InterSpec Familiarization

Will Johnson – wcjohns@sandia.gov

20220420

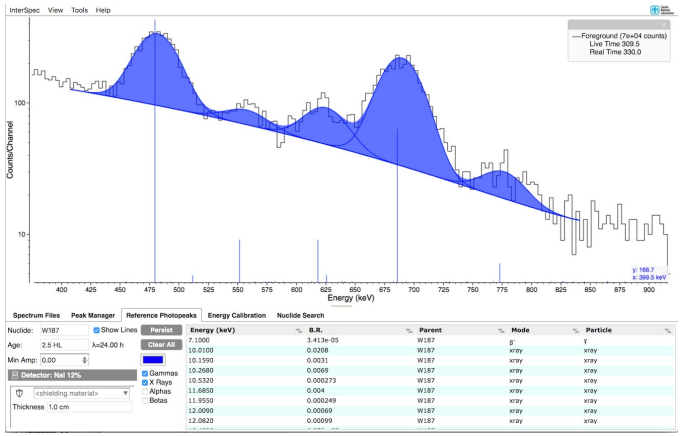
Help/Support: InterSpec@sandia.gov

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

SAND2022-4588 TR

Todays goals:

- Get you comfortable with opening and viewing spectrum files in InterSpec
- Get you familiar with basic peak-fitting, nuclide ID, energy calibration
- Have you be able to fit activity and shielding for a spectrum



Please work-along, or tinker around with InterSpec as we go along today

The example spectrum files at https://sandialabs.github.io/InterSpec/tutorials/

Some general information

This presentation uses InterSpec v1.0.10_rc3, but v1.0.9 is acceptable

- Windows, Linux, macOS: http://github.com/sandialabs/InterSpec/releases/
  - Windows Install: unzip downloaded file, and place resulting directory where ever you would like (e.x., C:\Program Files\InterSpec); manually pin to start-menu and associate file-types
- iPhone, iPad, Android, macOS: search the app-store for ”InterSpec”

InterSpec is completely open-source (LGPL v2.1), and code available from:

- https://github.com/sandialabs/InterSpec
- https://github.com/sandialabs/SandiaDecay
- https://github.com/sandialabs/SpecUtils

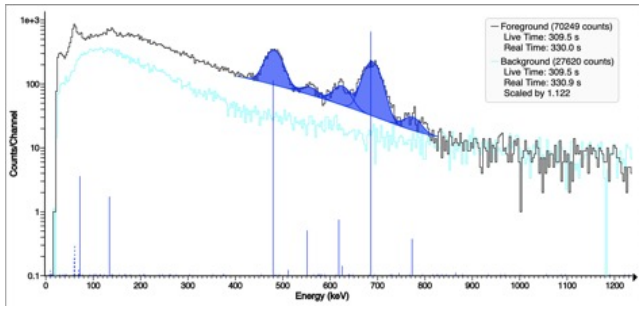
Support, bug reports, and requests: InterSpec@sandia.gov

Todays presentation should take ~1 hour

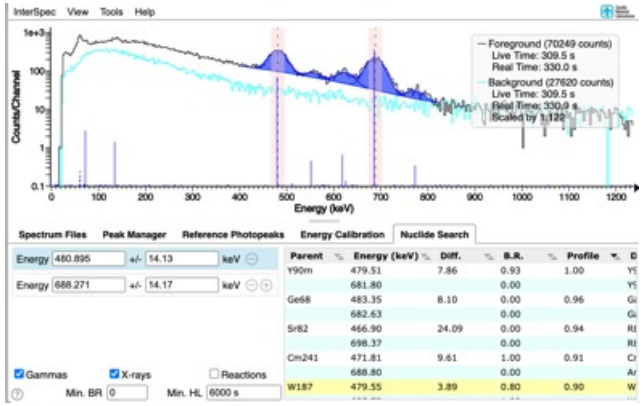
Introduction to InterSpec

general use

InterSpec Capabilities:



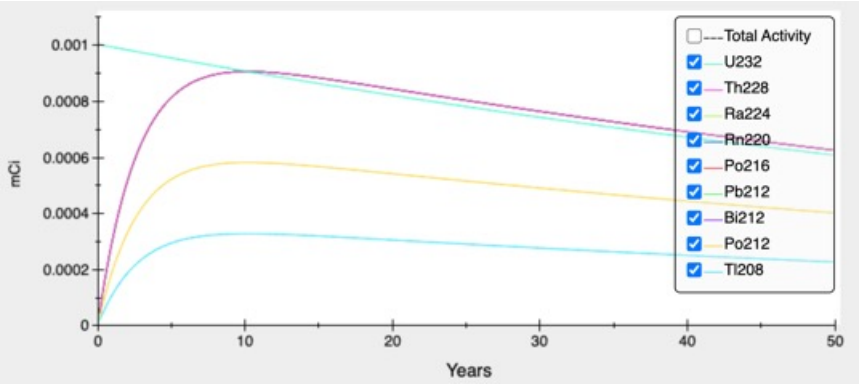
Quickly view spectrum files and fit peaks

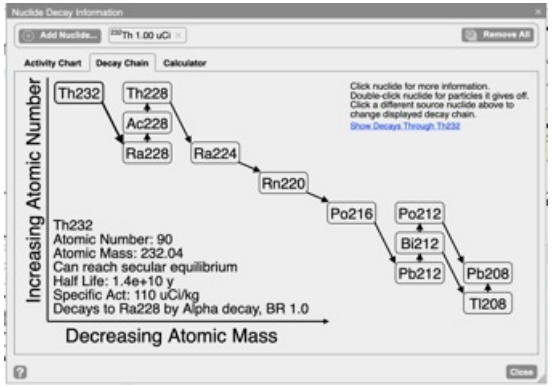


Perform nuclide ID

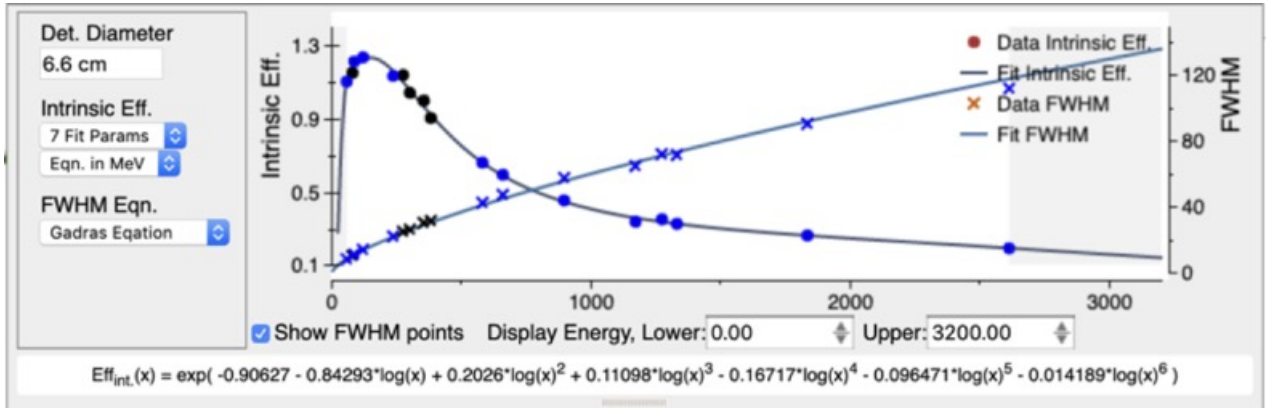
Determine nuclide activities, shielding amounts, isotopics, and ages

InterSpec Capabilities (continued):

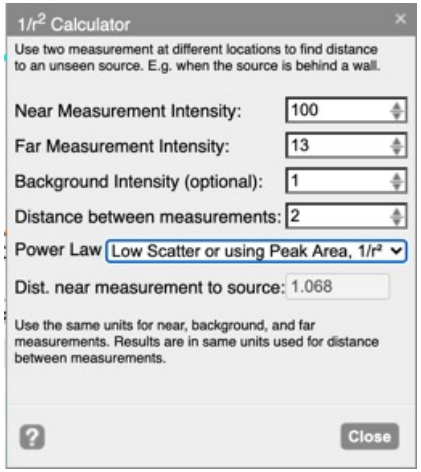




Perform nuclide decay calculations, get reference information, export inf as CSV, etc

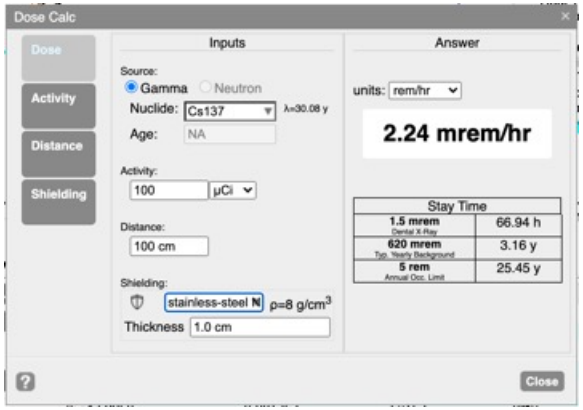


Develop detector response functions (efficiency + FWHM)

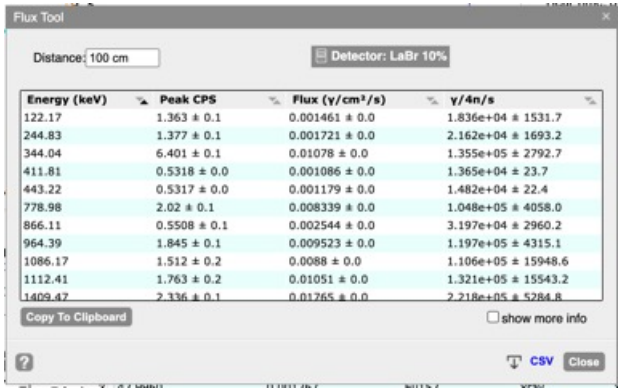


1/r² calculator

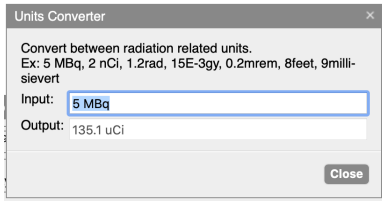
InterSpec Capabilities (continued):



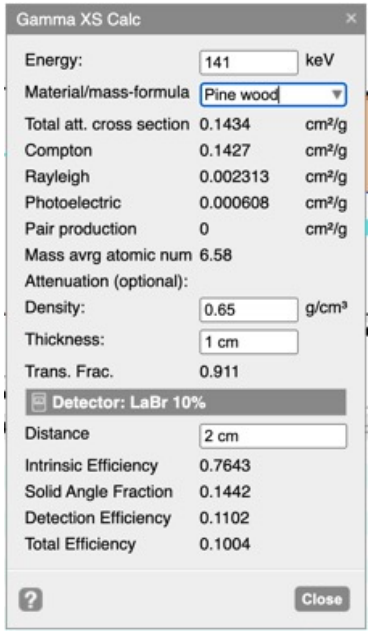
Flexible gamma dose calculations
Activity ←→ Dose
Activity ←→ Distance
Etc.



Gamma flux calculator



Convert radiation relevant units



Cross-section calculator

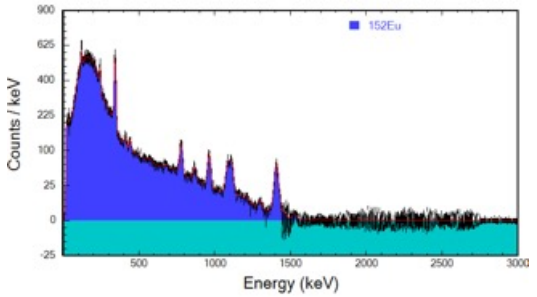
And more!

(and also more under active development)

What InterSpec is not:

InterSpec is not a magic easy button – all features are interactive – doesn't tell you the answer automatically, but assists the user to perform analysis

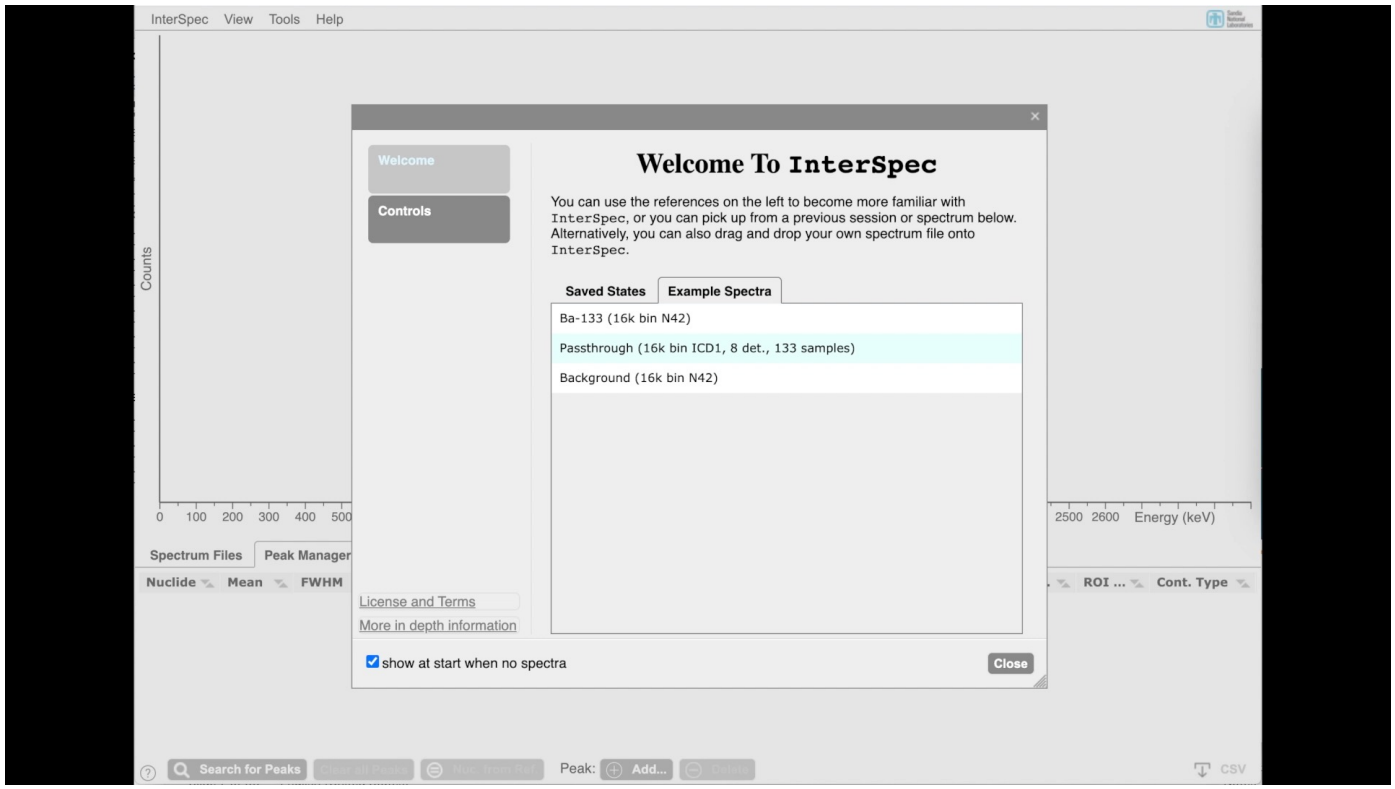
Not full-spectrum analysis



Does not do data acquisition - only accepts data already taken

Does not generate reports or adhere to standardized methodologies

Initial analysis example (about 4 minutes)



