR_PeakShape:PWIntercept, root:HR_PeakShape:PWSlope, root:HR_PeakShape:PeakShapeW)
A template command is at the bottom of the PK_PeakShape ipf.

*** This must be done for all peak shapes groups (each V group, each W group)