Within Pika, the compilation of uncertainties in stick calculation is under development

There are two uncertainty estimates that are somewhat easily accessible for you (as soon as you have done Pika peak fitting on a todo wave).

Uncertainty #1 “Residuals”
Uncertainties as viewed in Open, Closed, Diff from the HR_PeakHeights_gr are saved in a data set called HRResidNoiseOpen, HRResidNoiseClosed, HRResidNoiseDiff

HRResidNoiseDiff = mean (absolute value of residuals at 4 peak widths distance)
Within Pika, the compilation of uncertainties in stick calculation is under development.

Uncertainty #2 “Counting”
Uncertainties as optionally viewed in Diff from the HR_PeakHeights_gr are called HRCountErrorDiff
Formula for calculating this error is the same as for unit resolution sticks (sum of squares...)

For the difference spectra, one run, IF you have found multipeak fits for the raw difference spectra MSD, then the peak height values as calculated by the peak height of the open – peak height of closed (and it’s ‘error’) can be displayed.

To get the HR sticks for all runs (that were fit) in memory:

Go to the Pika panel, HR Results tab, Time Series Spectra section.

Leave the Mass list blank, Choose a todo wave (usually choosing all is easier in the long run, because rows = t_series).

Press the “Export Matricies” button

A 2D wave called HRMxD_sticks is put in memory.
HRMxD_sticks: rows = runs, columns = chosen HR fragment

For HR Clinic sample data set (Helsinki) I only found HR sticks for my V mode data, and the instrument was in V/W switching mode. So every other run is blank.

To get the 'Residual' uncertainties for all runs (that were fit) in memory:

Go to the Squirrel panel, Misc tab, HDF to Memory Transfer section.

Choose HRResidNoiseDiff in the Wave popup.

Choose a todo wave (usually choosing all is easier in the long run, because rows = t_series).

Press the “Dump to Memory” button

A 2D wave called HRResidNoiseDiff_d is put in memory
HRResidNoiseDiff_d : rows = runs, columns = chosen HR fragment

For HR Clinic sample data set (Helsinki) I only found HR sticks for my V mode data, and the instrument was in V/W switching mode. So every other run is blank.

To get the ‘Counting’ uncertainties for all runs (that were fit) in memory:

Two Steps:

(1) From the command line run:
squirrel_fetch(all, pk_CountingErrors, "","HROpenStick;HRClosedStick")

(2) Go to the Squirrel panel, Misc tab, HDF to Memory Transfer section.

Choose HRCountErrorDiff in the Wave popup.

Choose a todo wave (usually choosing all is easier in the long run, because rows = t_series).

Press the “Dump to Memory” button

A 2D wave called HRCountErrorDiff_d is put in memory
What are ‘Counting’ uncertainties? In Squirrel:

Sigma is one value, is defined by user in squirrel panel, ‘width of single ion’
Noise is one value, is defined by user in squirrel panel, ‘corresponds to electronic noise’
IntegrationWidthNs is wave, is squirrel stick integration region for each m/z in ns units
SI is single ion wave, in bits ns units, one value for each run
ToFPulserInHz is a wave, one value for each run, 99.99% will be constant value
samptimeClosed is the time spent in closed for each run.

Take abs value of sticks, multiply by sigma, divide by stick integration region, undo
duty cycle correction:
err_Closed =abs(MSSclosed)*sigma/samptimeClosed // for each run
err_Open=abs(MSSopen)*sigma/samptimeOpen // for each run
if (waveexists(corr_fact)) // if airbeam correction factor exists, use it
    err_Closed/=corr_fact
    err_Open/=corr_fact
endif
err_Closed*=sqrt(28/(q+1))
err_Open*=sqrt(28/(q+1))

Calc a noise error estimate in Hz-type units:
err_tmp =noise*noise*IntegrationWidthNs*28/(SI*ToFPulserInHz*m/z))

Add noise errors to sticks errors, take square root of sum of squares
err_Closed +=err_tmp
err_Open += err_tmp
err_Diff = sqrt(err_Open+err_Closed) = MSSDiff_p_err

How are ‘Counting’ uncertainties applied? In Squirrel:

Multiply the sticks error matrix by square of frag coefficients:
MSSD_all_Mat_Org_err = MSSDiff_p_err *OrgFragMatrix^2 // cross product

How are uncertainties applied? In Pika:

The ‘Residual’ nor the ‘Counting’ uncertainties do *not* incorporate an
airbeam correction. Also, the ‘Electronic Noise’ and ‘Sigma’ are hard-
coded, not user modifiable. Also, currently calculated Pika uncertainties
do include the ‘electronic noise’ error.

There is no HR frag table yet, so there is no code that ‘applies’ it to
species.