Sandia National Laboratories

Minimum Detectable Activity and Detection Limits in InterSpec

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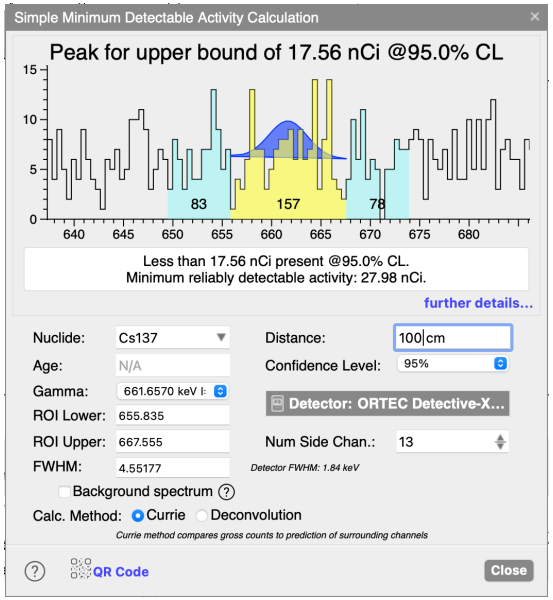
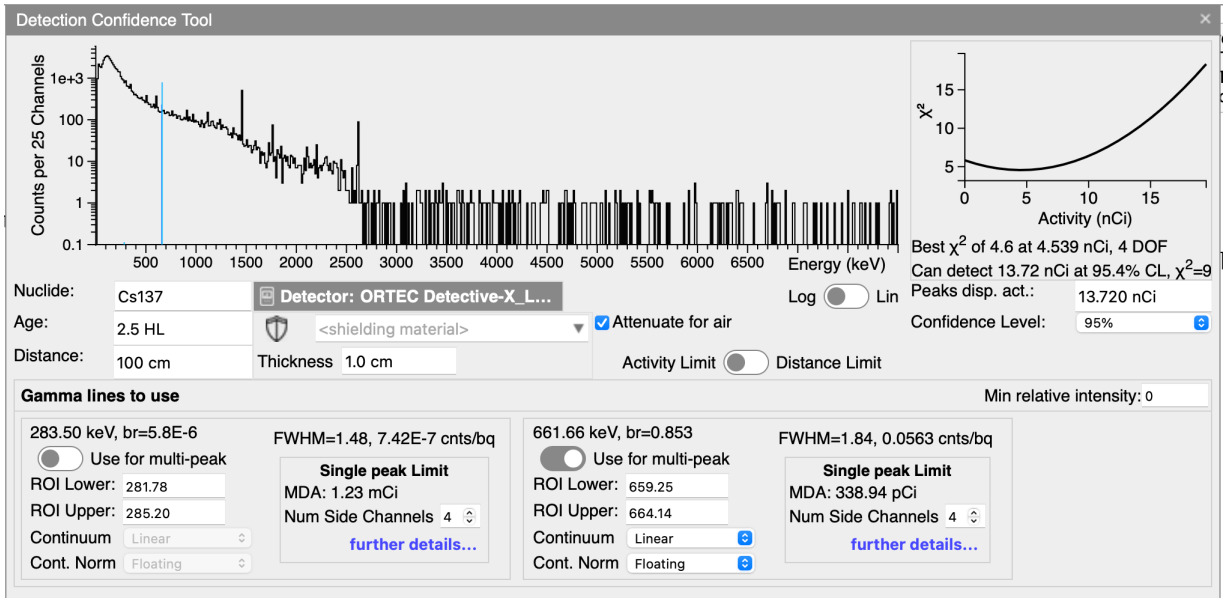
Detection limit tools in InterSpec

There are two tools in InterSpec to help place detection limits





A "simple" MDA tool:

- Single Region of Interest (ROI)
- Right-click on spectrum, at the ROI, and choose "Quick MDA..."
- Reasonable defaults

A more advanced detection limit tool

- Multiple ROIs can be used to increase sensitivity
- Place limits on activity, **or** on maximum detectable distances
- Uses a "Deconvolution" methodology, or you can get the simpler "Currie" style limits for each peak
- Under the "Tools" menu as "Detection Confidence Tool"

Some useful resources

Useful references for understanding MDA:

- CURRIE, L.A., *Limits for qualitative detection and quantitative determination*.
  https://pubs.acs.org/doi/10.1021/ac60259a007
  The original paper on detection limits – very accessible
- IAEA /AQ /48, *Determination and Interpretation of Characteristic Limits for Radioactivity Measurements*
  https://www-pub.iaea.org/MTCD/Publications/PDF/AQ-48_web.pdf
  Very in-depth, with lots of examples
- ISO 11929-1:2019, ISO 11929-3:2019, ISO 11929-4:2020
  Paid specifications – in practice AQ48 is probably sufficient
- P.A. Zyla et al. (Particle Data Group), *Prog. Theor. Exp. Phys. 2020, 083C01*
  https://pdg.lbl.gov
  Doesn't directly address gamma spectroscopy, but has more general and advanced statistical concepts. The "Deconvolution" methodology in InterSpec derived from this reference, although the ISO specification does include something similar.

Obtaining InterSpec with these tools

- Available as of v1.0.13, or June 2024 in the “bleeding edge” build of InterSpec
  - https://github.com/sandialabs/InterSpec/releases/tag/bleeding-edge
  - This is an automated build that is updated every time new code is pushed to github
  - Both tools are currently very “alpha” – so use with caution

Limit methods

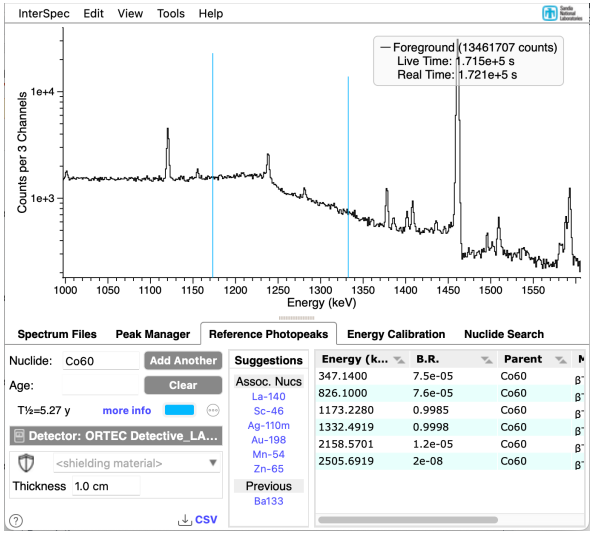
InterSpec offers two methods to compute limits:

- Currie Limit:
  - Standard single peak calculation that uses the gross-counts in a energy region of interest (ROI), and compares it to what would be predicted by a few channels on either side of the ROI
- Deconvolution:
  - Uses peak shape information, and can use multiple peaks to place better limits
  - At a given activity/shielding/distance, the peak(s) are compared to data to generate a χ^2 value. The most likely value of activity or distance is found, and then that quantity is varied until the χ^2 changes an amount corresponding to desired confidence level (CL)

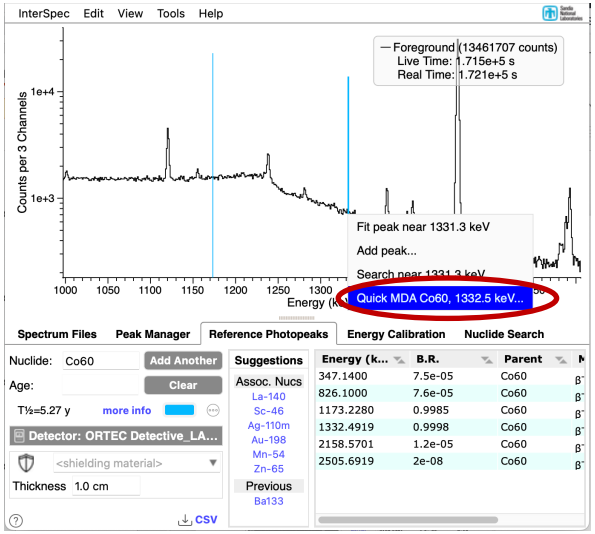
“Simple” MDA Method

Using the Simple detection limit tool

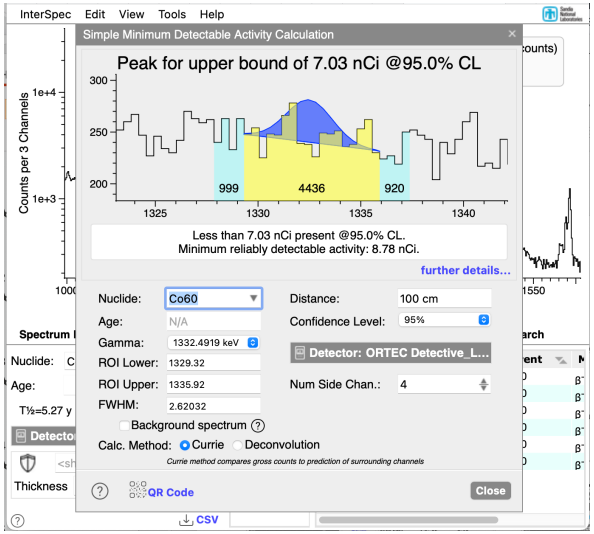
To use:



1) Load spectrum, and optionally show reference lines

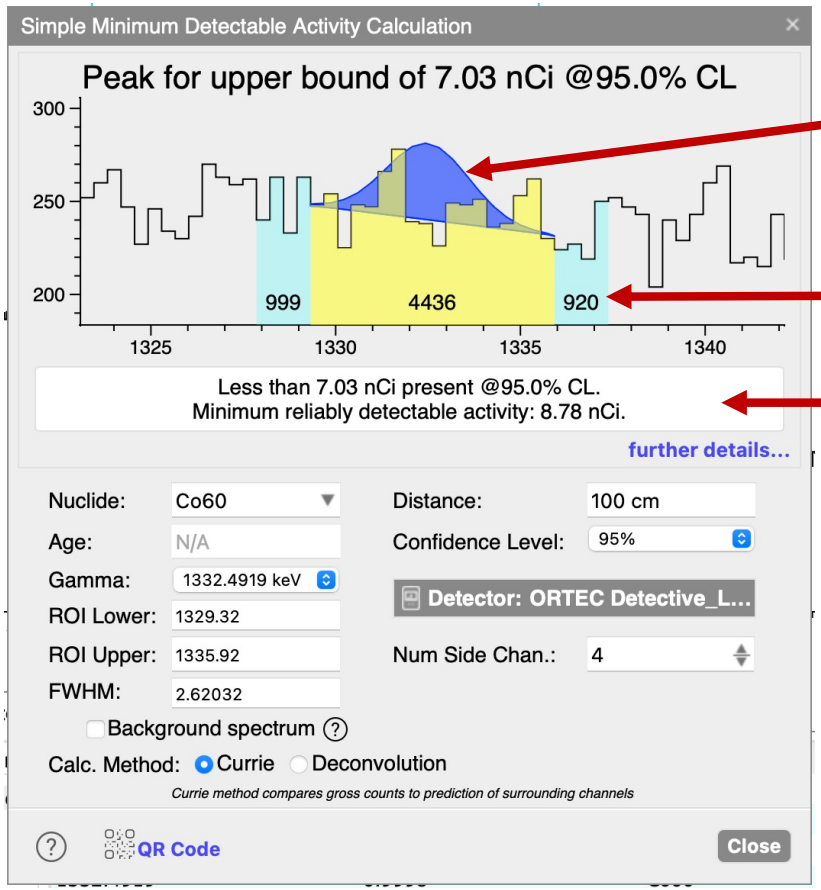


2) Right-click on the spectrum near the energy of interest. (but not near a peak. Select “Quick MDA…” option.



3) Input distance, and optionally adjust other options.

Using the simple detection limit tool – brief result explanation

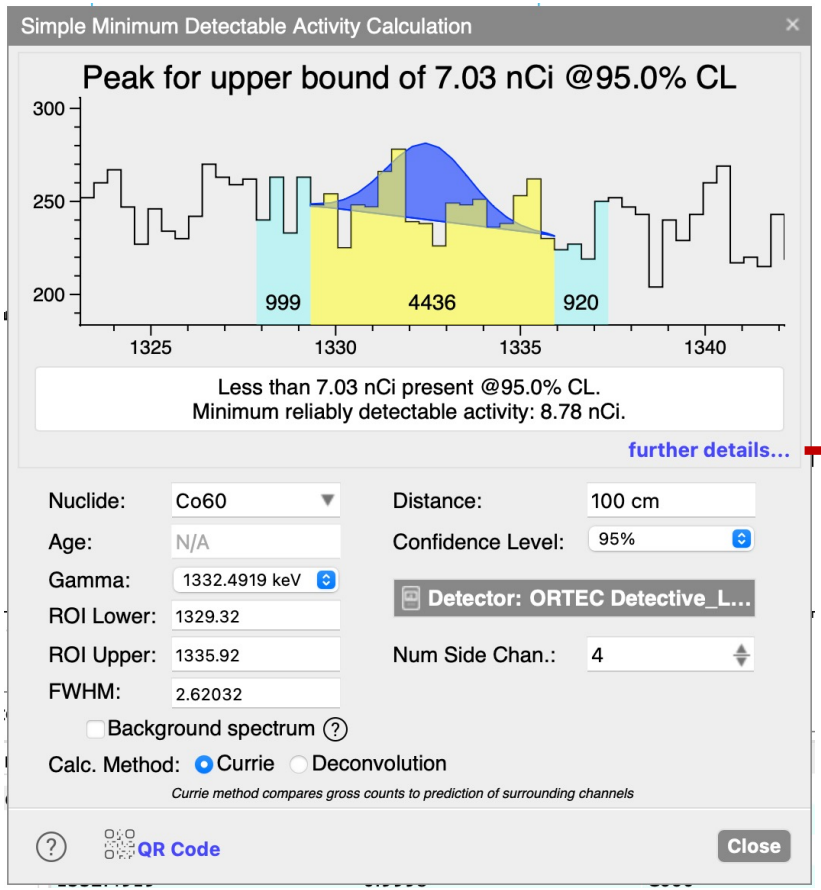


The displayed peak is plotted at the amplitude of the limit, to give you a visual sanity check on the limit

Counts of the data areas are given on chart

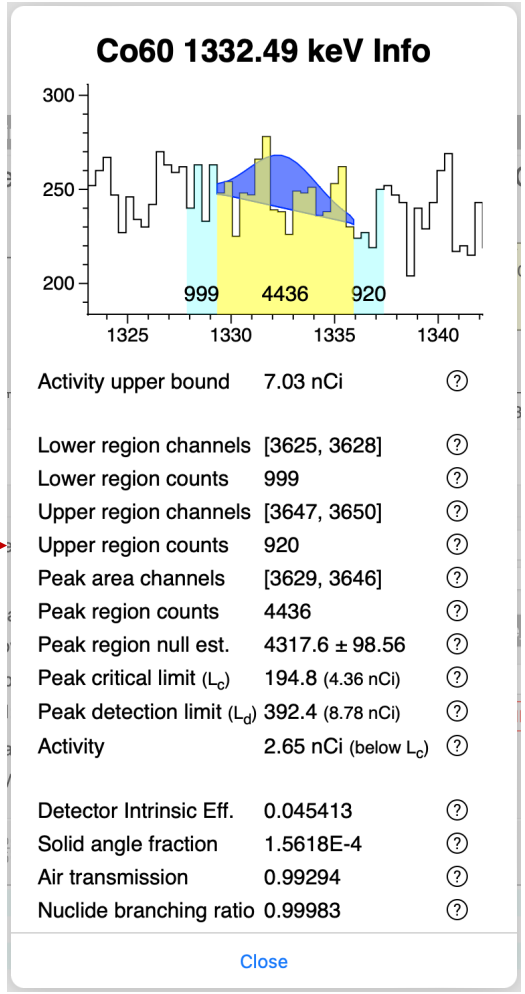
The result text tries to give plain-language explanation (for those of us that forget the domain-specific terminology)

Using the Simple MDA tool – further details



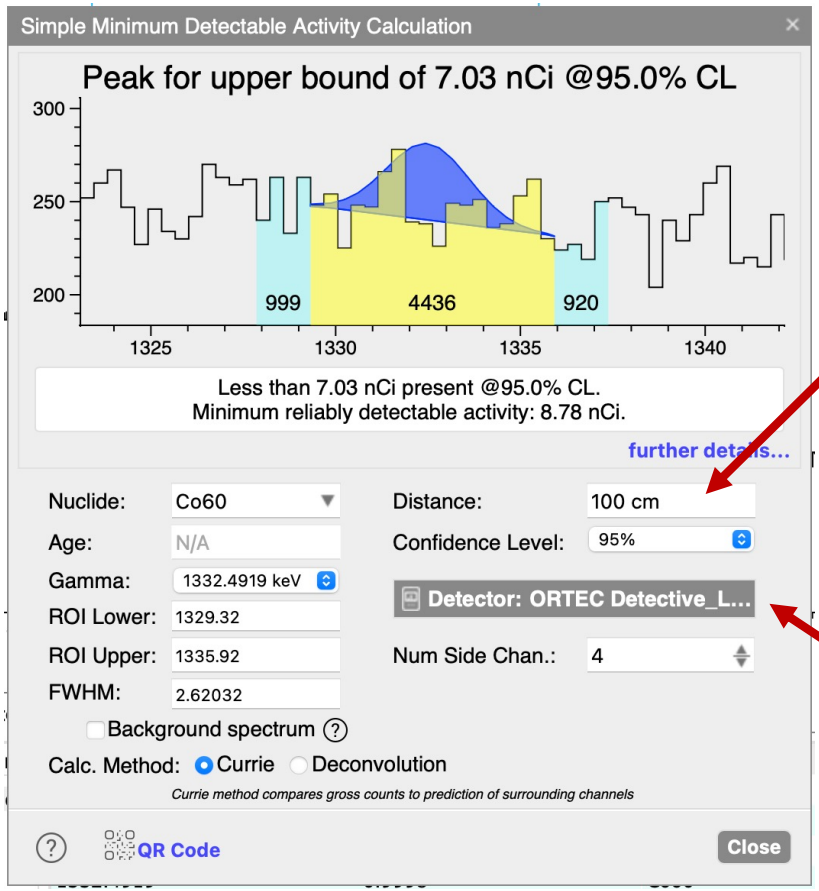
The "further details..." link gives you all the information that leads to the limit.