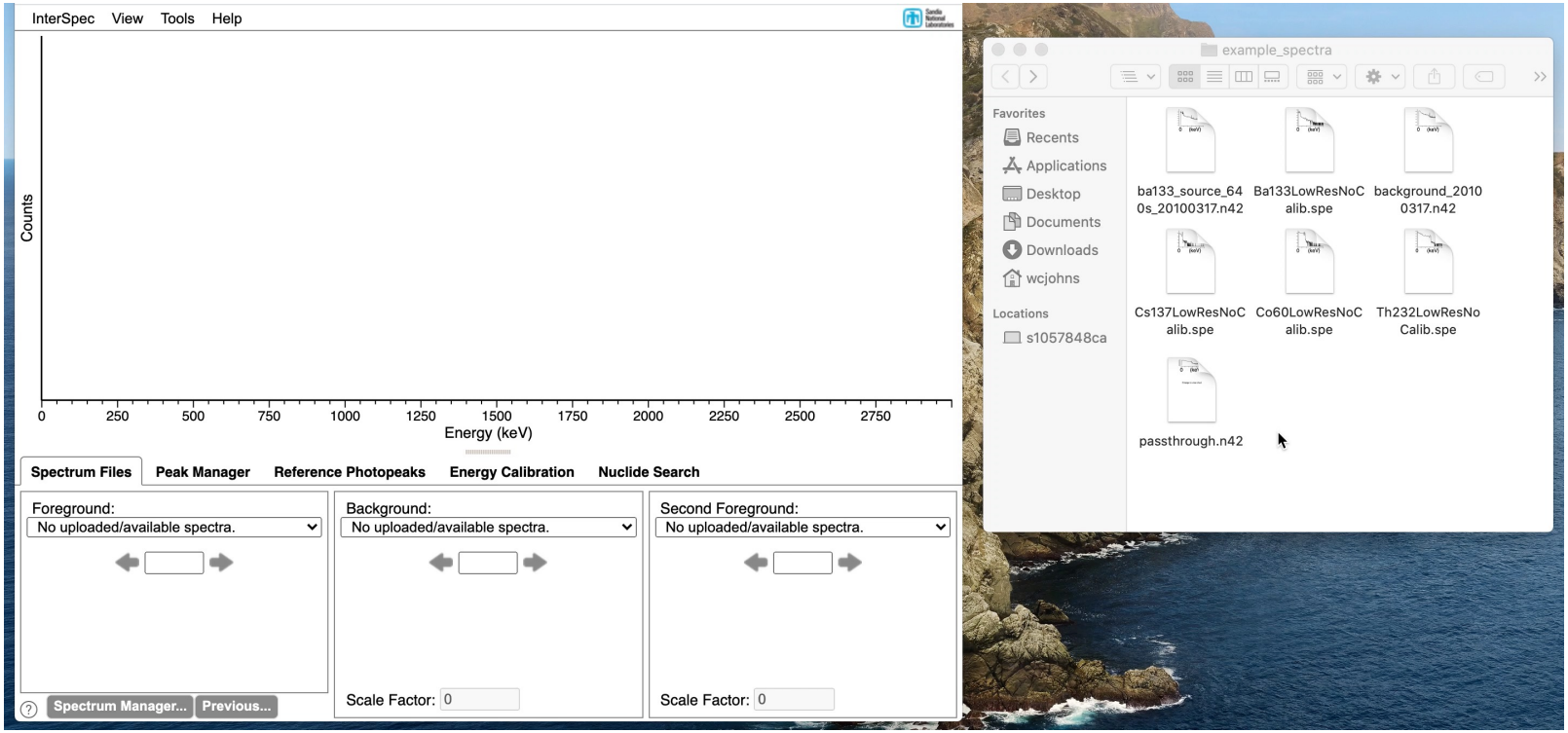
Result: 46 uCi of Ir-192 with 6.20 mm of Pb shielding

Truth: 51 uCi of Ir-192 with 6.35 mm of Pb shielding

How to use InterSpec

Interacting with spectra

Loading Spectra

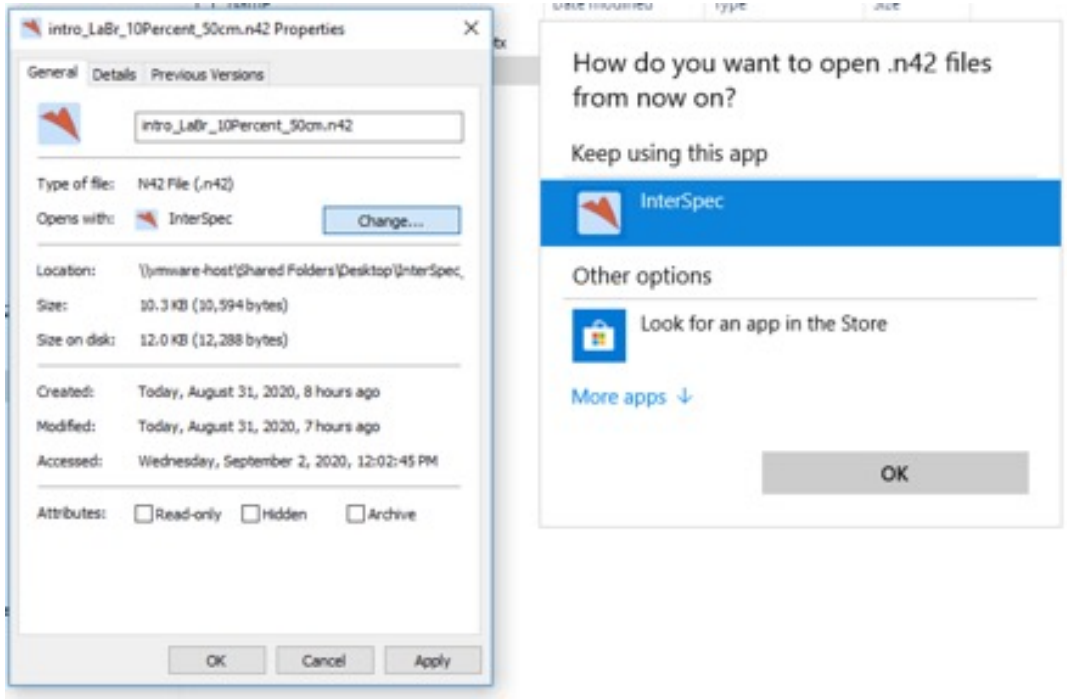


To load a spectrum file: drag-n-drop from your computer

- When file is over InterSpec, you can choose to open it as Foreground, Background, or Secondary

The **InterSpec→Open File...** menu option lets you browse for files

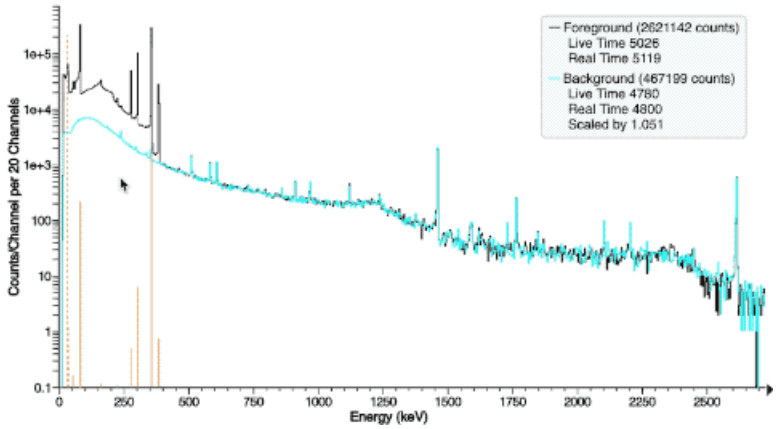
Loading Spectra (continued)



You can double-click on spectrum files in the operating system to open them in InterSpec

Window: you have to manually associate file types with InterSpec first
macOS/iOS/Android: spectrum files are automatically associated with InterSpec

Interacting with spectra



Zoom in: click and drag to the right - let go of the mouse to zoom in.

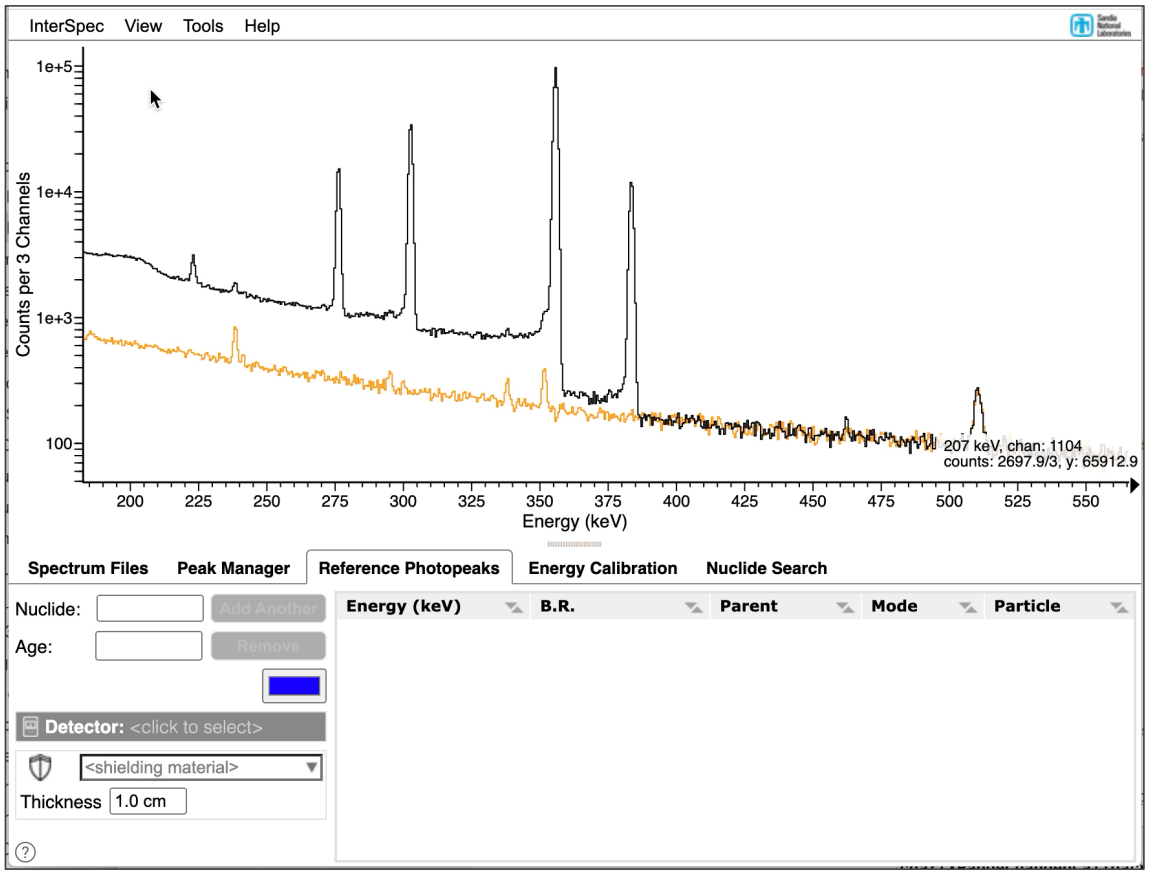
Zoom out: click and drag to left; zooming out happens continuously

To pan left or right: click and drag with right mouse-button. Or click and drag x-axis labels

Mouse wheel: up/down zooms in; left/right pans energy

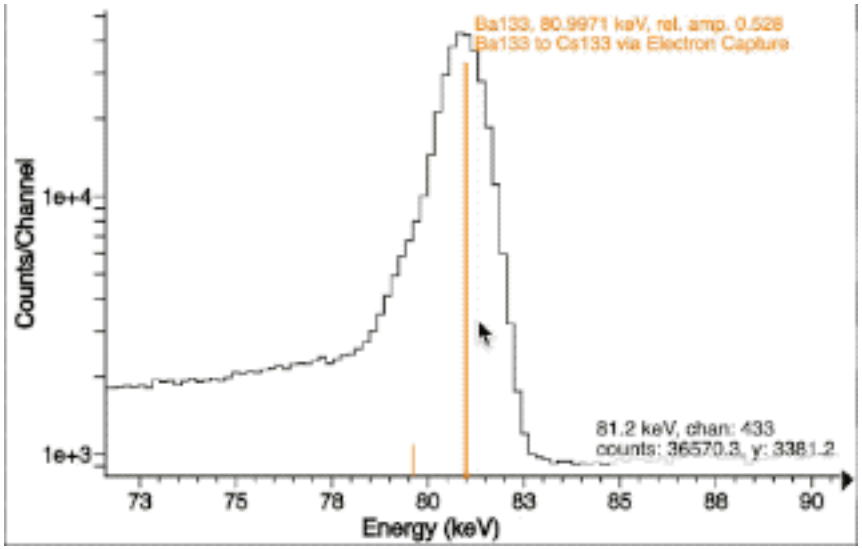
Touch screens: one finger pans left/right, two horizontal fingers zoom in/out

Interacting with spectra (cont)



View → “Show Energy Slider” will bring up a strip chart

Basic peak-fitting



To fit a peak, double click near it.

