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BATCH PEAK, ACTIVITY, AND SHIELDING FITTING IN INTERSPEC – REV 2

Automating in-situ analysis, common lab measurement, or analysis of larger datasets

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Org. 08647

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U.S. DEPARTMENT OF ENERGY | NNSA

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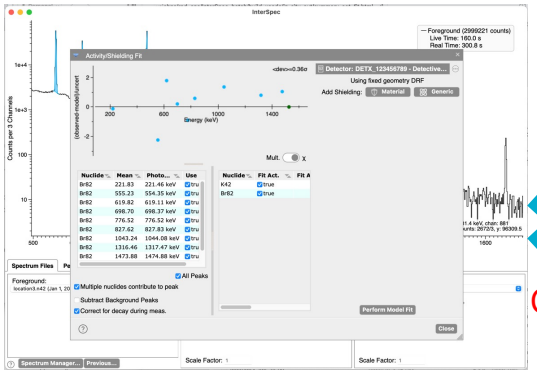
SOME NOTES

- This presentation is using the “bleeding edge” build of InterSpec, available as of 20250611
  - https://github.com/sandialabs/InterSpec/releases/tag/bleeding-edge
    - This is an automated build that gets updated every time code is pushed to the repository
  - V1.0.13 contains the “command line” batch tool, and it is expected v1.0.14 will contain the GUI version of the tool (including for macOS)
- This presentation also assumes basic working knowledge of using InterSpec
  - See https://sandialabs.github.io/InterSpec/ for tutorials and short use videos
- This “batch” processing feature is brand new, and still being tested
  - Bug reports, feature requests, suggestions, and complaints are greatly appreciated!
    - InterSpec@sandia.gov

GENERAL IDEA

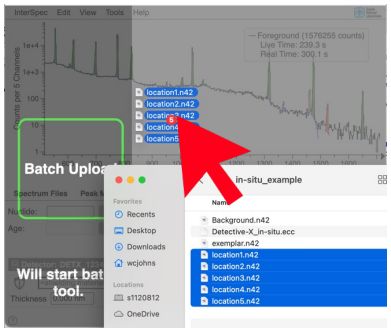
GENERAL PROCESS

Assuming you have many similar measurements you would like to analyze, you can either use GUI or command line tools

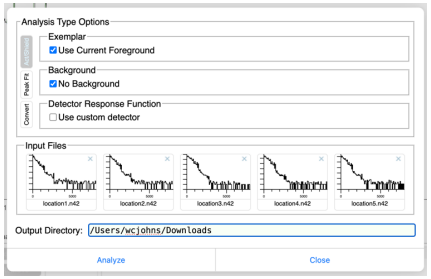


Perform an analysis, on a representative spectrum, referred to as the “exemplar”, as normal in InterSpec

GUI

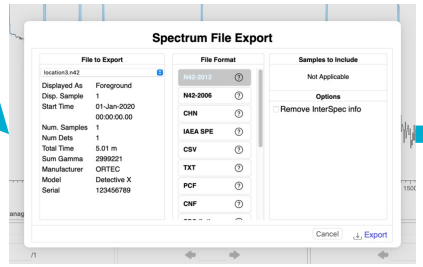


Drag all the files you want to analyze onto InterSpec



Set the options you want in GUI and hit “Analyze”

Command Line

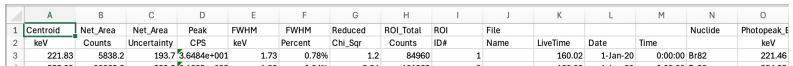


Export the spectrum as a N42-2012 file. This will save all fit peaks, nuclide IDs, Energy calibration, detector efficiency function, and your Activity/Shielding fit, into a N42 file

From the command line, tell `InterSpec_batch`, where the exemplar file is, where the other input files are, and any other options – all other files will then be quickly analyzed in a similar fashion to the exemplar

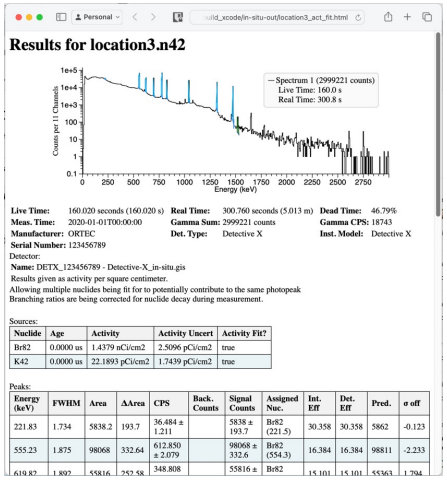
WHAT YOU'LL GET OUT – BY DEFAULT

A text file, for each input-file, that contains results + lots of calculation details