Hovering the mouse over the ⓘ icons gives further explanation of each quantity



Using the Simple MDA tool – necessary inputs

At a minimum, you will need to input the distance, and make sure you have a detector efficiency selected



You will need to input the distance you care about

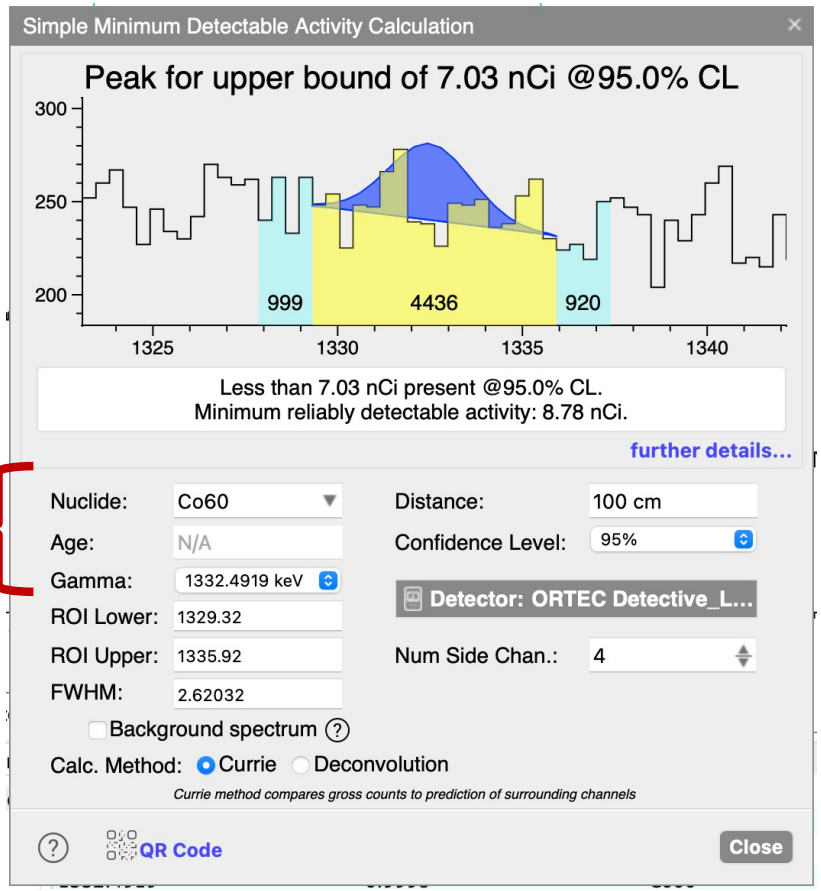
Most other settings are usually reasonable

If you need, you can also change your detector efficiency function by clicking here

Using the Simple MDA tool – selecting nuclide and gamma

Inputting nuclide, gamma, and nuclide age is similar to other places in InterSpec

If you were showing reference photopeak lines, nuclide and gamma will be filled out – if not, you can change

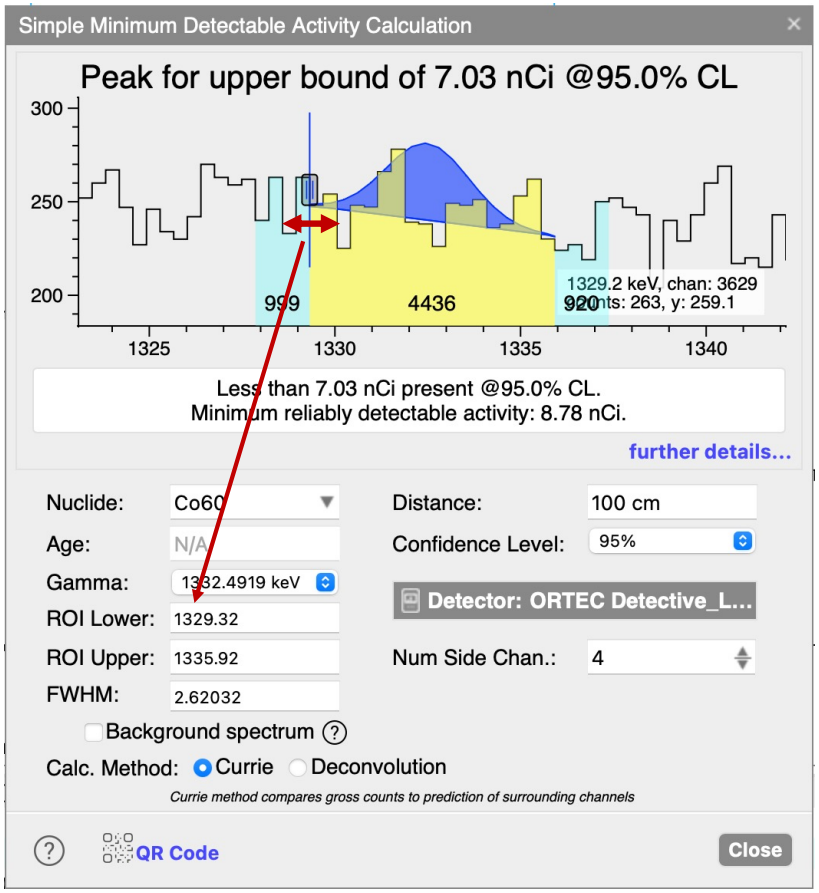


Selecting different gammas will update the ROI limits, centering the ROI on the selected gamma.

However, all gammas from the nuclide in the ROI will be used to compute expected contribution, and thus be accounted for

Using the Simple MDA tool – adjusting Region of Interest

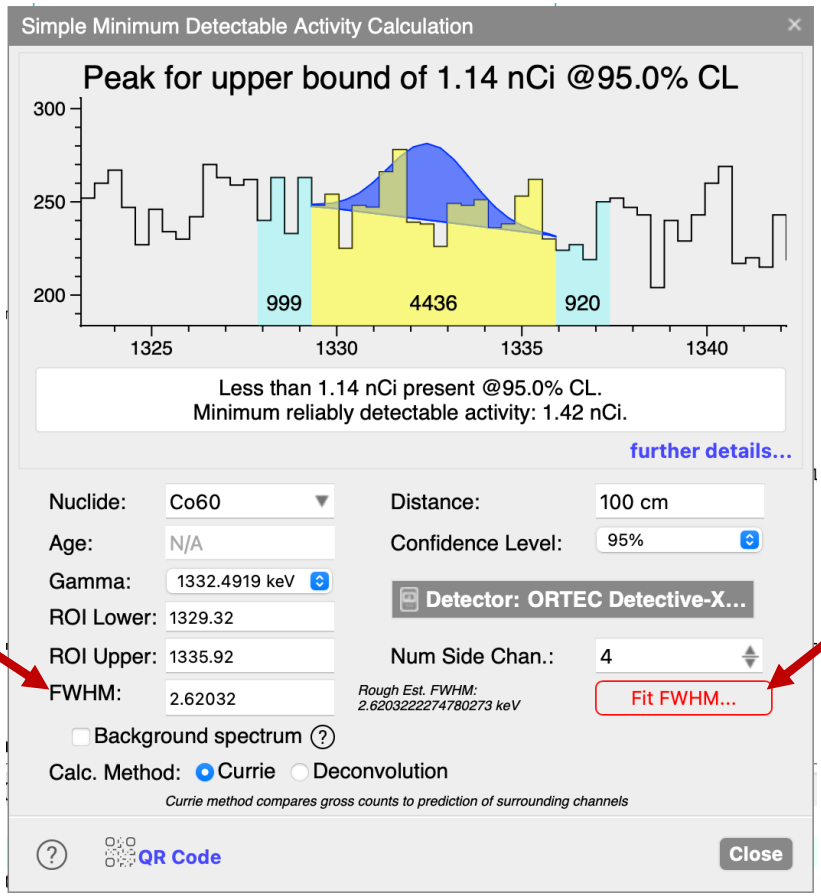
You can adjust the ROI lower and upper bounds by either typing in numbers, or by using the mouse and hovering over the edge of the ROI like normally on the spectrum



Using the Simple MDA tool - FWHM

For Currie method, FWHM is used to estimate ROI width – for Deconvolution it is integral to the calculation

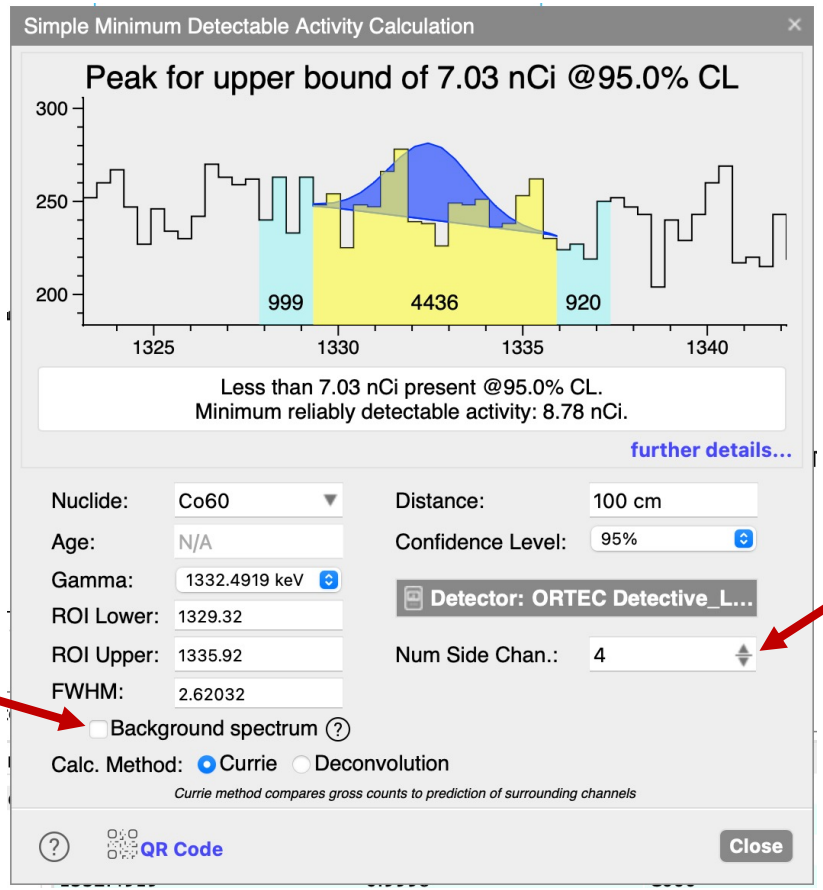
By default, the FWHM is derived from the currently loaded detector efficiency function, if it has that info – otherwise a reasonable guess is used.