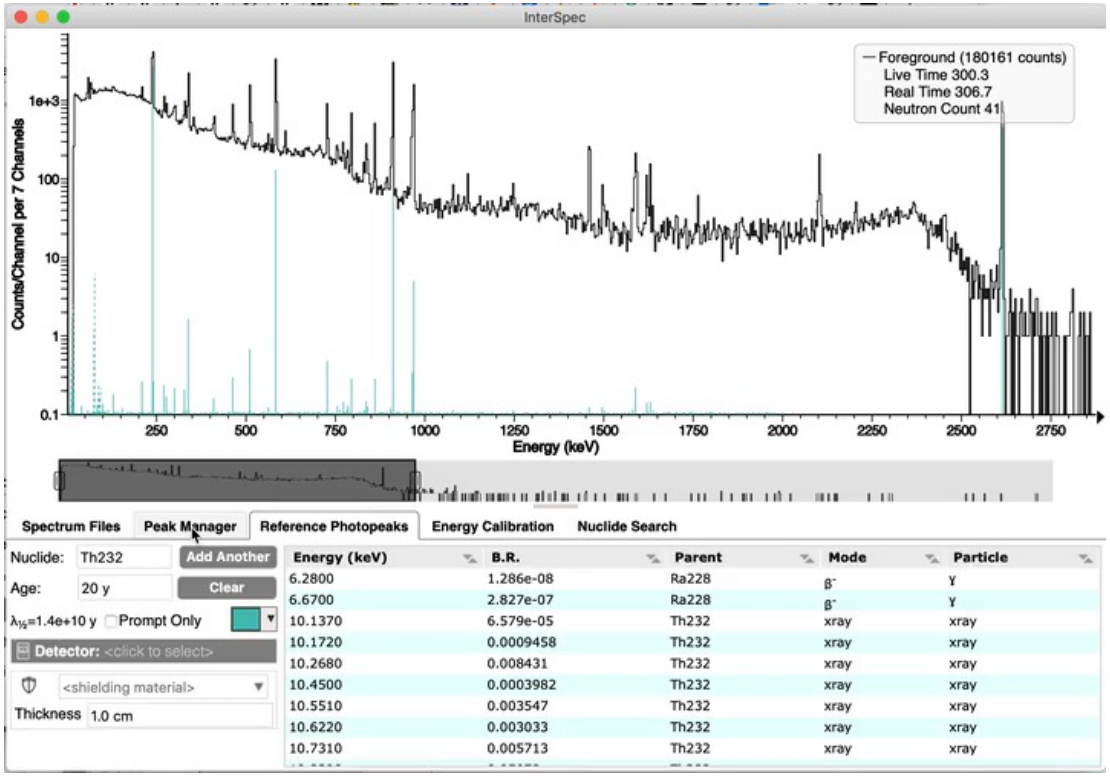
Double clicking again will add another peak.

You can adjust the Region Of Interest (ROI), by moving mouse to edge of ROI

Right-click on a peak to get a menu to add or remove a peak from a ROI

Holding control and dragging across a region lets you fit for multiple peaks in a ROI

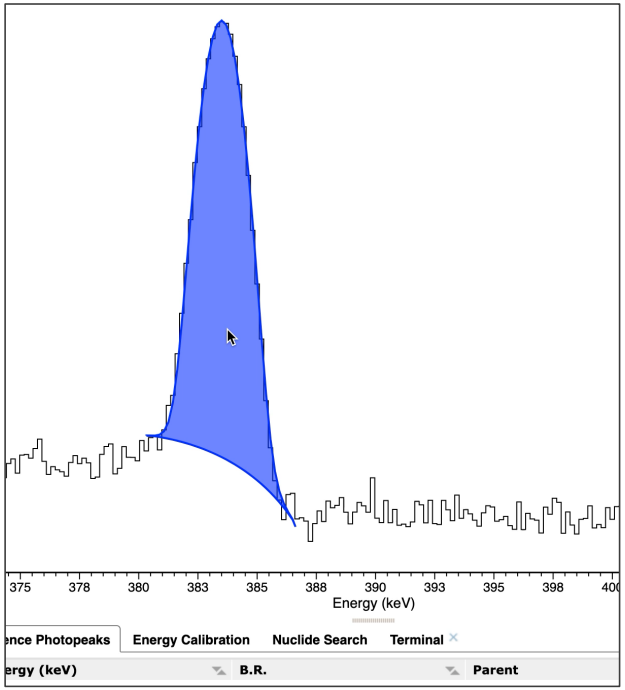
Peak Fitting (cont)



There is also an automated peak search that works decent, especially for HPGe

- Gets you to the ~80% level for HPGe spectra – e.g., may require some "clean-up"
- Does not use the currently showing reference lines, or detector response function (DRF) to identify peaks

Peak Fitting (cont)



You can also right-click on a peak and choose “Peak Editor…” from the popup menu to have more control over fitting a peak.

You can fix some of the peak quantities, and fit for other ones, manually adjust some of the parameters, select a continuum type, and more

If you forget how to do something:

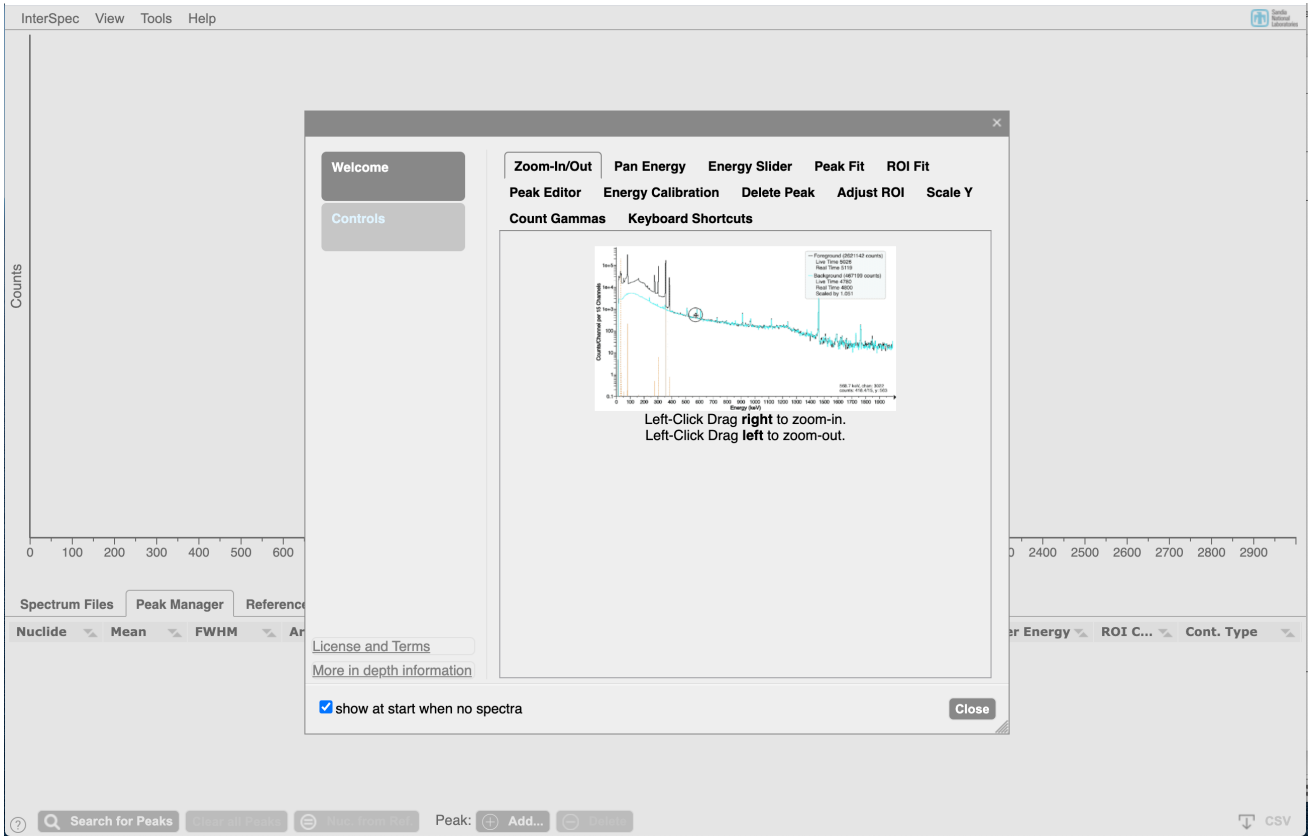
Help → Welcome → Controls

or

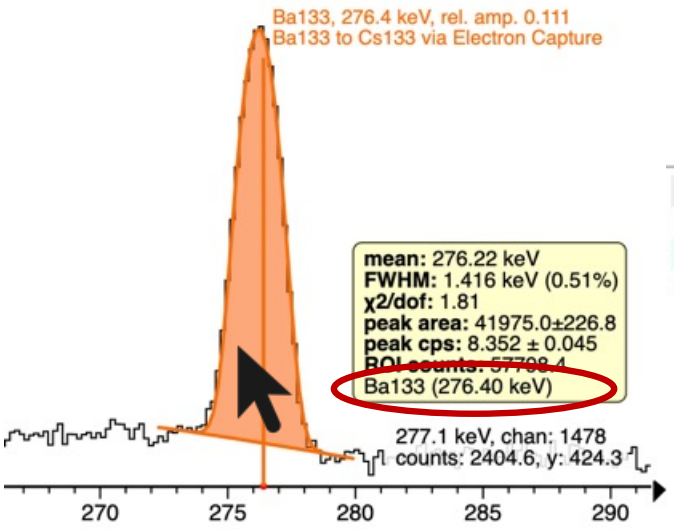
Help→ "Help Contents…"

or

There is often a ⓘ icon in lower-left of tools you can click on



Important concept!



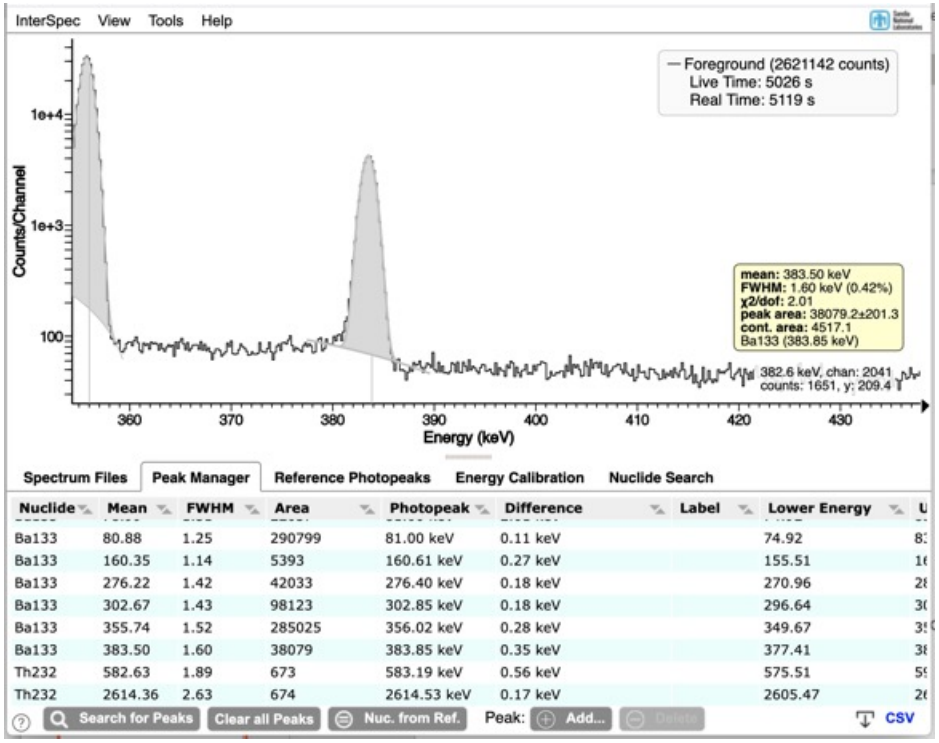
Spectrum Files | Peak Manager | Reference Photopeaks | Energy Calibration | Nuclide Search

Nuclide	Mean	FWHM	Area	CPS	Photopeak	Differ...
Ba133	79.54	1.16	22002	4.378 ± 0.074	79.61 keV	0.07 keV
Ba133	80.92	1.18	277536	55.22 ± 0.12	81.00 keV	0.07 keV
Ba133	276.22	1.42	41975	8.352 ± 0.045	276.40 keV	0.18 keV

Peaks can get associated with a nuclide, x-ray, or reaction

- The peak is actually associated with a specific gamma-line of the nuclide/x-ray/reaction

Associating peaks with a nuclide/reaction/x-ray

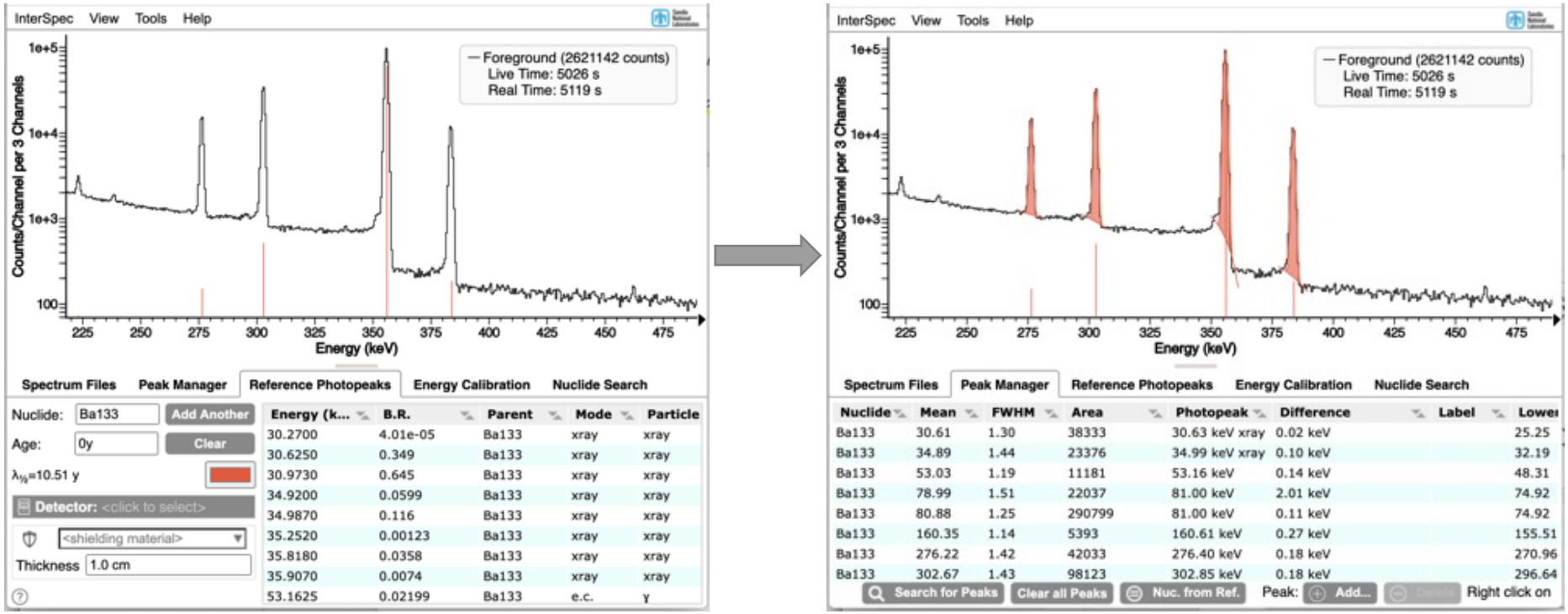


Nuclide	Mean	FWHM	Area	Photopeak	Difference	Label	Lower Energy
Ba133	80.88	1.25	290799	81.00 keV	0.11 keV		74.92
Ba133	160.35	1.14	5393	160.61 keV	0.27 keV		155.51
Ba133	276.22	1.42	42033	276.40 keV	0.18 keV		270.96
Ba133	302.67	1.43	98123	302.85 keV	0.18 keV		296.64
Ba133	355.74	1.52	285025	356.02 keV	0.28 keV		349.67
Ba133	383.50	1.60	38079	383.85 keV	0.35 keV		377.41
Th232	582.63	1.89	673	583.19 keV	0.56 keV		575.51
Th232	2614.36	2.63	674	2614.53 keV	0.17 keV		2605.47