Centroid	Net_Area	Net_Area	Peak	FWHM	FWHM	Reduced	ROI_Total	ROI	File				Nuclide	Photopeak_E
keV	Counts	Uncertainty	CPS	keV	Percent	Chi_Sqr	Counts	ID#	Name	LiveTime	Date	Time		keV
221.83	5838.2	193.7	5.6484e+001	1.73	0.78%	1.2	84960	1		160.02	1-Jan-20	0:00:00	Br82	221.46
555.23	98068.3	332.6	6.1285e+002	1.88	0.34%	2.64	121969	2		160.02	1-Jan-20	0:00:00	Br82	554.35
619.82	55816.2	252.6	3.4881e+002	1.89	0.31%	1.23	70917	3		160.02	1-Jan-20	0:00:00	Br82	619.11
698.7	33250.7	194.7	2.0779e+002	1.93	0.28%	1.44	41782	4		160.02	1-Jan-20	0:00:00	Br82	698.37
776.52	91184.8	310.4	5.6983e+002	1.97	0.25%	4.63	98517	5		160.02	1-Jan-20	0:00:00	Br82	776.52
827.62	25229.6	170.4	1.5767e+002	2	0.24%	1.28	30822	6		160.02	1-Jan-20	0:00:00	Br82	827.83
1043.24	24814.6	164.8	1.5507e+002	2.08	0.20%	2.65	28549	7		160.02	1-Jan-20	0:00:00	Br82	1044.08
1316.46	20796.5	147.5	1.2996e+002	2.2	0.17%	1.71	22130	8		160.02	1-Jan-20	0:00:00	Br82	1317.47
1473.88	11889.3	110	7.4299e+001	2.32	0.16%	1.45	12440	9		160.02	1-Jan-20	0:00:00	Br82	1474.88
1523.66	200.8	15.8	1.2546e+000	2.58	0.17%	1.47	333	10		160.02	1-Jan-20	0:00:00	K42	1524.6

For each input file, a CSV of peak fits



For each input file, a stand-alone HTML file with tables of info, and an interactive spectrum (zoom in/out) you can inspect peak fits with

A single HTML file with spectra and results summary for all input files

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	Setup													
2	Analysis time : 20240916T225201.133174													
3	Working dir : /Users/wcjohns/rad_ana/InterSpec_batch/build_xcode													
4	Exe build date : InterSpec build date: Sep 16 2024													
5	Exe build date : InterSpec build date: 20240913													
6	Exe path : /Users/wcjohns/rad_ana/InterSpec_batch/build_xcode/Debug/InterSpec													
7														
8	Exemplar File : ./in-situ_example/exemplar.n42													
9														
10														
11														
12	Filename	Nuclide	Activity	ActivityUnce	ActivityUnce	Activity (uCi	ActivityUnce	Activity (pCi	ActivityUnce	Activity (bq)	ActivityUnce	Activity (me	ActivityUnce	NuclideAge
13	Warnings:													
14	No peak assigne	not using this nuclide.												
15	location1.n42	Br82	37.4927 pCi/	313.3859 fCi	0.84%	3.74926933	3.13385860	37.4926933	0.31338586	1.38722965	0.01159527	1.38722965	1.15952766	0.0000 us
16	location2.n42	Br82	118.5423 pC	548.7810 fCi	0.46%	0.00011854	5.48780928	118.542295	0.54878096	4.38606492	0.03030649	4.38606492	2.03048566	0.0000 us
17	location2.n42	K42	1.3040 pCi/c	343.4347 fCi	26.34%	1.30396213	0.43434743	1.30396213	0.43434743	0.04824658	0.01270708	4.82465988	1.27070854	0.0000 us
18	location3.n42	Br82	1.4379 nCi/c	2.5096 pCi/c	0.17%	0.00143789	2.50961034	1437.89120	2.50961035	53.2019746	0.09285558	5.32019746	9.28555828	0.0000 us
19	location3.n42	K42	22.1893 pCi/	1.7439 pCi/c	7.86%	2.21893130	1.74390244	22.1893130	1.74390244	0.82100400	0.06452439	8.21004006	6.45243906	0.0000 us
20	location4.n42	Br82	501.4257 pC	1.2094 pCi/c	0.24%	0.00050143	1.20941436	501.425679	1.20941436	18.5527501	0.04474833	1.85527501	4.47483308	0.0000 us
21	location4.n42	K42	6.9501 pCi/c	796.8582 fCi	11.46%	6.95014275	7.96858225	6.95014275	7.96858225	0.25715528	0.02946375	2.57155281	2.94837543	0.0000 us
22	location5.n42	Br82	164.2800 pC	644.8082 fCi	0.39%	0.00016428	6.44808235	164.279966	6.64808235	0.07835676	0.02385795	6.07835676	1.38579046	0.0000 us
23	location5.n42	K42	1.6748 pCi/c	370.6350 fCi	22.13%	1.67483018	0.37083027	1.67483018	0.37083027	0.06196871	0.01371349	6.19687168	1.37134900	0.0000 us

A CSV file with analysis summary of all files

For each input file, peak fits are also saved to an N42 file.