If no FWHM is available, an option to fit the functional form from the current spectrum will appear

Using the Simple MDA tool – background estimation options

If you know there is no signal in the spectrum, then you can select ”Background spectrum”. This will use only the ROI channels – and no side channels – to derive the limit.
If selected, the side channel option will be hidden

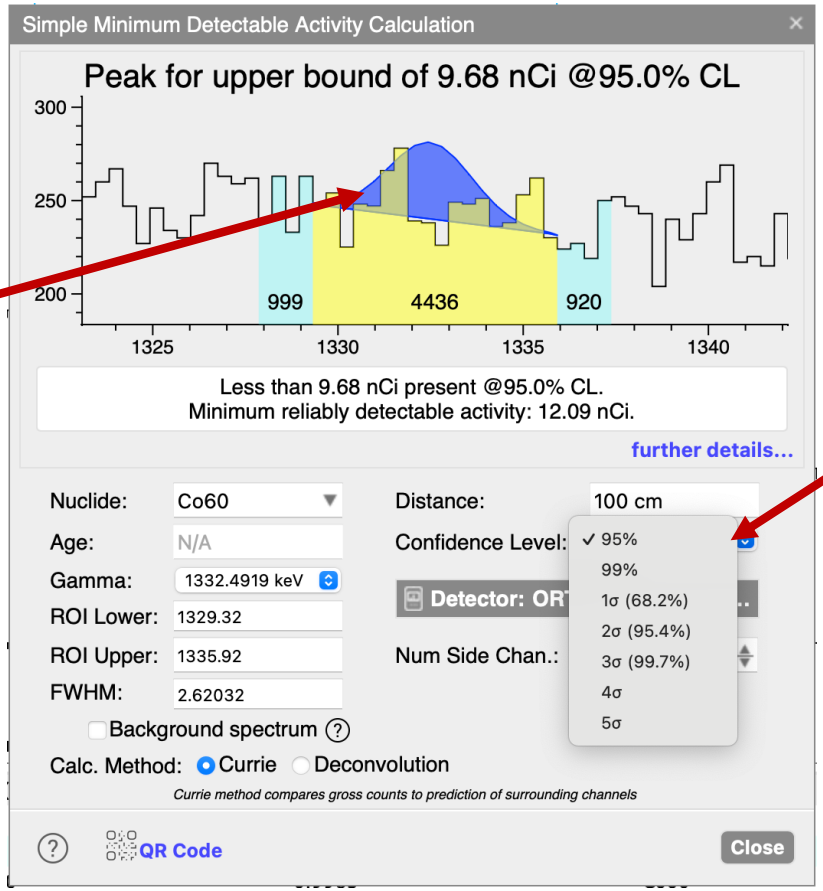


You can select the number of side channels to use to estimate the expected counts in ROI – more channels will decrease uncertainty, improving limits, but may then cause a bias by picking up features in the spectrum

Using the Simple MDA tool – Confidence Level

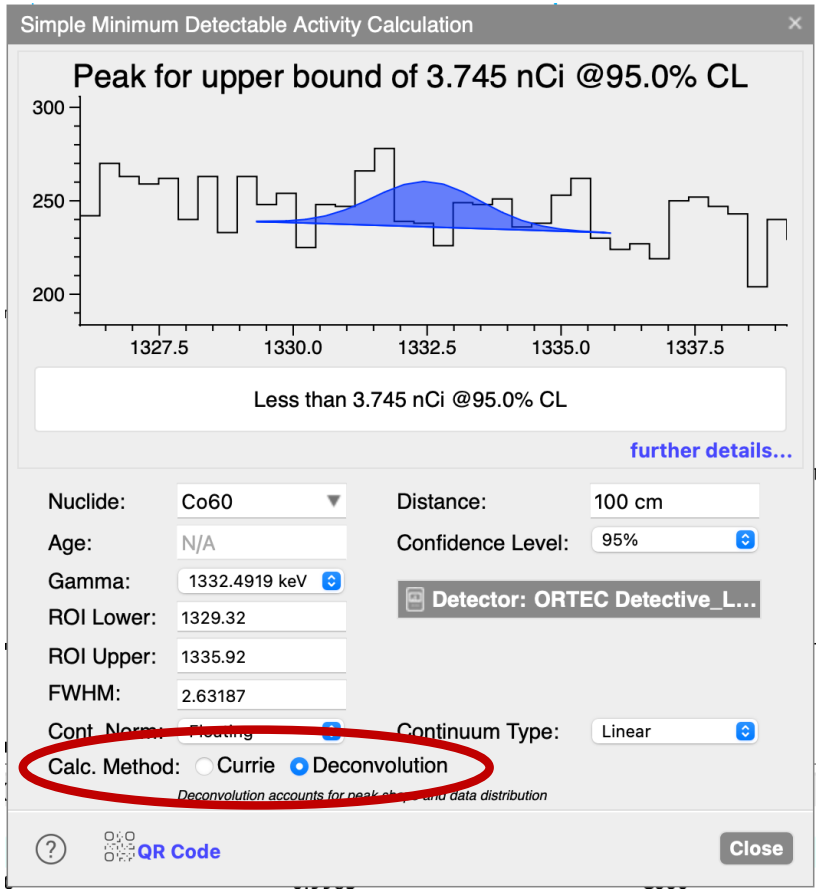
Although reporting at 95% C.L. is common, you may wish to select different C.L.s to find the level at which the plotted peak gives you confidence , that it is not there. E.g. 99% C.L.

The shown peak is the amplitude expected, for the given limit C.L. – judgement “by eye” is perhaps as important as a given numerical C.L.



You can select the confidence level you would like here

Using the Simple MDA tool – Calculation method



Two method for computing limits are offered:

1. **Currie**: default, and most commonly used method. The counts expected in the ROI is estimated using neighboring channels. This value is compared against observed counts, and simple Poisson statistics are used to quote limits. Simple and robust.

2. **Deconvolution**: Shape of the peak, and data, are taken into account, by scanning over activities and calculating χ^2 of the fit peak at each activity. Limits are quoted based on deviation from the best χ^2.
   This method often results in higher sensitivities, but given the higher implementation complexity, it is not as widely used*.

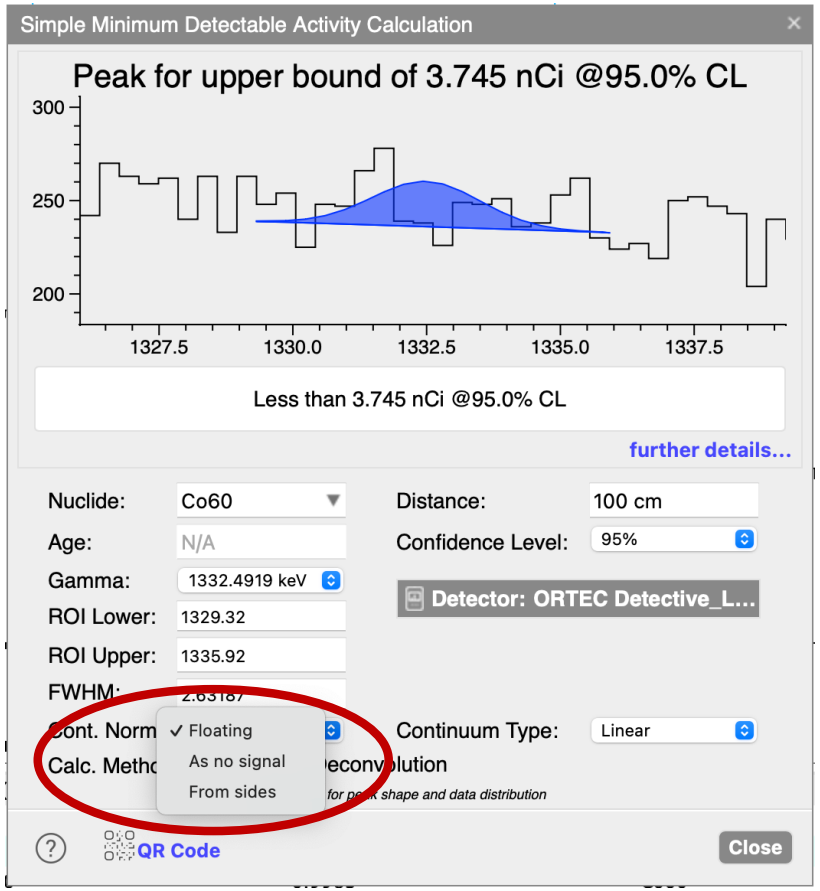
*This method, or something very similar, is specified in ISO-11929 but the InterSpec author is not aware of any other gamma spectroscopy programs that implements this methodology for comparison