Associating a peak with a nuclide/reaction/x-ray:

- Keep track of nuclide ID
- Enables easy energy calibration, nuclide activity, isotope age, shielding, detector response function, calculate fluxes, …

Associating a peak with a nuclide/x-ray/reaction – best method

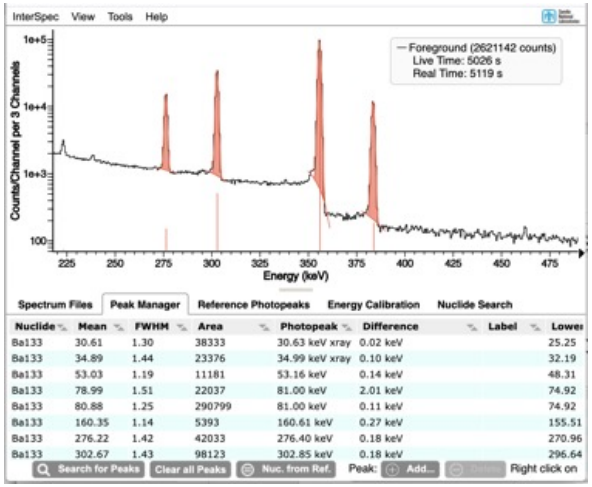


Show reference lines **before** fitting for peaks

- Association will automatically be made when you fit the peak if there is a gamma-line near peak
- Peak color will be the same as the reference line, to help track ID

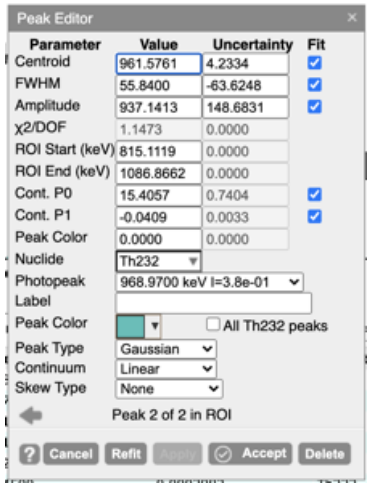
Associating a peak with a nuclide/x-ray/reaction – other methods

Right-click peak and going to “Change Nuclide” item will bring up some suggested nuclides

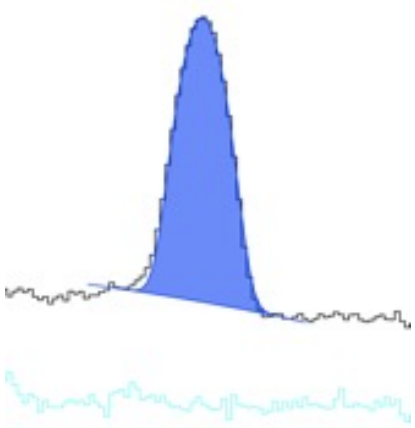


Tables listing peak information are all directly editable

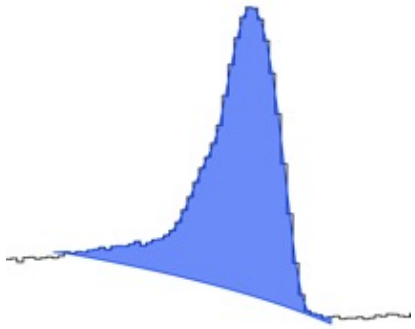
The peak-editor also lets you select the nuclide and energy



Peaks



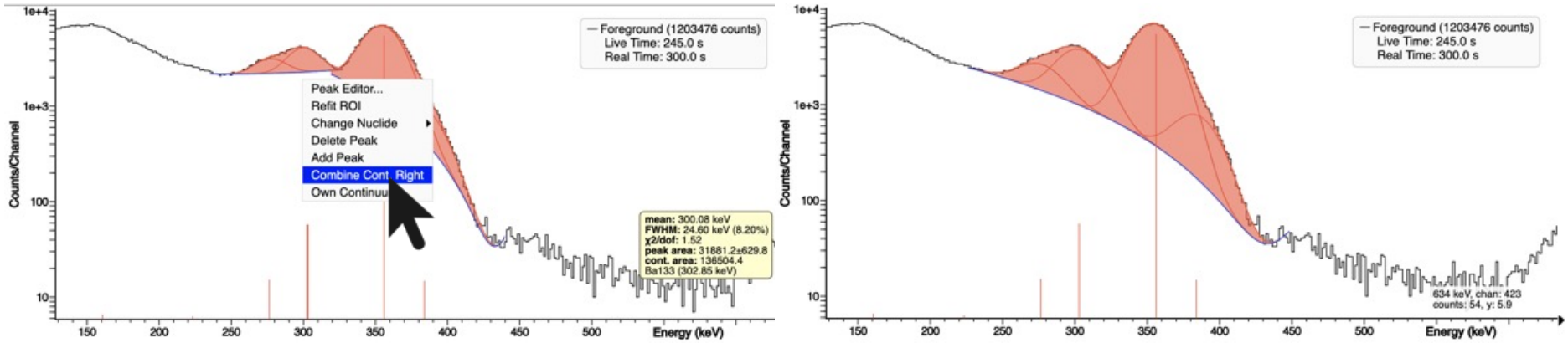
By default peaks are Gaussians sitting on top of a polynomial continuum



Peaks can also be “data defined” meaning their amplitude is the area between the continuum observed counts

Recommend sticking with Gaussian + Polynomial unless bad fit

Peaks (continued)

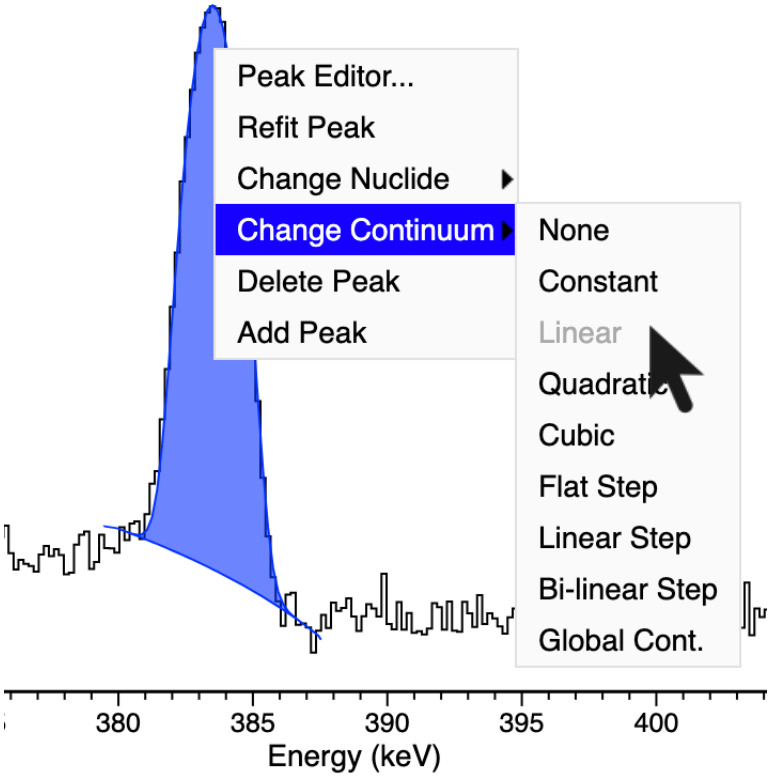


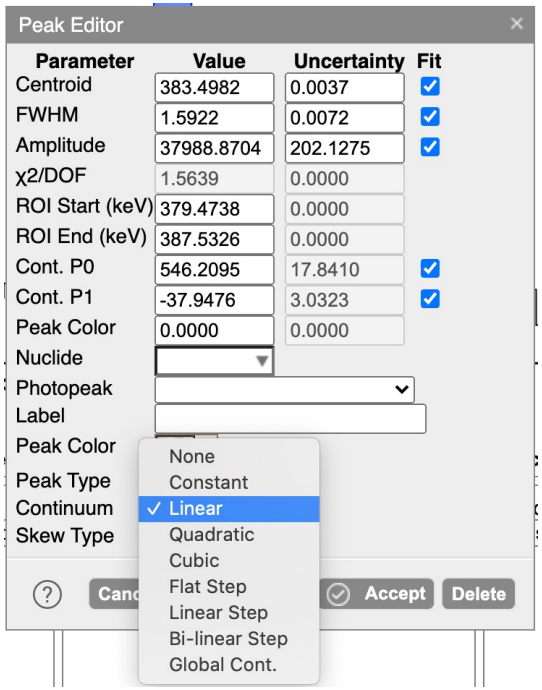
Peaks can share a continuum

- If InterSpec doesn't automatically have peaks share a continuum: right-click on a peak, and choose to "Combine Cont. Right/Left" or "Own Continuum".

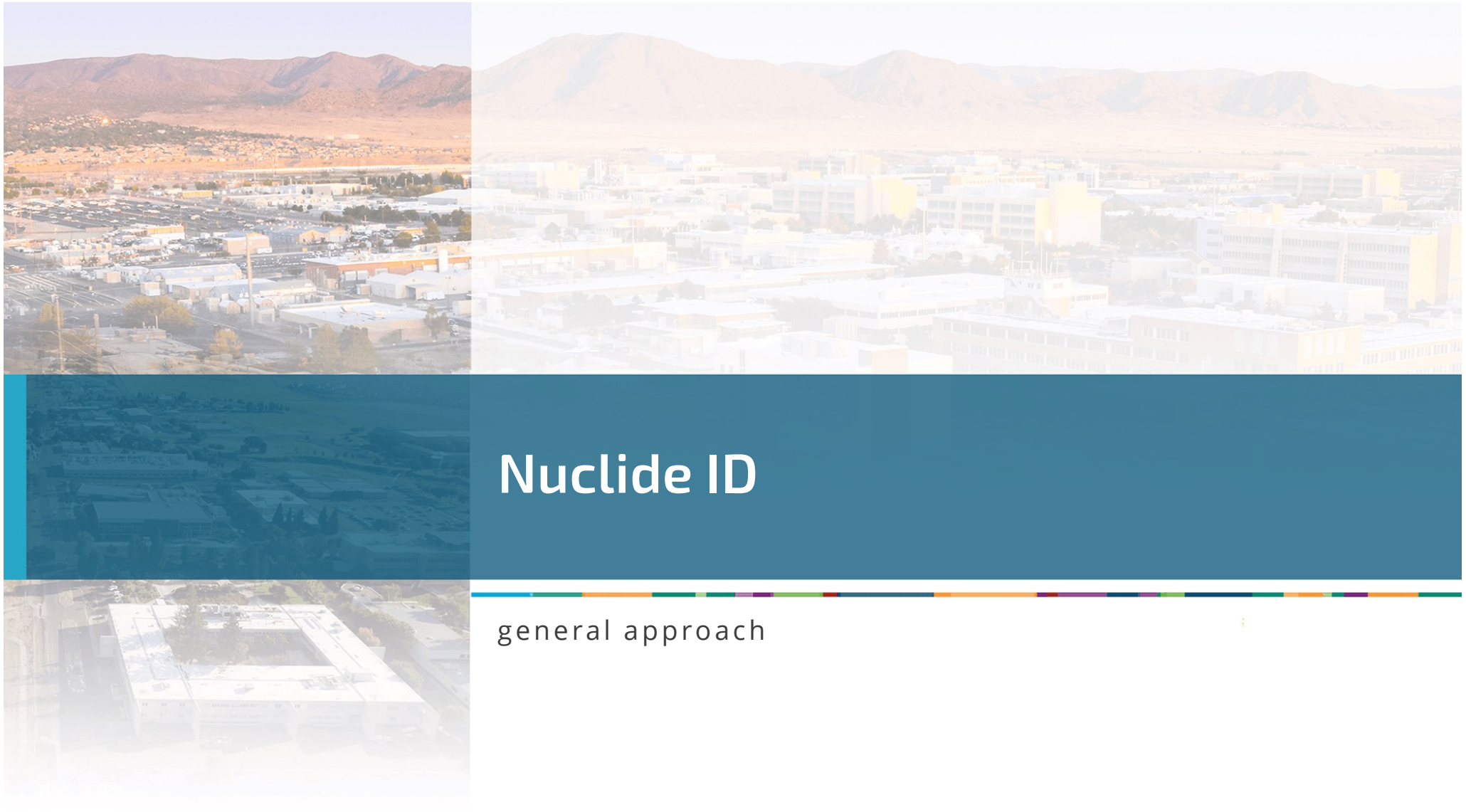
Peak continuum types

You can select different types of continuums by right-clicking on peak, or in "Peak Editor"





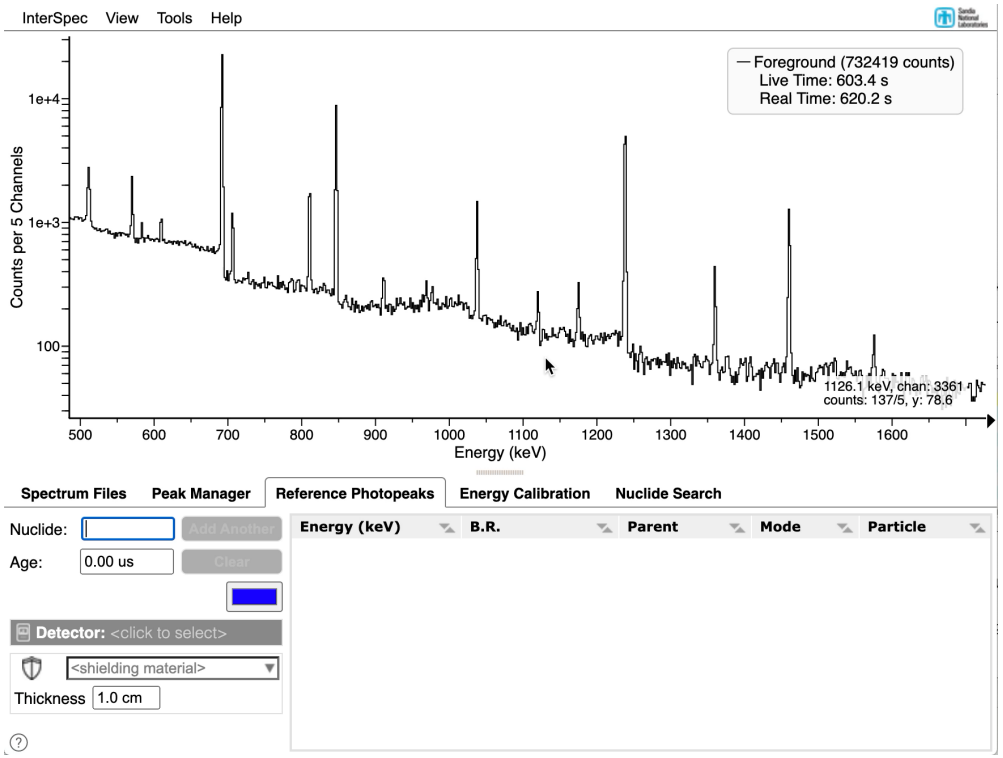
More detailed and advanced peak-fitting will be covered in part two