You can also create custom report output format

OPERATIONS AVAILABLE FOR BATCH ANALYSIS:

- All features of the Activity/Shielding fit tool can be used in batch mode
  - Fitting for activities, nuclide ages, accounting for interferences between nuclides, trace sources, self-attenuating sources, shielding thicknesses, spherical, cylindrical (end and side-on), and rectangular geometries, enrichments, etc
- The energy calibration (that you possibly corrected) of the exemplar can be used with the other input files
  - You can also get minor updates to that by having the batch analysis fit for energy calibration based off the fit peaks
- All peak-fitting possibilities are allowed (various peak skews, sharing ROIs, continua type, fixing FWHM, etc)
- You can specify background file to either peak-by-peak subtraction, or a “hard” background subtraction (i.e., channel-by-channel)
- You can also choose to just fit for peaks, instead of activities and such

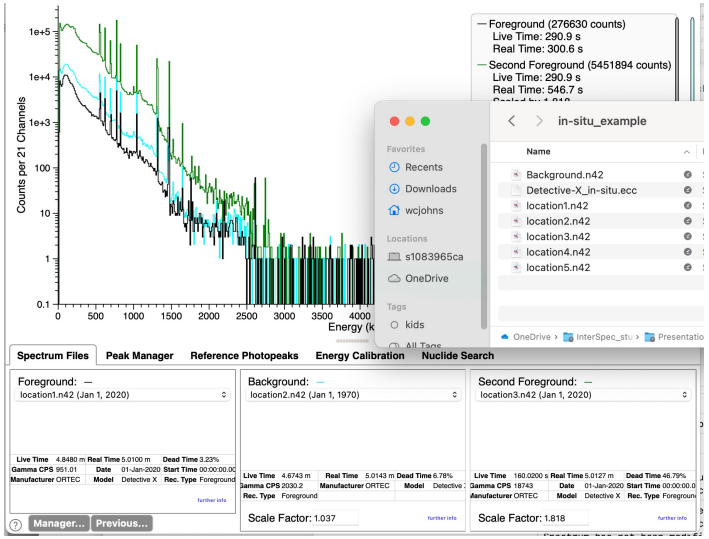
LIMITATIONS OF THE BATCH ANALYSIS

- Only peaks, and nuclides in the “exemplar” file are fit for
- The activity and shielding fit setup has to be the same for all similar input files
- You have to perform the analysis in the exemplar file first in InterSpec
- Use and testing has so far been pretty limited – let us know if you find issues
- The “Isotopics from peaks”, “Isotopics by nuclides”, “Detection Confidence Tool”, or “Flux Tool” have not been implements for batch analysis
  - Let InterSpec@sandia.gov know if these would be useful to you

IN-SITU EXAMPLE

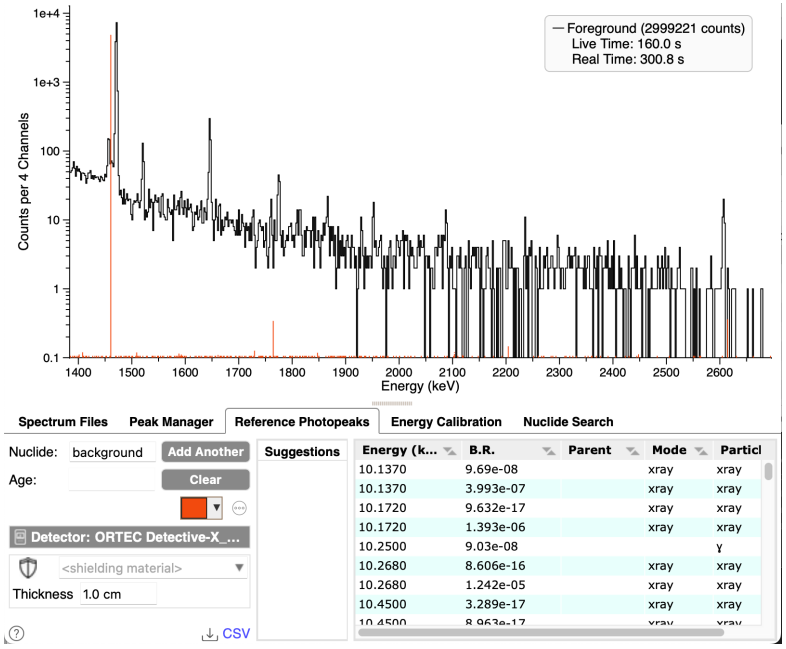
- Setup: there was a contamination event and in-situ measurements where taken at various places throughout the region, with a Detective-X detector, 1 meter from the ground, pointed down.
- Please see the included “in-situ_example” directory for 5 data files, a background, and the “Detective-X_in-situ.ecc” file, which is the expected full-energy peak efficiency for the detector for surface contamination, computed using ISOCs
- We will step through the batch analysis process in the following slides