Using the Simple MDA tool – Deconvolution continuum norm

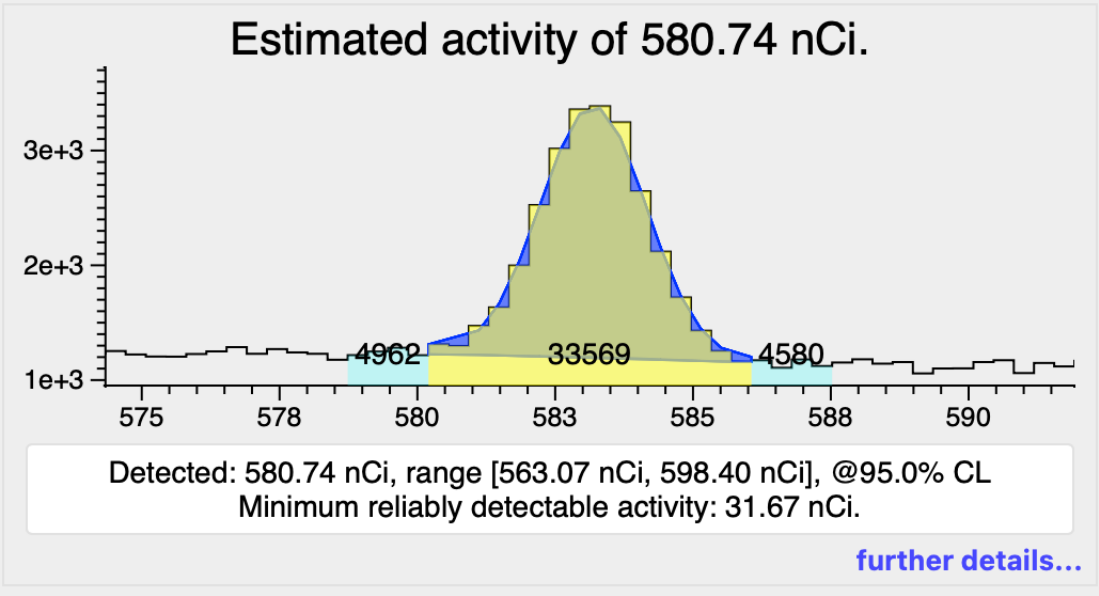
The primary additional option Deconvolution style continuum is “Cont. Norm.” method.

When scanning activities, to compute χ^2, this option lets you select how the peak should be normalized to the data:

1. **Floating**: At a specific activity, the Gaussian + Polynomial continuum is fit to determine best χ^2. Most conservative and default option – if no signal present, then continuum will be pushed a little below data by the Gaussian.
2. **As no signal**: This option asserts no signal is present, so the polynomial continuum is first fit to the data in the ROI, then the Gaussian is added to that line, and finally the χ^2 computed.
3. **From sides**: channels adjacent to ROI are used to estimate the straight-line continuum; Gaussian is added on top of this, then χ^2 computed.



Using the Simple MDA tool – signal present



If signal is detected, the nominal activity is provided, as well as range at the desired C.L.

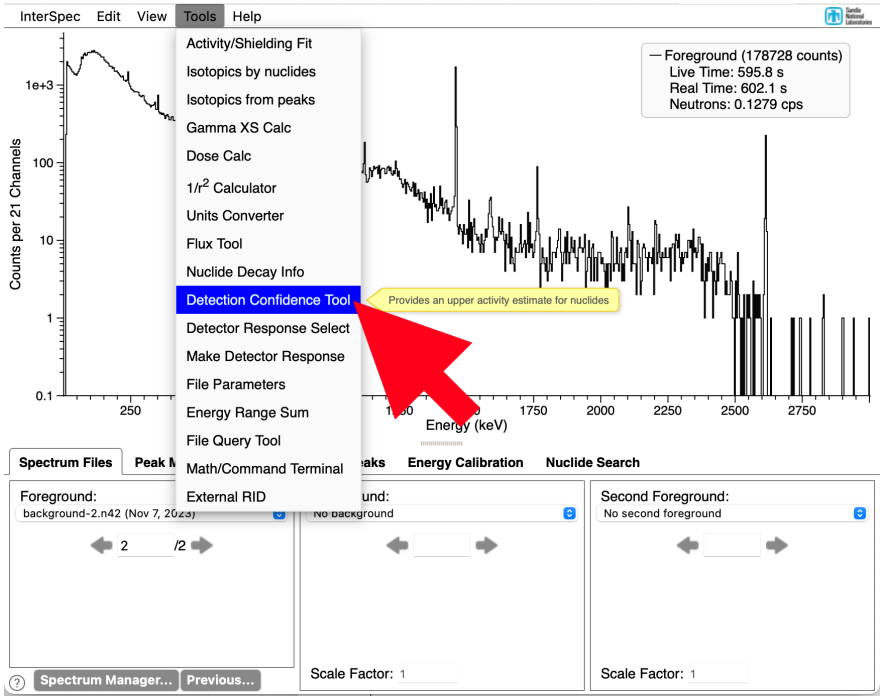
- Only statistical uncertainties are taken into account – e.g., no energy calibration, detector efficiency, FWHM, distance, etc uncertainties are taken into account

“Advanced” detection limits tool

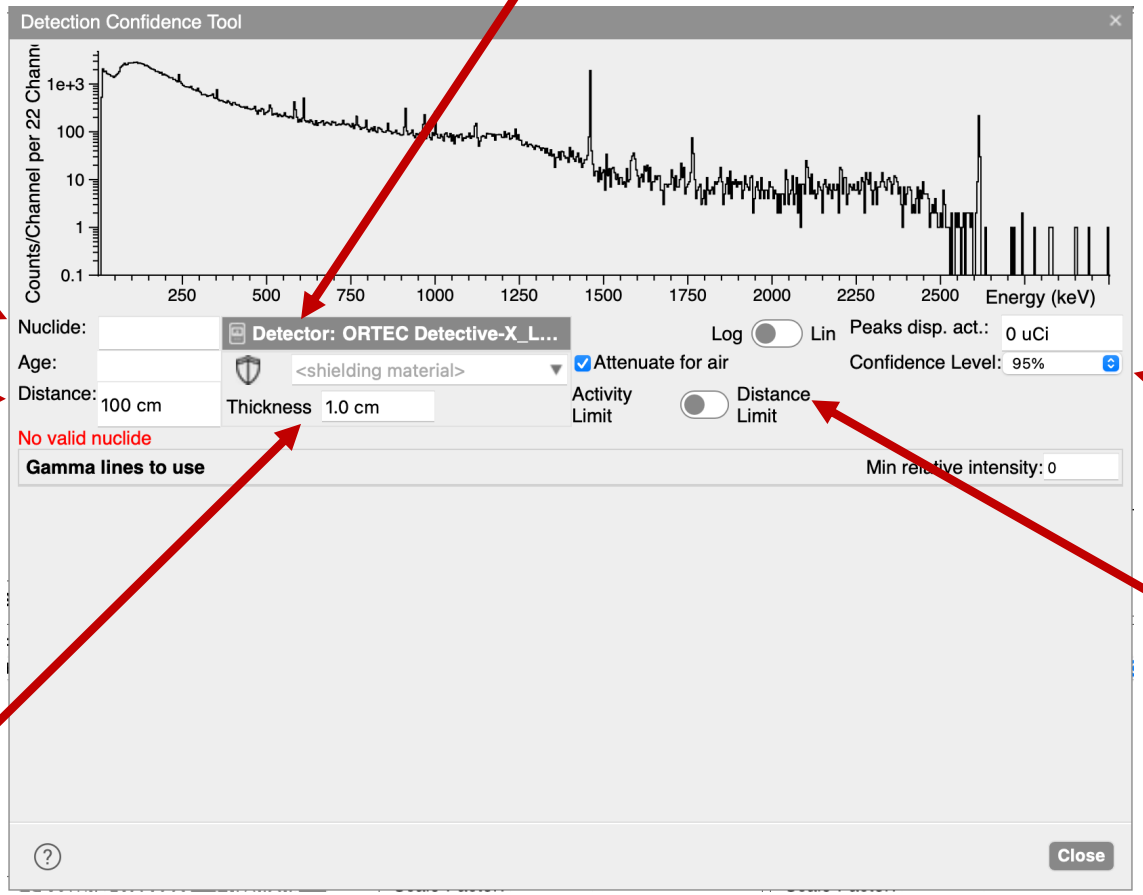
Using this tool is a bit more involved, but also more flexible

The “advanced” tool

- Can place limit on either activity or distance
- Can use multiple ROIs to increase sensitivity
- Can include shielding
- To use:
  - For detection limits, open a representative background, or at least a spectrum without the signal present
  - To place activity or distance limits, use spectrum file with signal present
- “Tools” → “Detection Confidence Tool”