Nuclide ID

general approach

Nuclide ID



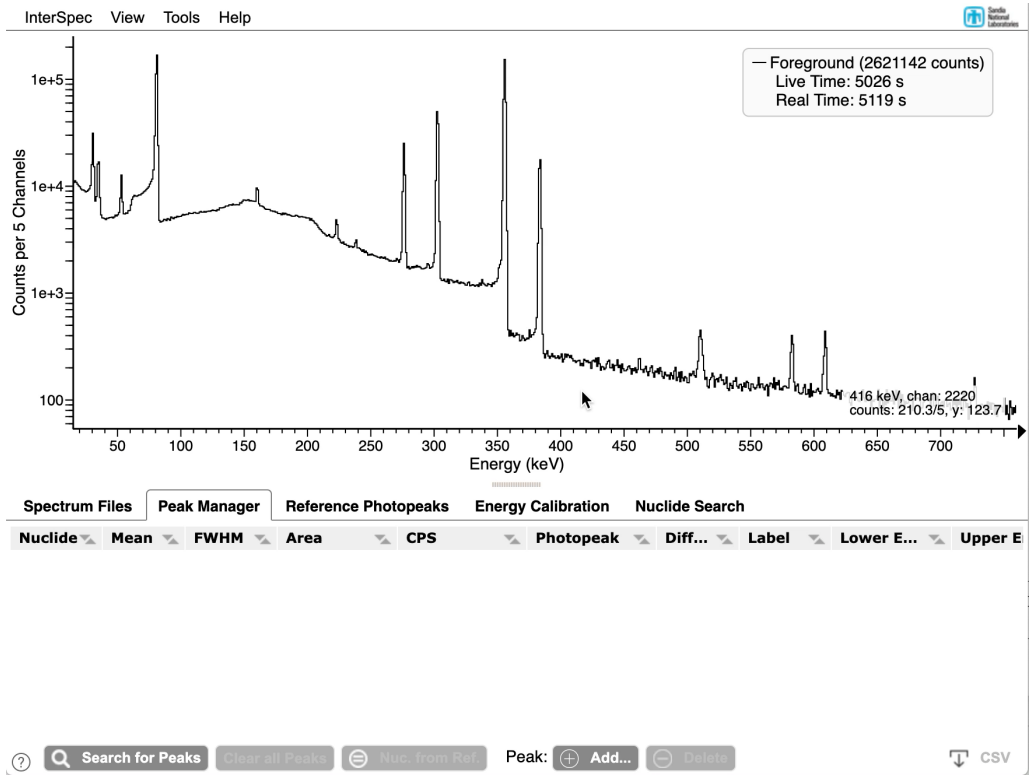
The “Nuclide Search” tab lets you search on one or more energies

You can enter an energy and search window manually, or by clicking on a peak, or the spectrum

By default search-results ordered by “Profile” which generally is the best, but can also be ordered by any table column

Clicking on a result row in table will show reference lines for that nuclide, on the spectrum

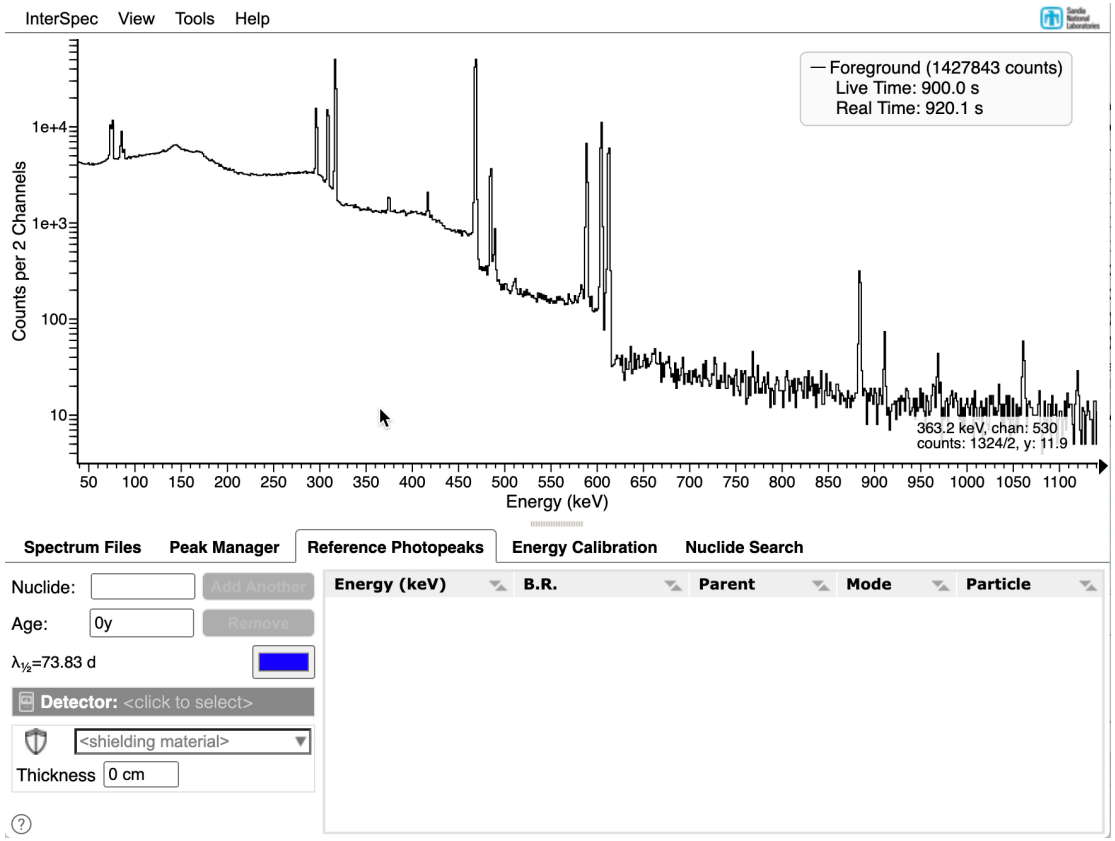
Nuclide ID (continued)



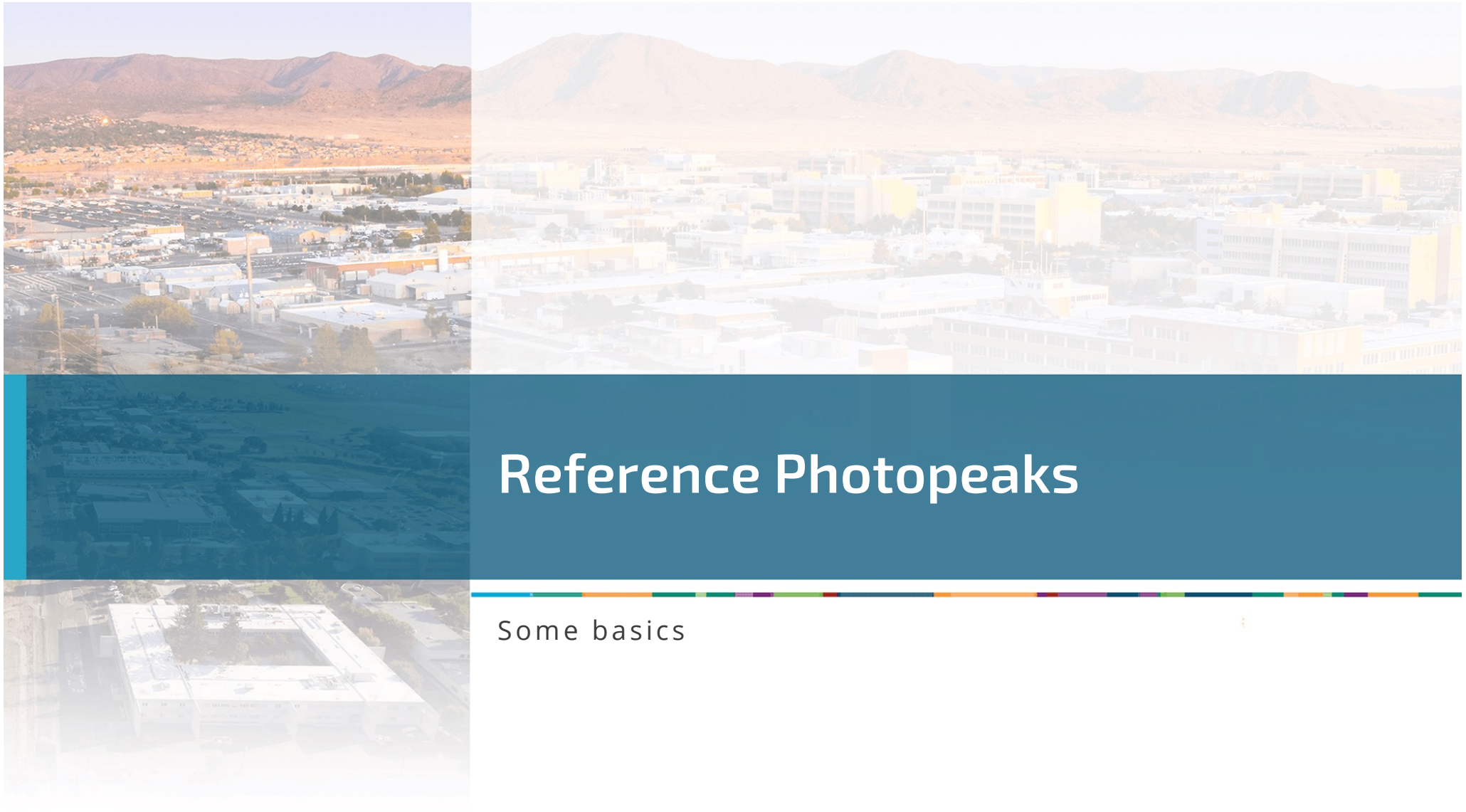
Right-clicking on a peak after fitting it will also show you some suggestions

- Suggestions are meant to assist you – they are not a automated identification
- Especially useful for catching sum-peaks, or escape peaks

Nuclide ID (continued):



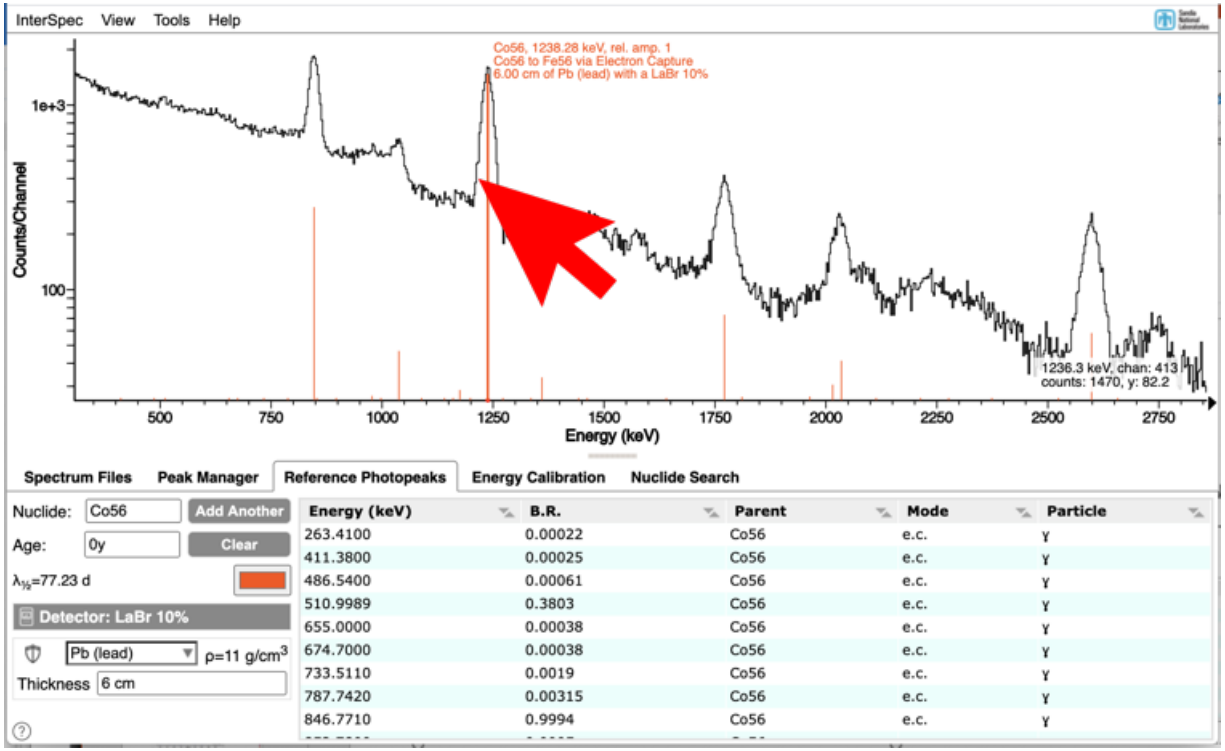
The “Reference Photopeaks” tab (covered next) is also really useful for nuclide ID



Reference Photopeaks

Some basics

Reference Photopeaks



The “Reference Photopeaks” tab might be the most useful tool in InterSpec

- Gives you access to all >4000 nuclides, all x-rays, and ~200 reactions
- You can age nuclides, add shielding, DRF, and when appropriate just prompt products
- The reference lines on the spectrum provide additional information when you mouse-over them

Reference Photopeaks (continued)