Enter information



Select detector efficiency function by clicking here

Nuclide of interest

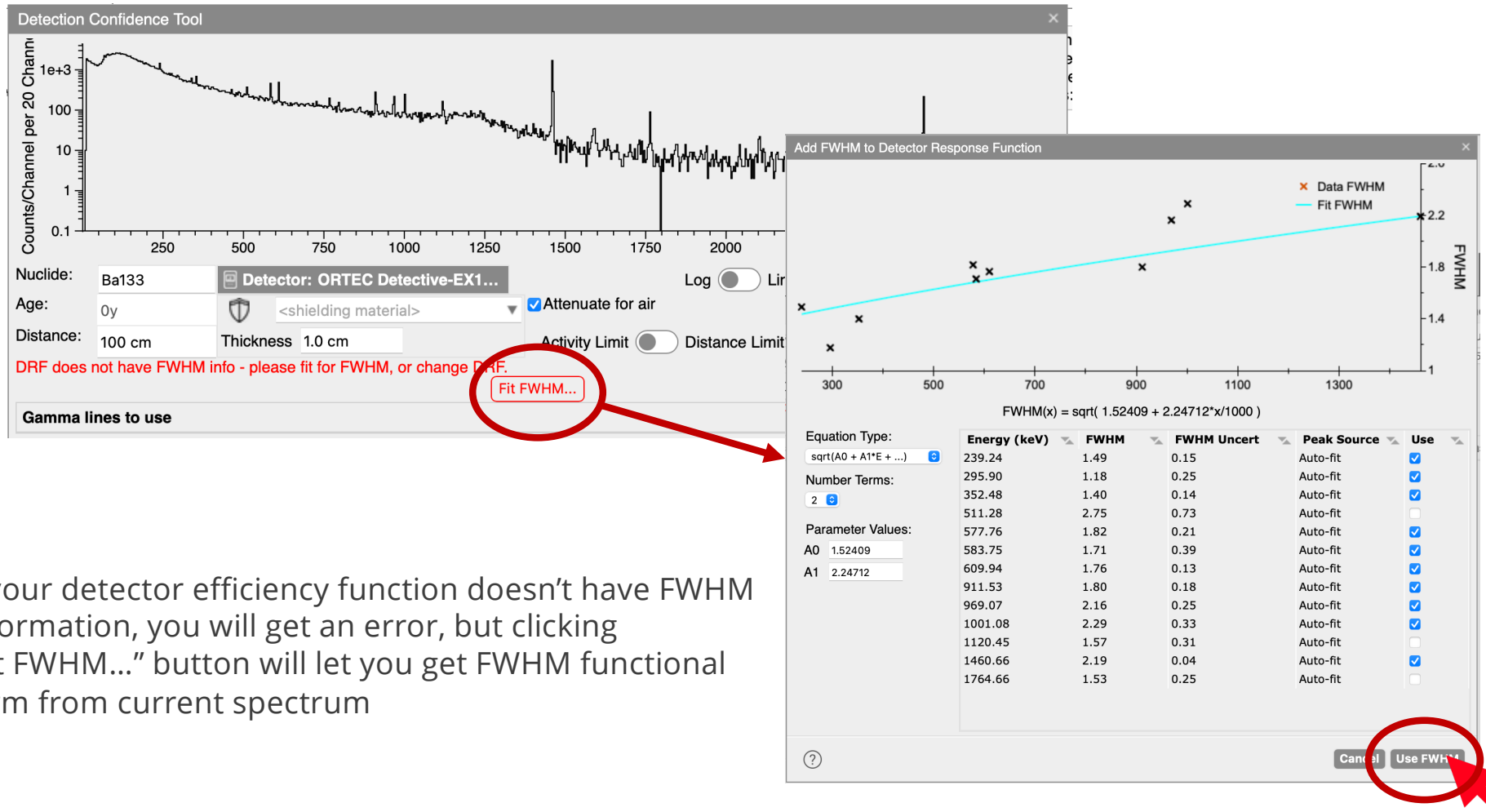
Distance

Confidence Level you want

Select if you want activity or distance limit

Add some shielding, if you want

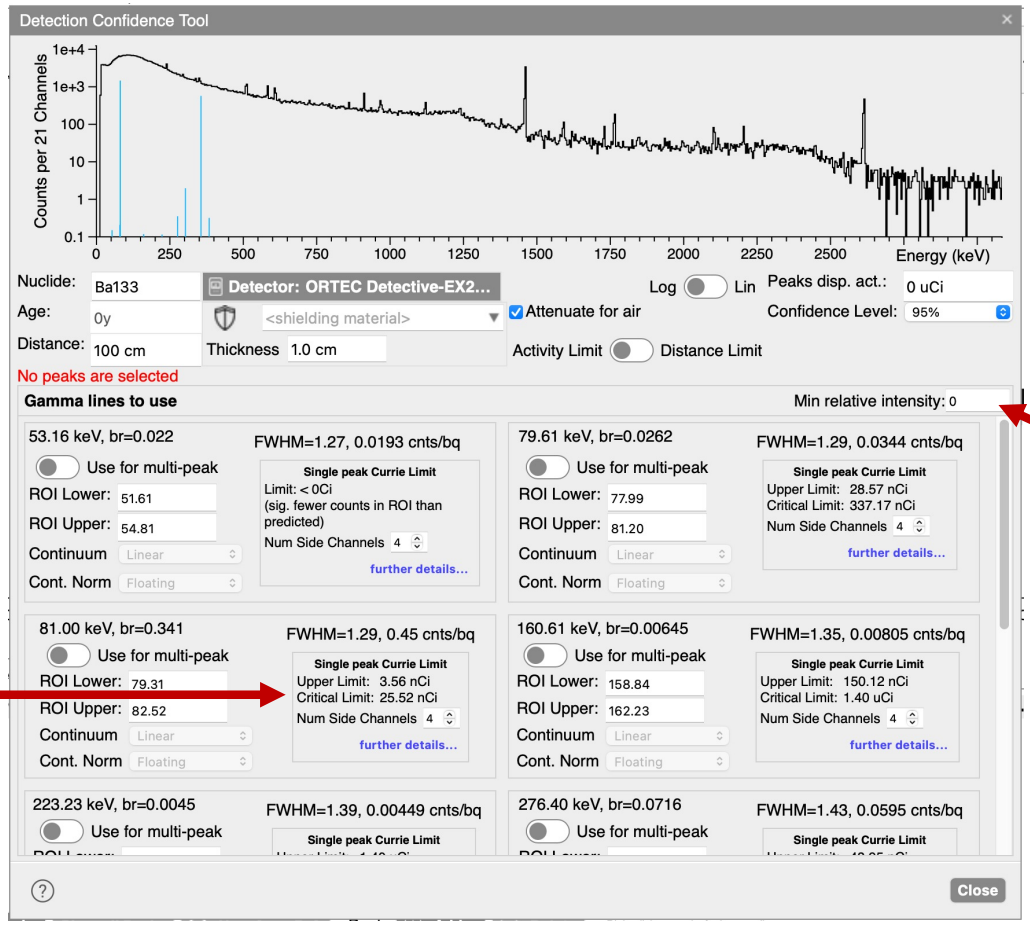
FWHM Response



If your detector efficiency function doesn't have FWHM information, you will get an error, but clicking "Fit FWHM…" button will let you get FWHM functional form from current spectrum

Selecting peaks to use

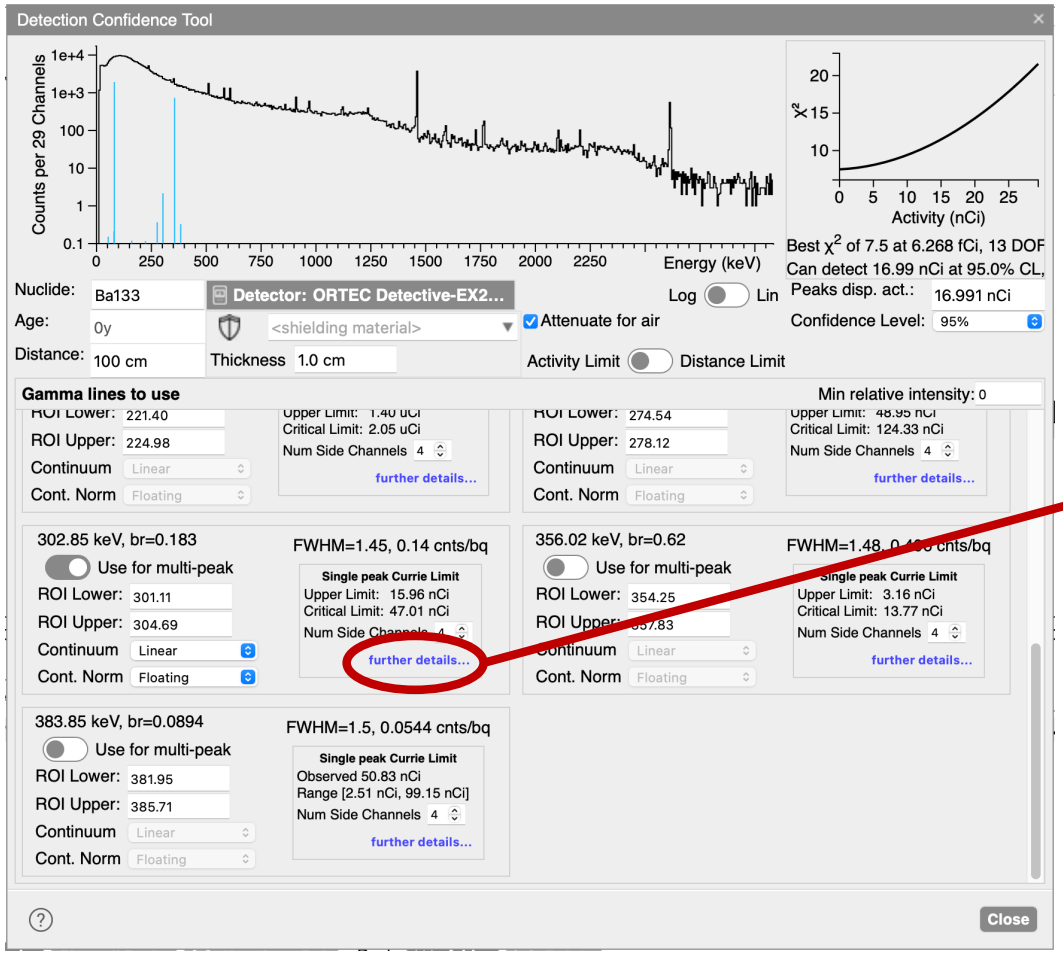
Once you have entered a nuclide and selected a DRF, you will be presented with all gammas for that nuclides decay chain