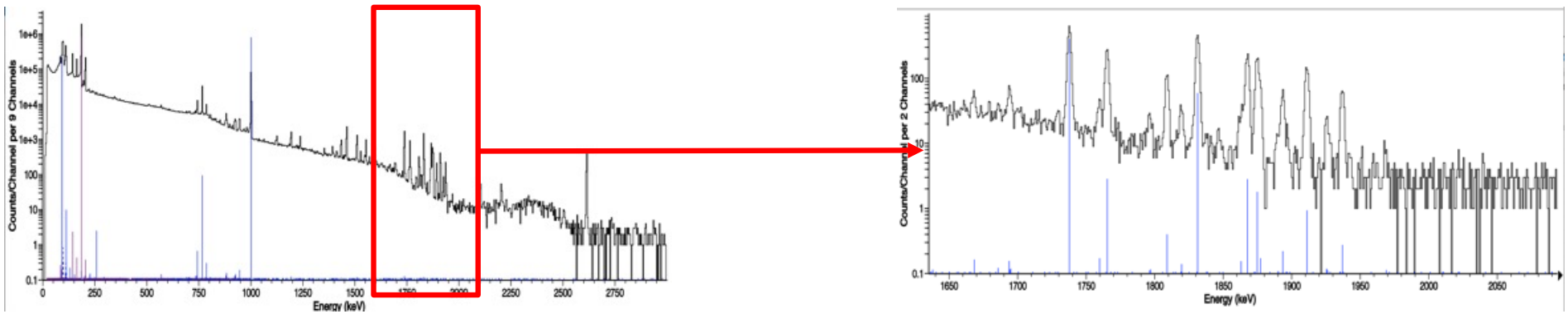
You can enter “nuclides” in fairly flexible, e.g., all the following are valid:

- Co56, Co-56, 56Co, 56 Co, 56-Co, cobalt 56, 56 Cobalt.
- Ho166m, Ho-166 meta, 166m Ho, 166m-Ho, holmium 166m
- Once you finish entering, will be converted to format like “Co56”

Reactions are entered like: “H(n,g)”, “Ge(n,n)”, etc

You can also enter “Background”, or an element name/symbol for its florescence x-rays

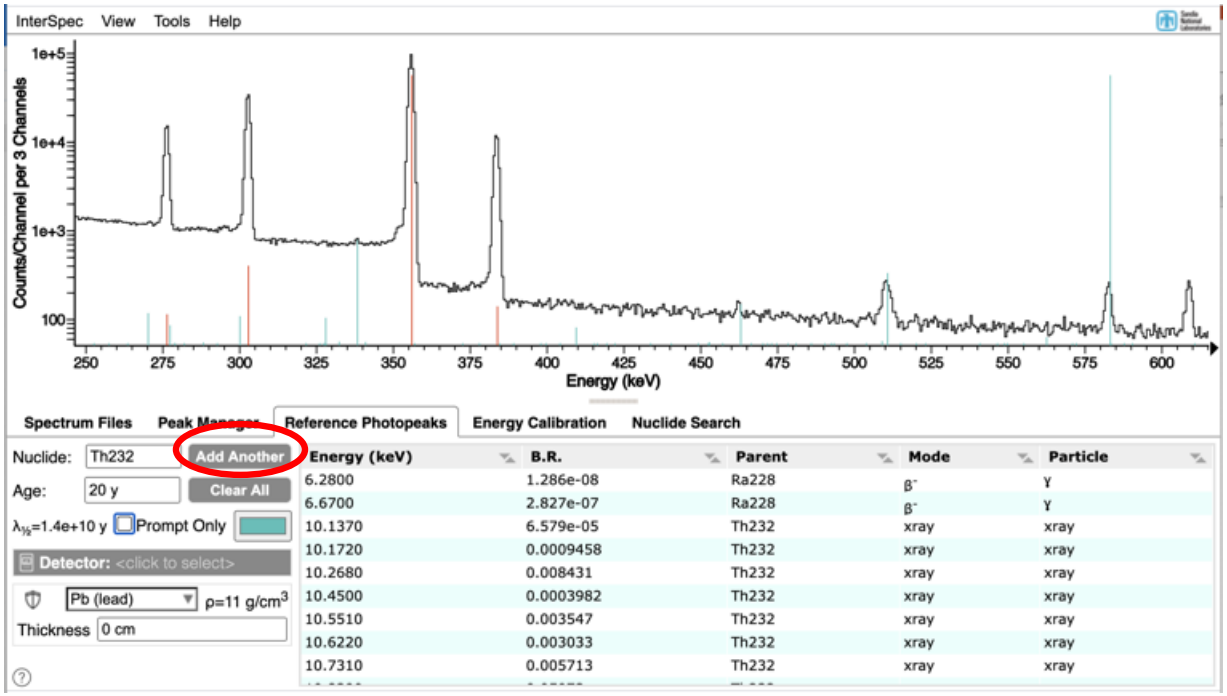
Reference Photopeaks (cont.)



The height of the lines on the spectrum indicate relative intensity of gammas/x-rays

- The heights are scaled so the highest intensity gamma line in currently displayed energy range has a height of 1, and all other lines are scaled linearly relative to this
  - Even if the spectrum y-axis is log, reference lines are linear – this best matches what is seen in the data-spectrum, given the continuum counts
- Shielding and DRF (if entered) are taken into account in the chart-line amplitudes, but not on table values

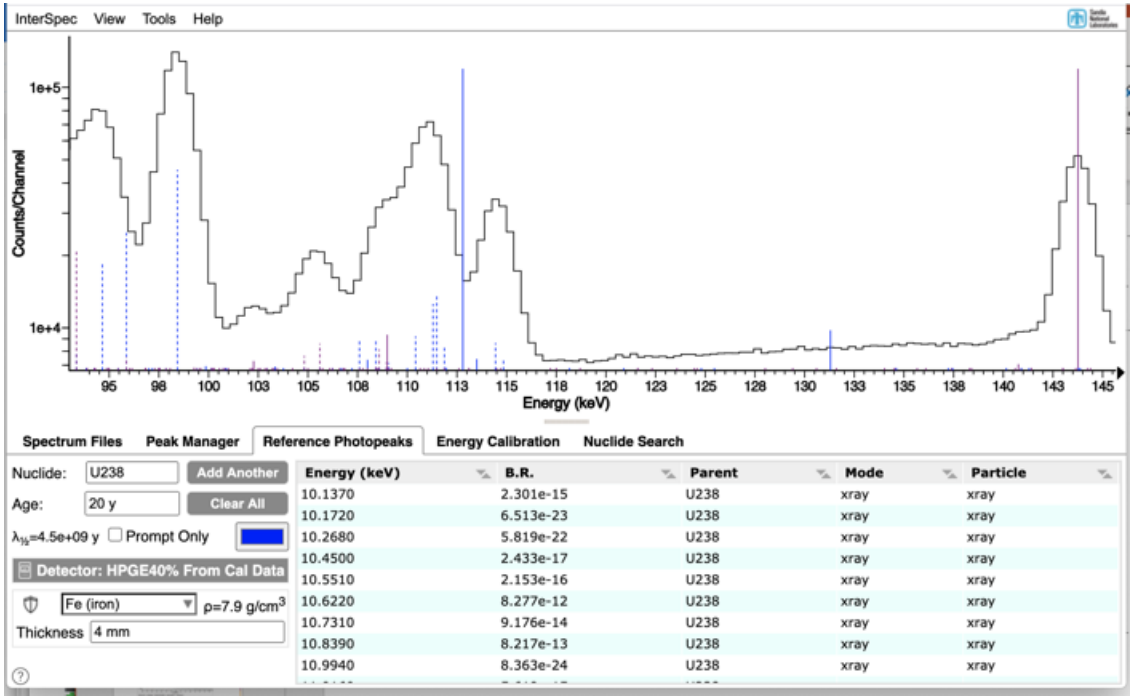
Reference Photopeaks (cont.)



To display lines for multiple isotopes, click “Add Another” and enter a new nuclide in

- Each nuclide can have a different shielding, age, etc. Changing these fields only changes the current nuclide, if you want to alter a previously entered set of reference lines, just type that name into the “Nuclide” field
- Line height scaling for currently visible energy range happens on a per-nuclide level
- If you fit a peak while showing multiple nuclides, usually the best one is chosen to associate with a peak

Reference Photopeaks (cont.)



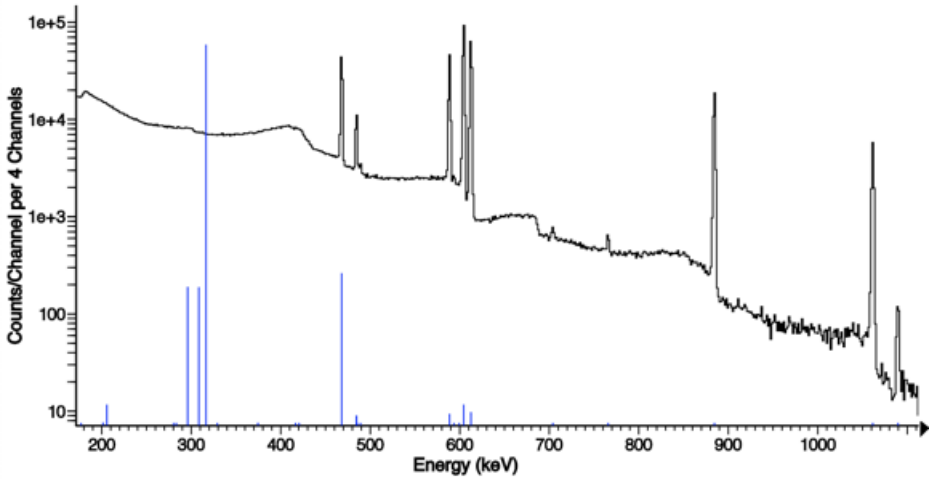
Reference lines for nuclides will also include x-rays that are emitted during decays

- x-ray intensities are computed during decay calculations so their intensities are comparable to the gammas
  - But be aware of geometry or florescence effects

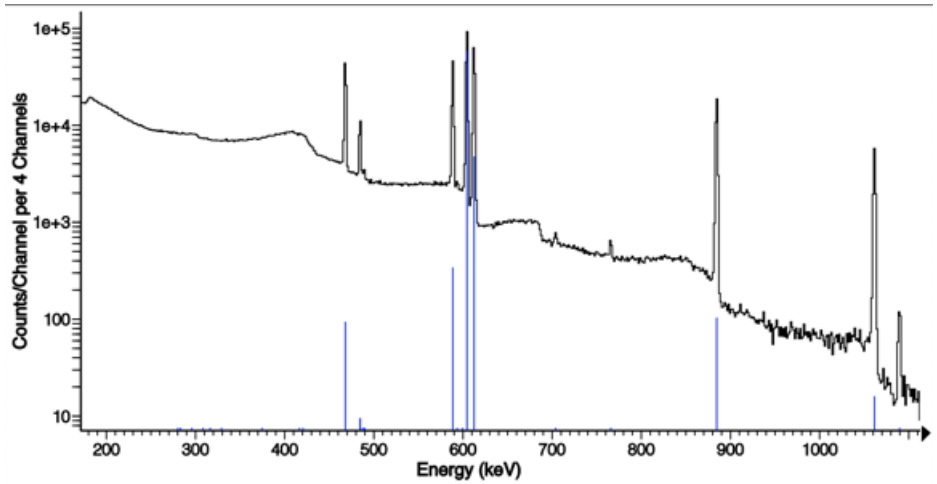
X-rays are shown as dotted lines on the spectrum

If you just enter a element, its florescence x-rays are shown

Reference Photopeaks (cont.)



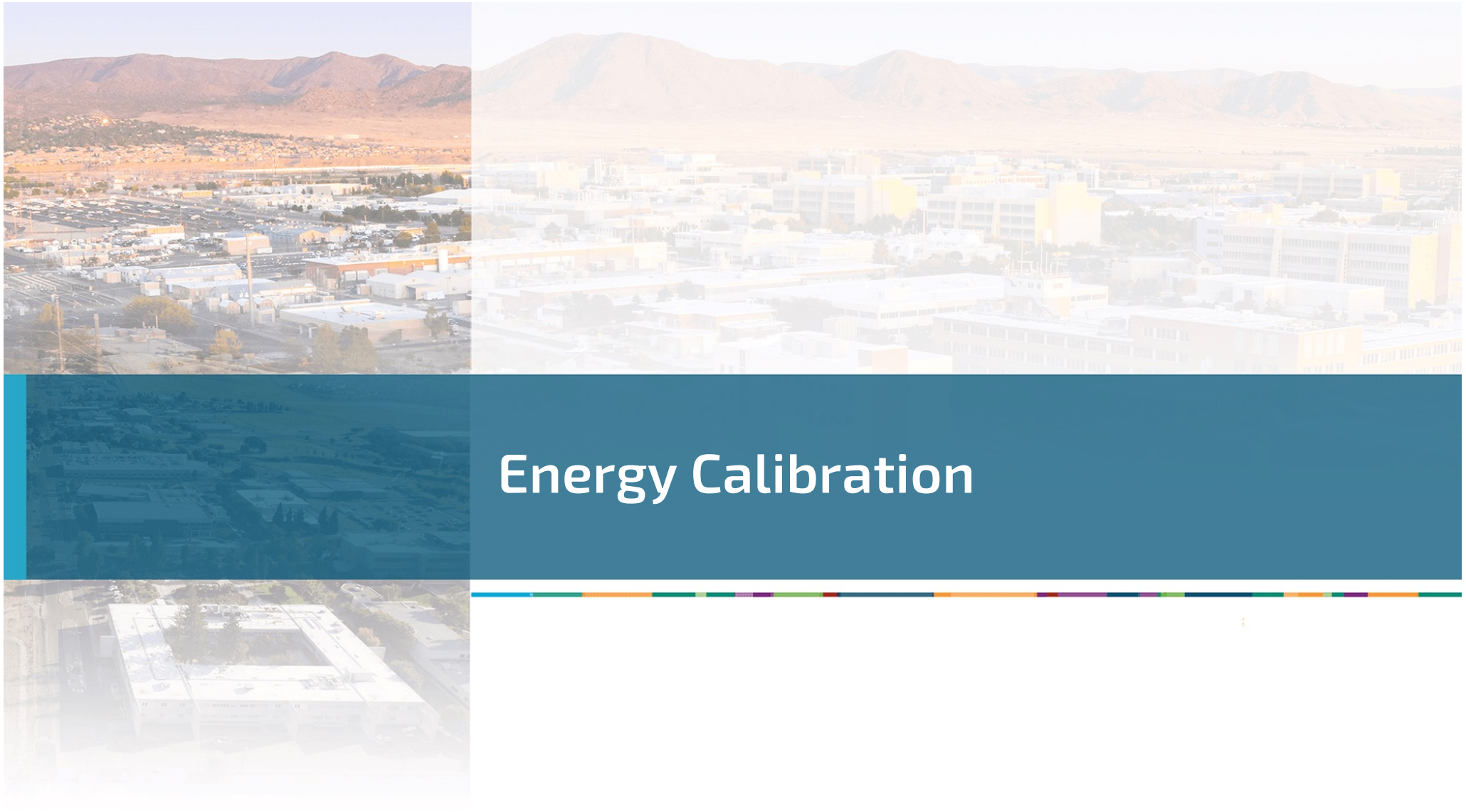
Ir-192 reference lines with no shielding



Ir-192 reference lines with heavy shielding

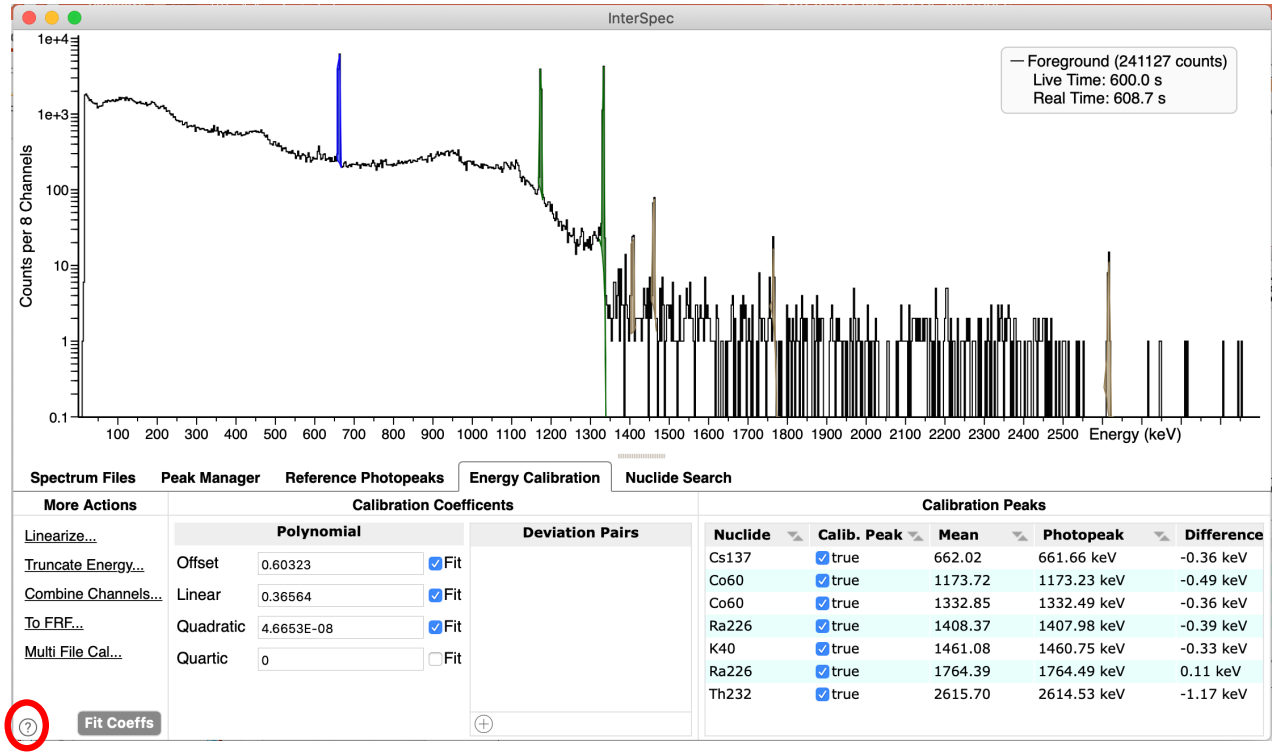
Adding shielding can be useful to:

- Knock down high-intensity low-energy lines that are easily shielded
- Account for large amounts of shielding



Energy Calibration

Energy Calibration



The “Energy Calibration” tab provides extensive energy calibration capabilities

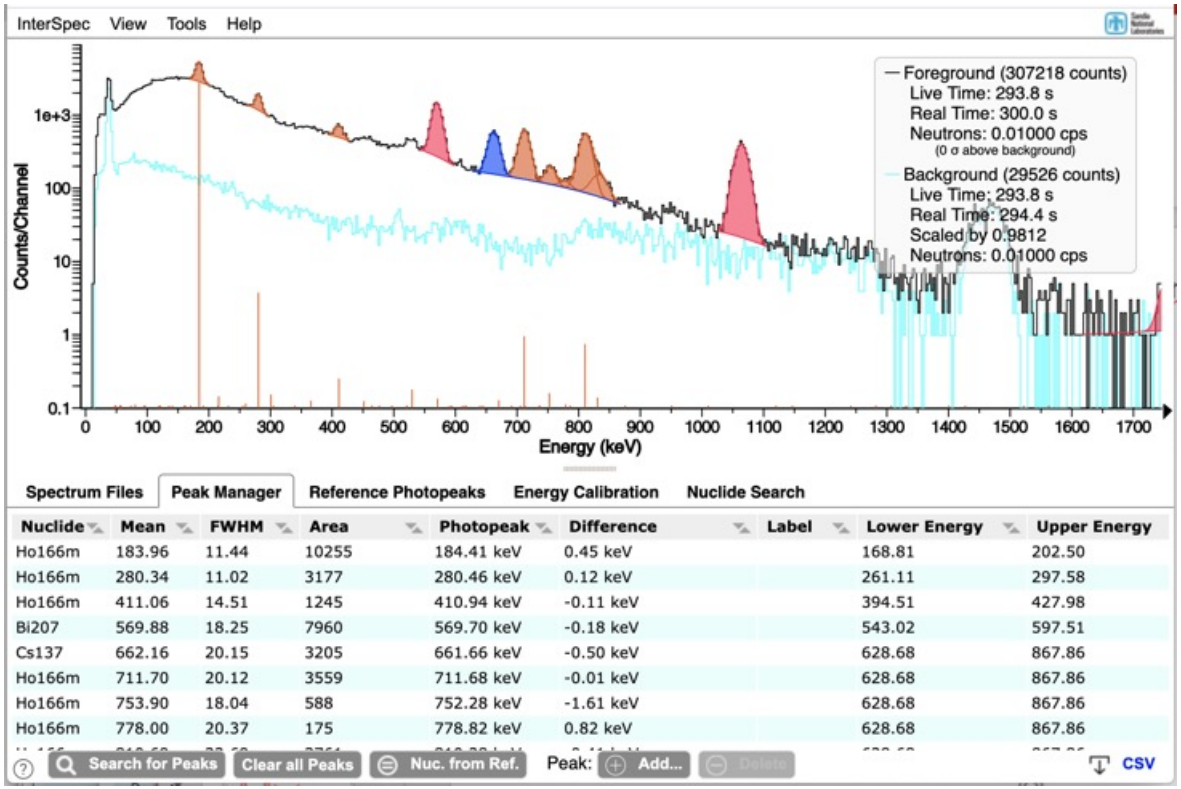
Fitting energy calibration coefficients, using peaks associated with nuclides is particularly useful

Will cover energy calibration more next week – you can also click ? in lower-left of tab

Fitting activity and shielding based on peaks in the spectrum

A quick introduction – not covering theory, or many, many details

Fitting activity, shielding, and age in InterSpec

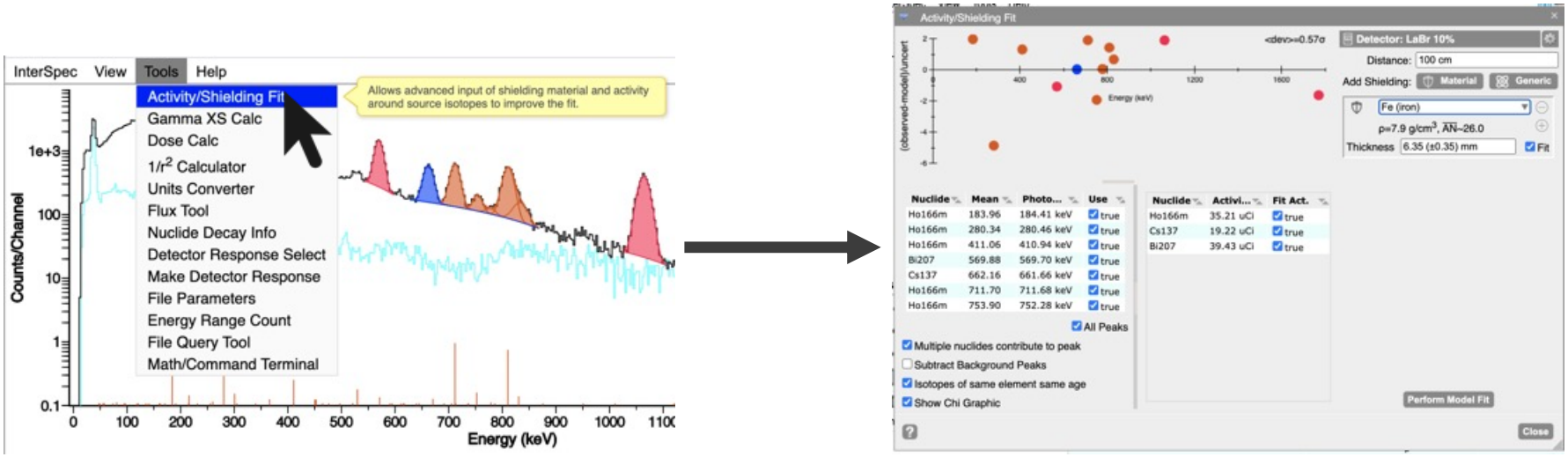


Nuclide	Mean	FWHM	Area	Photopeak	Difference	Label	Lower Energy	Upper Energy
Ho166m	183.96	11.44	10255	184.41 keV	0.45 keV		168.81	202.50
Ho166m	280.34	11.02	3177	280.46 keV	0.12 keV		261.11	297.58
Ho166m	411.06	14.51	1245	410.94 keV	-0.11 keV		394.51	427.98
Bi207	569.88	18.25	7960	569.70 keV	-0.18 keV		543.02	597.51
Cs137	662.16	20.15	3205	661.66 keV	-0.50 keV		628.68	867.86
Ho166m	711.70	20.12	3559	711.68 keV	-0.01 keV		628.68	867.86
Ho166m	753.90	18.04	588	752.28 keV	-1.61 keV		628.68	867.86
Ho166m	778.00	20.37	175	778.82 keV	0.82 keV		628.68	867.86

First: fit peaks, associating them with nuclides

- Peaks that are in both the background and foreground do not need to be fit. Or if a peak is for a nuclide you don't care about you can skip it
- If you have lots of peaks for a nuclide, like a HPGe spectrum of Ra-226, you can maybe fit for just the larger ones

Fitting activity, shielding, and age in InterSpec (cont.)



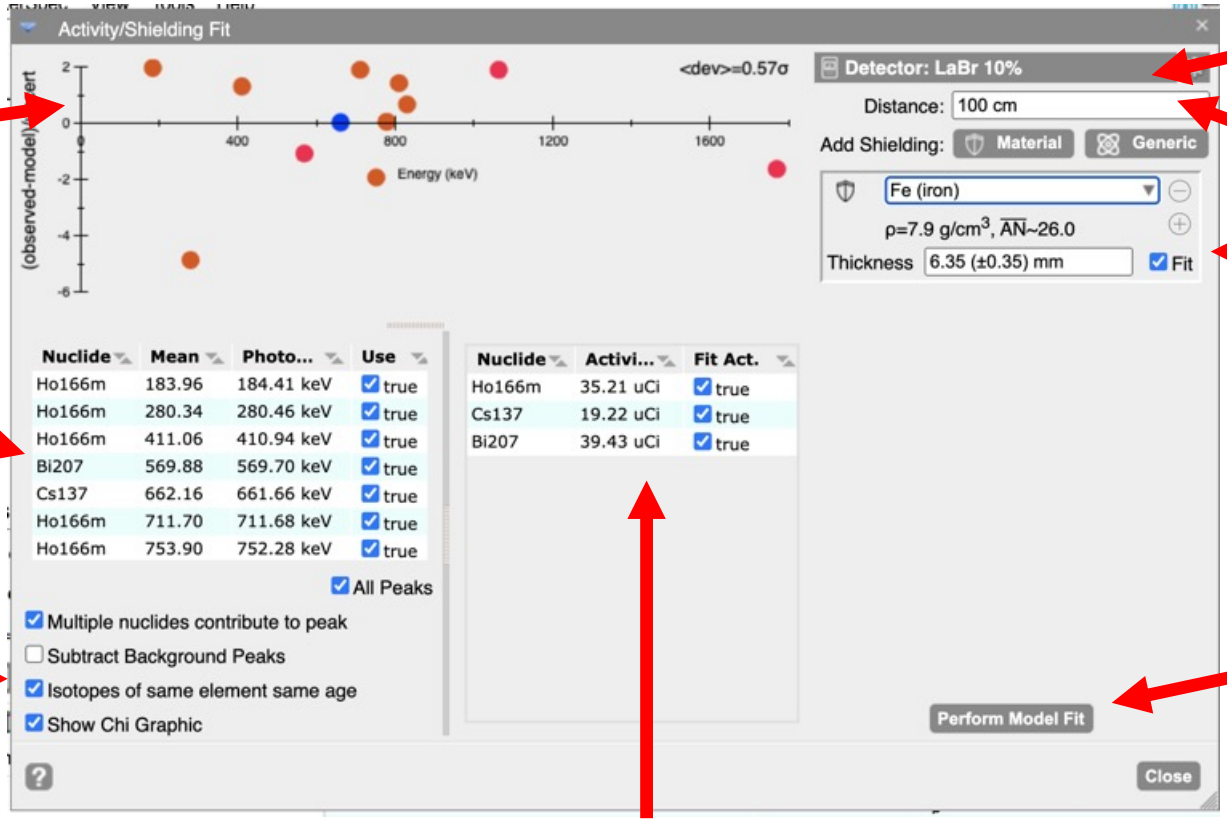
From the “Tools” menu, select “Activity/Shielding Fit”

Activity/Shielding Fit Tool

Get an idea of how good the fit is

You can select peaks to use in the fit

Some options



Select DRF

Enter distance

Select shielding(s)

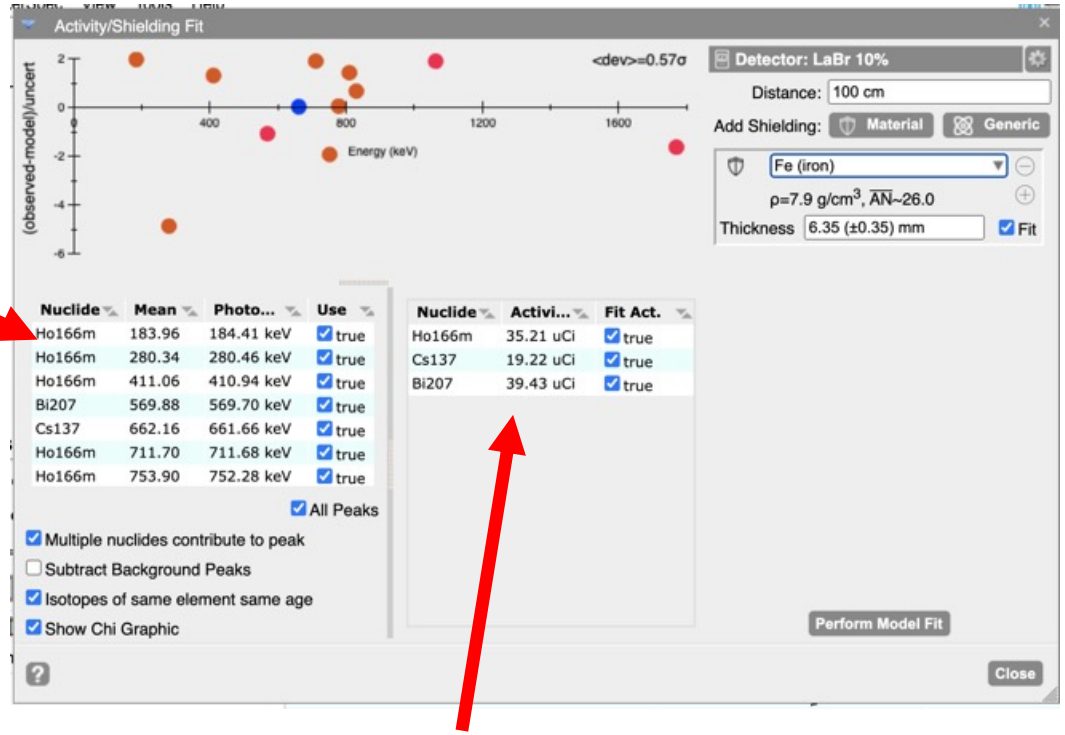
Fit for the quantities you want

Decide if you want activity and/or age fixed for each nuclide

Activity/Shielding Fit Tool (peaks to use)

All of the peaks you have fit for in the foreground will appear in this list.