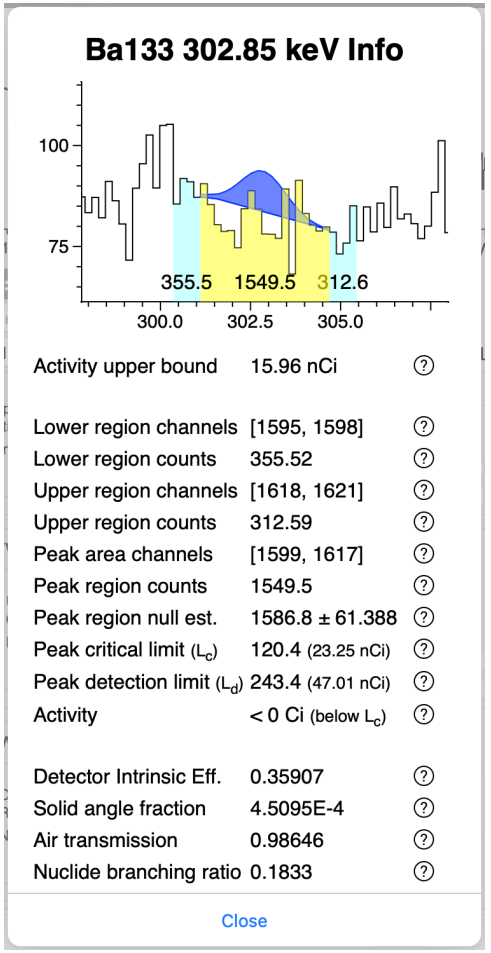


The Currie-style limits are computed for each peak

Too many peaks? Filter here

More information on Currie Limit counts



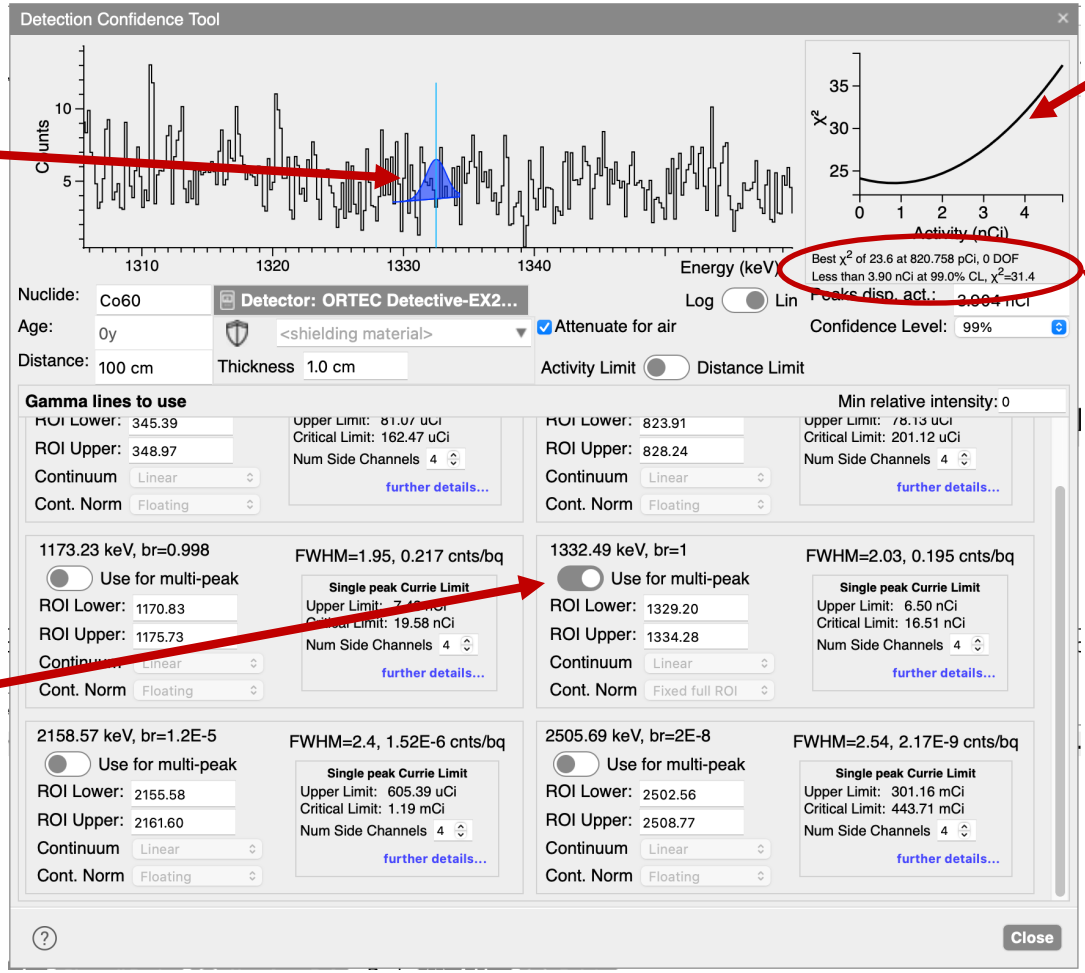


(same information as the “simple” tools “further details...”)

Using a peak with “deconvolution” style limit

Peaks being used will be plotted on chart (by default, at limit)

To use a peak for the deconvolution style limit, toggle the sliders

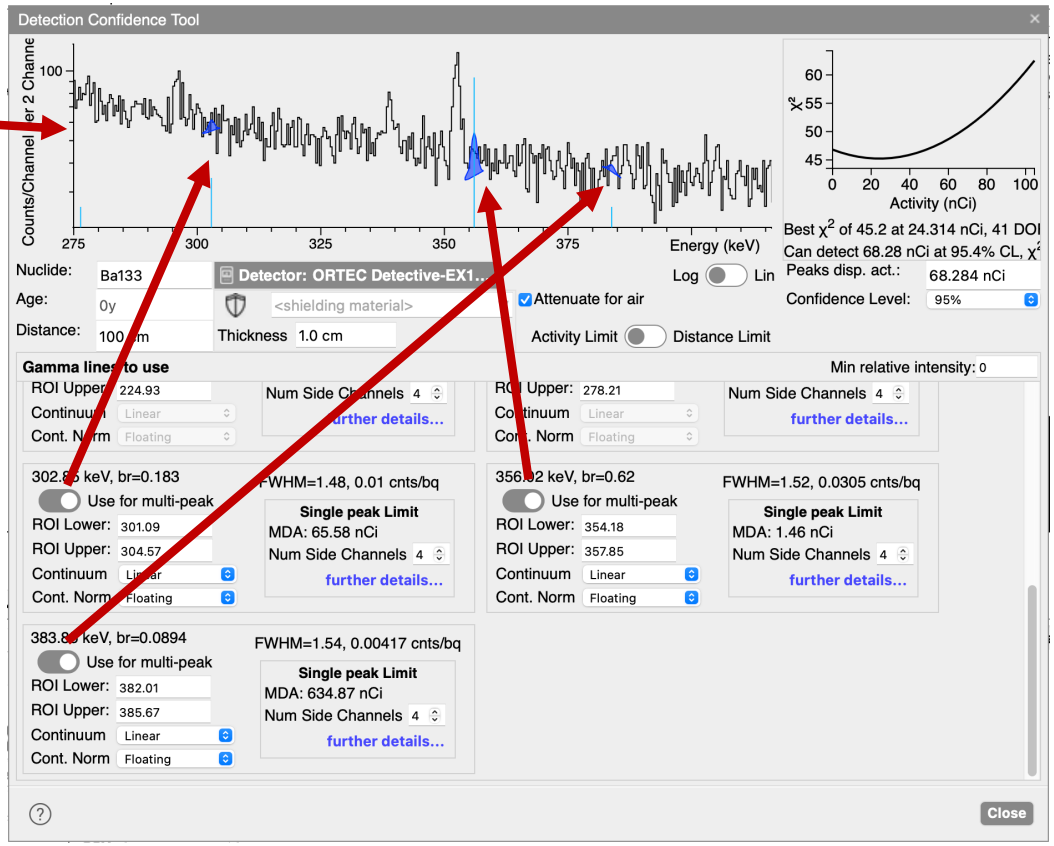


A χ^2 chart, as a function of energy or distance will appear

Limit, or range to desired CL is given here.
This is your answer from deconvolution method
If signal is detected as present, you will get a nominal activity and range.
If null-hypothesis is not excluded at given CL, then an upper limit is given

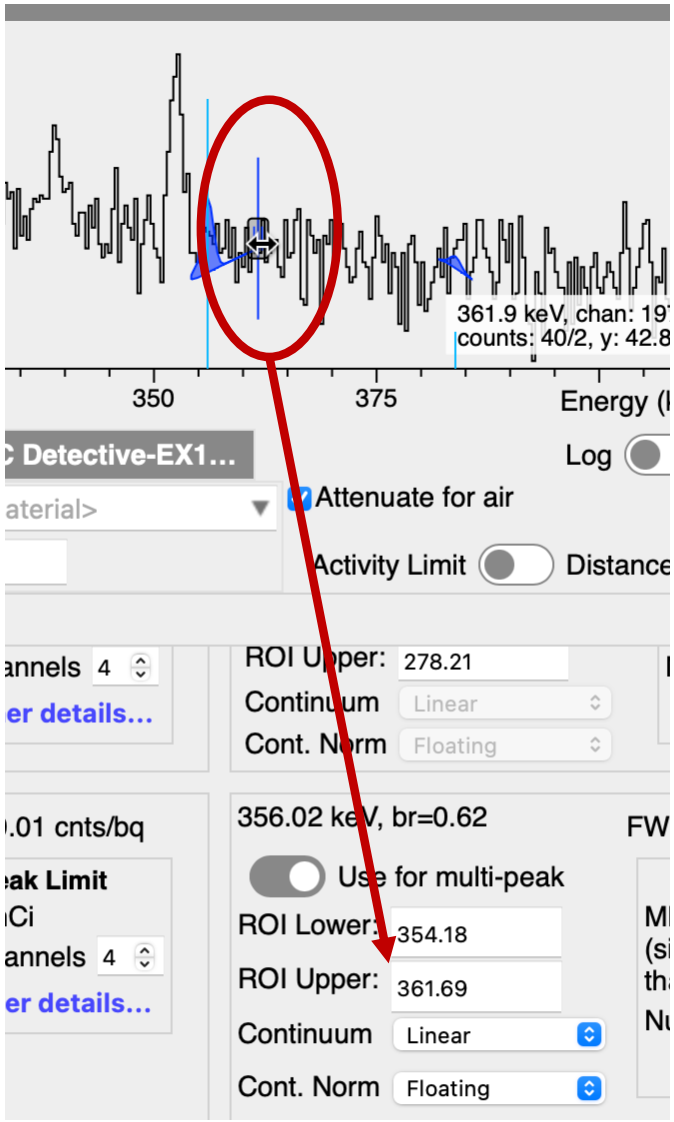
Using multiple peaks (may!) help sensitivity

You can zoom in/out on this spectrum the same as the primary spectrum in InterSpec



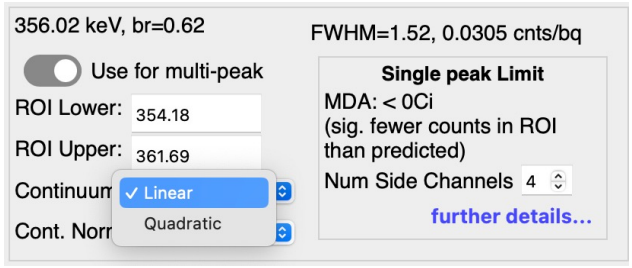
Deconvolution options

You can use the mouse at the edge of a ROI to adjust width,
Or you can type in numbers

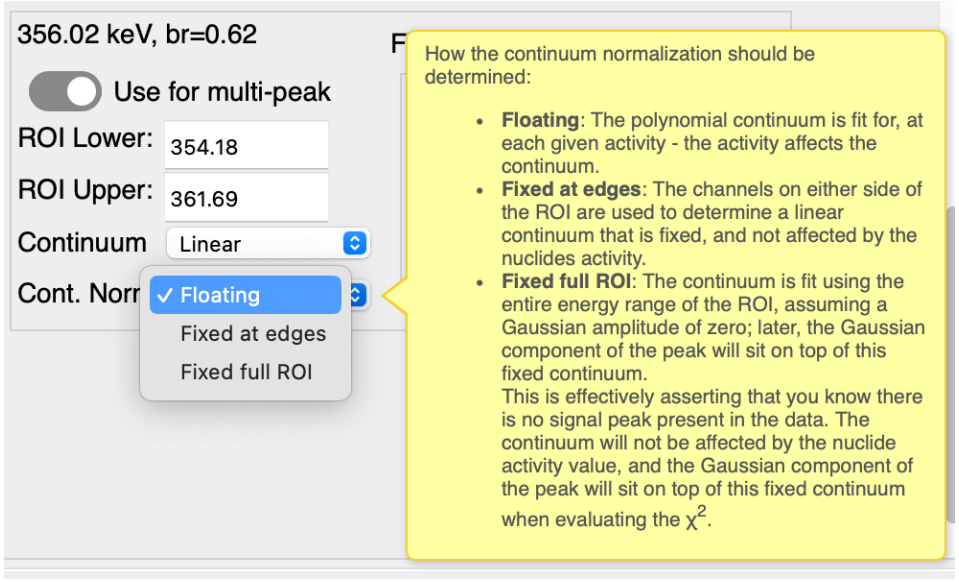


Deconvolution options (cont)

Peaks can use linear or quadratic continuums

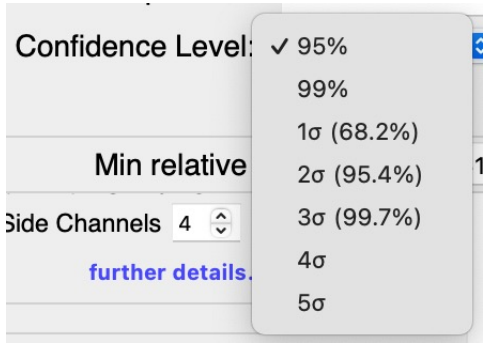


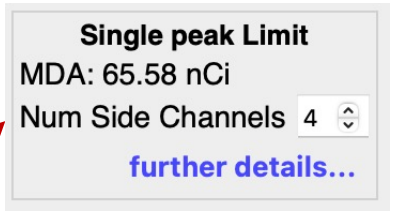
You can also choose how the continuum is normalized. Essentially asserting if you don't know if signal is in spectrum or not, or asserting you know it is not



More options:

You can select the confidence level you want. This applies to both deconvolution and Currie methods
(99% seems to correspond to my "by eye" limit)





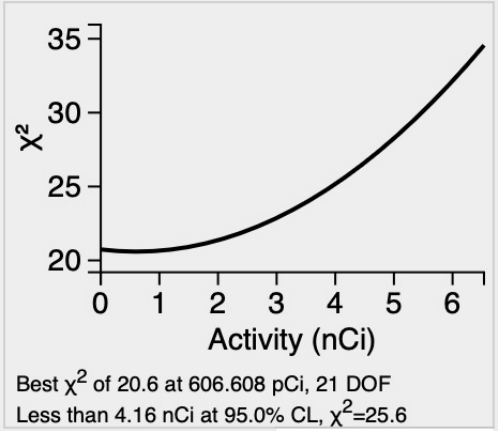
The number of side channels is used for Currie limit, and it's the number of channels, on each side of the ROI, used to estimate expected counts in ROI

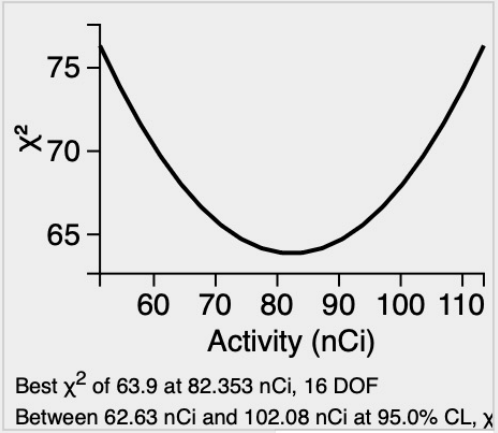
By default peaks are displayed on the chart at the limit (if no signal present), or at nominal activity/distance (if present) – but you can change this to quickly get an idea of what different values look like

Sometimes you want to know how far away you can detect a source at, or how far away a detected source is – this toggle lets you do that
(but you need to know activity and shielding)

The χ^2 chart:

The χ^2 chart gives you an idea of the likelihood as a function of activity or distance





If the χ^2 is not smooth (i.e., discontinuities, irregular shapes, etc), results are not trustable

- This is rare, but can happen if (some of) the peak(s) are near a feature in the spectrum – adjusting ROI, or using different energies will likely fix

Caveats

These tools have only been tested and used a minimal amount; they were developed an hour here and there over a few years – so there is likely bugs, and even logic issues that could lead to incorrect answers being given – please use with caution.

Besides for this Power Point, the only other documentation for the tool can be found at:

https://github.com/sandialabs/InterSpec/blob/master/InterSpec/DetectionLimitCalc.h

Future features

- Ability to scale measurement time (e.g., use 30 minute background to predict sensitivity of 5 minute measurement)
- Take into account uncertainties in energy calibration, distance, detector efficiency, and shielding
- The Deconvolution method does not currently give the critical detection limit (i.e., the activity above which signal will be reliable recognized as “detected”)
- Improvements to the UX of the advanced tool
- Comparisons to other tools
- Further validation and testing

References used in creating tool

- Determination and Interpretation of Characteristic Limits for Radioactivity Measurements, IAEA /AQ /48, https://www-pub.iaea.org/MTCD/Publications/PDF/AQ-48_web.pdf
- ISO 11929, 1 through 4, (2019, 2020) https://www.iso.org/standard/69579.html (IAEA/AQ/48 effectively covers these standards)
- The Particle Data Groups references on statistics and probability – primarily for development of the deconvolution calculations https://pdg.lbl.gov/2021/reviews/rpp2021-rev-probability.pdf https://pdg.lbl.gov/2021/reviews/rpp2021-rev-statistics.pdf