- You can choose if a peak should participate in the fitting process.

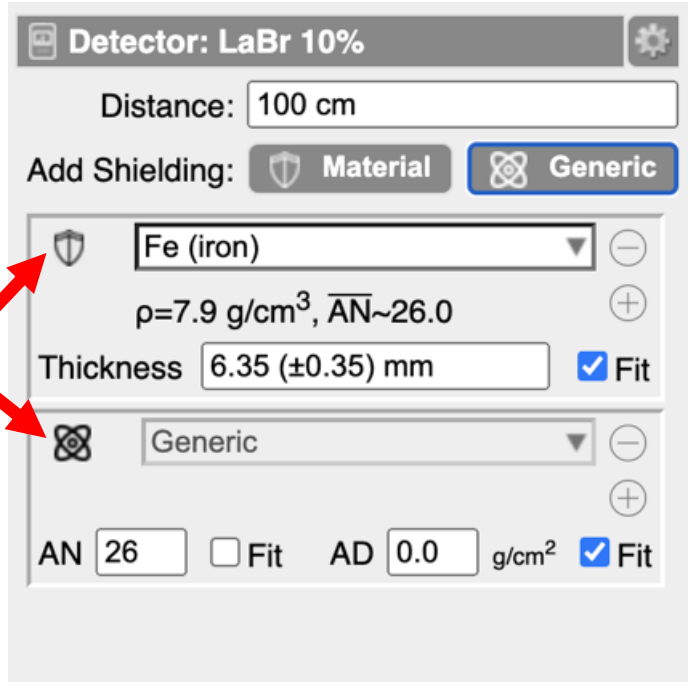


Any nuclides associated with the peaks you have selected, will appear here

- You can manually edit an activity, and choose not to fit it, if you happen to know it, but not the shielding
- Not shown above, but age of nuclides is also editable, or fittable for applicable nuclides

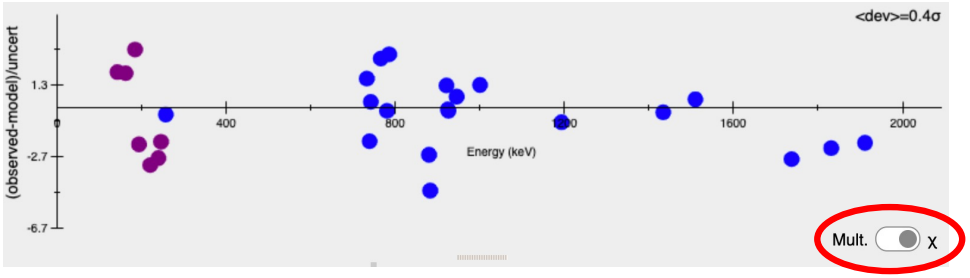
Activity/Shielding Fit Tool (shielding)

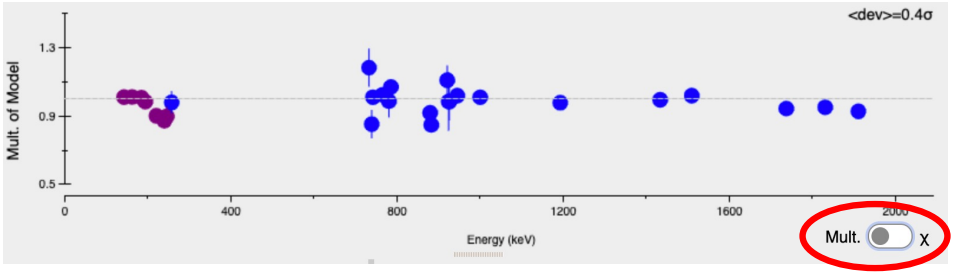
Clicking on these icons will toggle between shielding types



- The shielding can be either a specific type of material from InterSpecs database, or it can be a generic material where you specify the atomic number (AN) and areal density (AD), or you can enter a chemical formula and density.
  - You can choose to fit for, or fix, thickness, AN, and AD
- You can have multiple shielding's, but of course this can get degenerate to fit for multiple of them, especially if they have similar effective atomic numbers

Activity/Shielding Fit Tool: Graphic



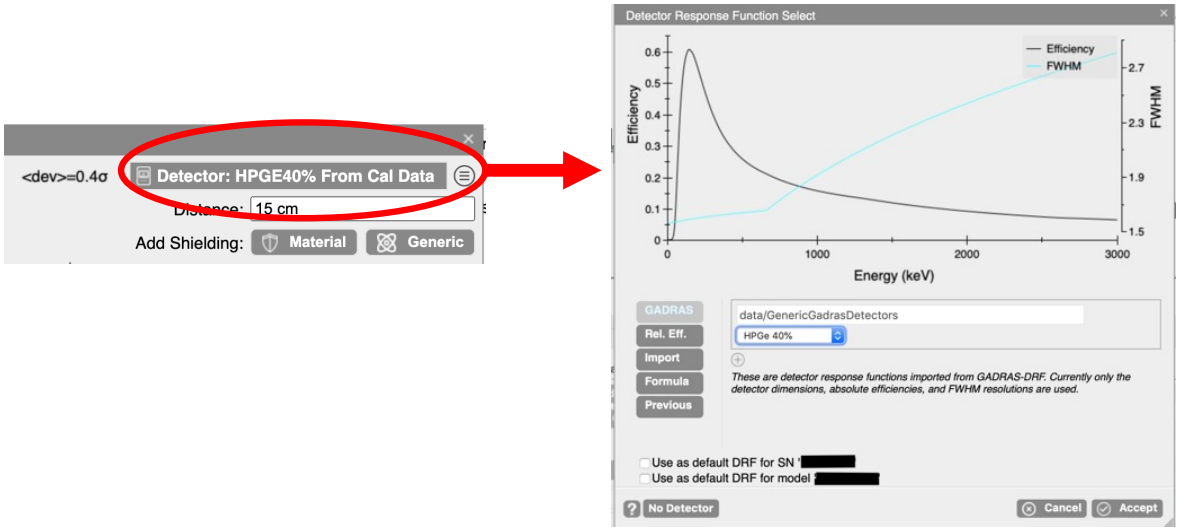


The graphic in this tool is to help provide you an idea of how well the data lines up to the model

- Left: chart shows you how many statistical deviations each peak is away from the best-estimate answer
- Right: chart shows you the multiple of how far away from the model each peak-area is. The error bars are 1-sigma statistical uncertainties.
  - E.x., if the dot corresponding to a peak is at 2.0, that indicates that peak would give double the activity that is currently showing

Generally, if after doing a "Perform Model Fit," a peak is greater than maybe 5-or-so-sigma away from the nominal value, you should consider removing that peak from the fit, or checking that its associated with the correct gamma line, or that there isn't an interfering nuclide that you aren't currently fitting for

Activity/Shielding Fit Tool: Detector Response Functions



If you click/tap on the detector area, it will bring up this dialog

- InterSpec includes a few generic Detector Response Functions (DRF)
- You can load DRFs from a few different common sources
- You can enter a mathematical formula for efficiency as a function of energy

The “Make Detector Response” tool can also be used to create your own DRF from characterization data

Generally the same DRF can be used for all detectors of the same model

Detector response functions not further covered in this presentation

Activity/Shielding Fit Tool – some words of caution

This tool really does require your critical thinking and spectroscopy knowledge.

You can shoot yourself in the foot.

And its also not magic. You can only fit for as many quantities as you have peaks for. So for Cs137, you can only fit for activity or shielding thickness; not both, or not the atomic number of shielding.

If you are fitting for the atomic number of shielding, you generally will need one or more peaks below 300 keV.

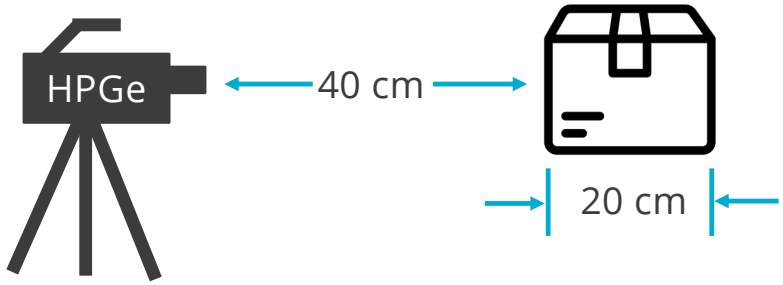
And you always need to ask yourself if the result makes sense.

And you should always add additional uncertainties for things like distance, or the detector response function, or a million other things.

Example Problem setup:

A 20cm x 20cm x 20cm package is found to be radioactive

A 20 minute spectrum is taken, 40 cm from surface of package using HPGe detector

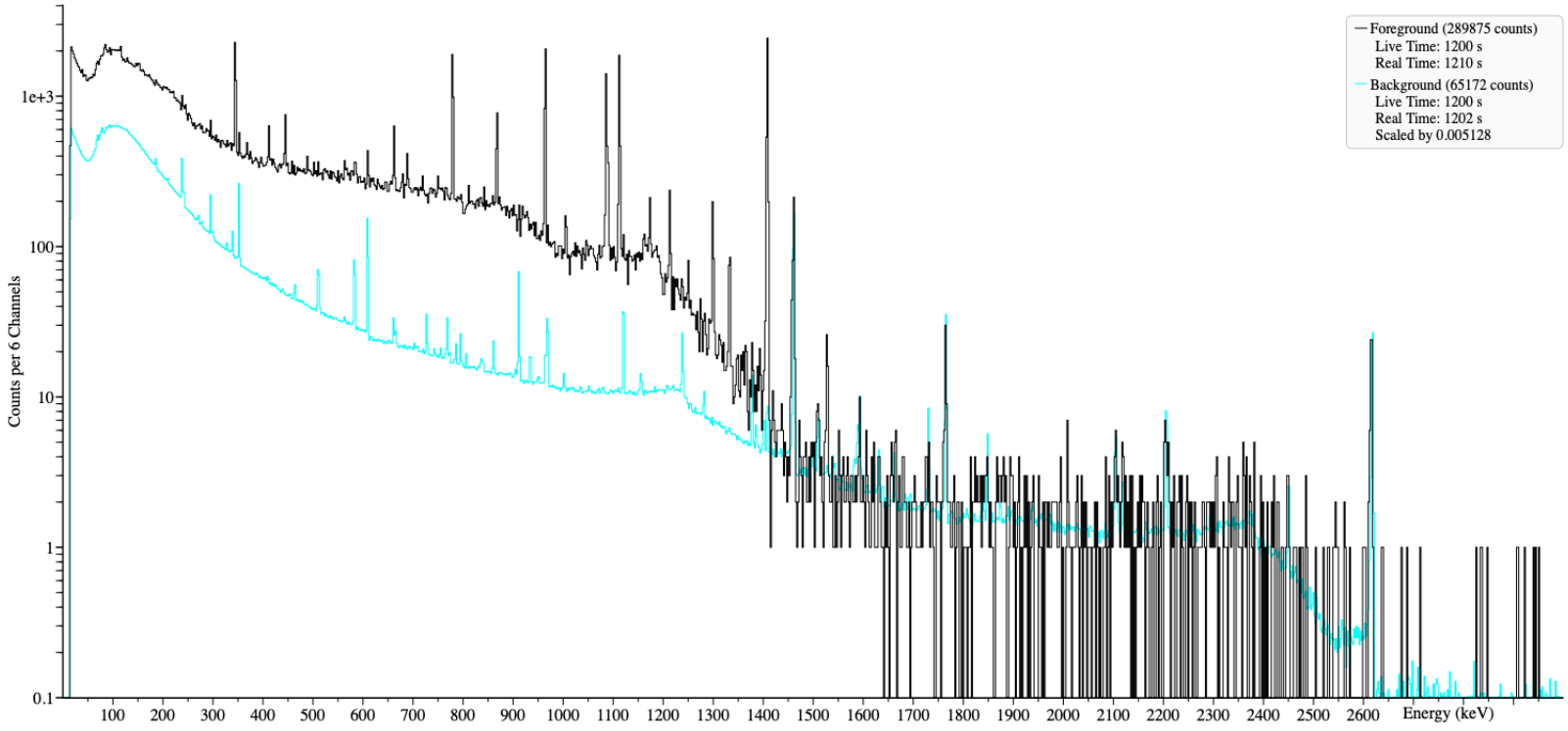


Please: open ”example_problem_1.n42”, perform nuclide identification and quantification

Assume Lead (Pb) shielding, and source is centered in box

For convenience, the detector response function and background spectrum is included in the N42 file

Spectrum to be evaluates (only contains Eu152)



True Answer:

Eu-152

Result: 449 ± 6 kBq (12.1 ± 0.2 μCi)

6.3 ± 0.1 mm Pb shielding

Truth: 451 ± 3 kBq (12.2 ± 0.1 μCi)

7.0 mm Pb shielding

Uncertainties are 1-σ, statistical only.