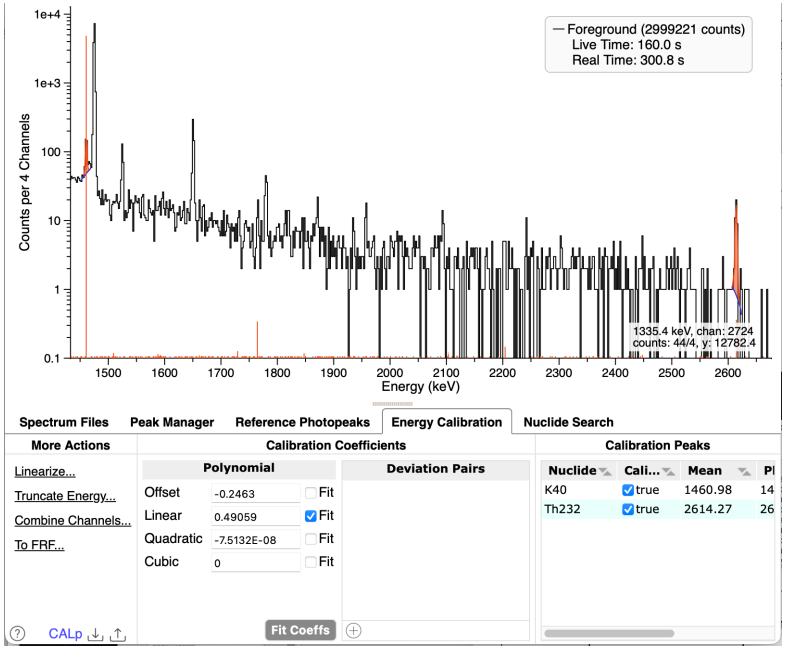
IN-SITU EXAMPLE – STEP 1: PICK EXEMPLAR



- Pick the file to use as as the “exemplar”
  - This file should have all the peaks you might want to use for activity analysis
  - Usually you can just quickly compare the spectra against each other, and use the file with the most peaks, if it even matters
- After picking the “exemplar”, load that file as the foreground, using the “Spectrum Files” tab

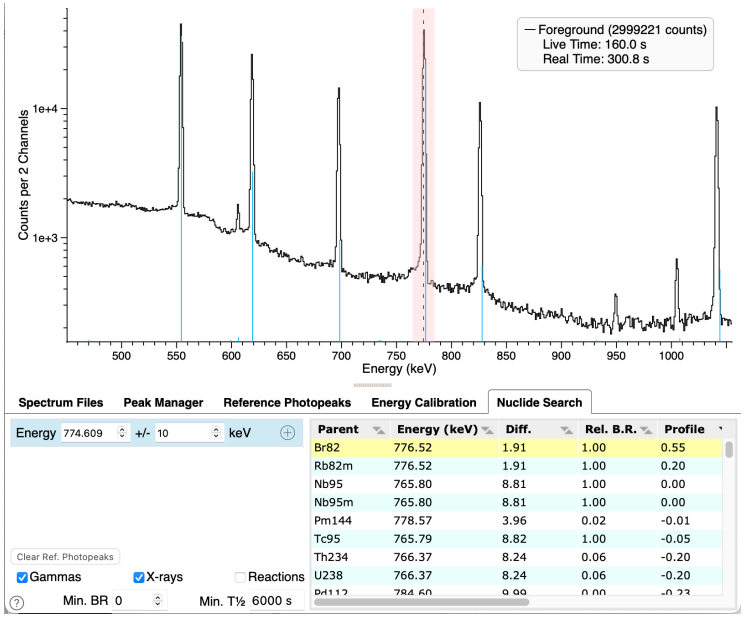
IN-SITU EXAMPLE – STEP 2: CHECK ENERGY CAL





- Check, and fix, the energy calibration
  - For these spectra, show either the “background” or “K40” reference lines, and then double click on what should be the 1460 keV peak and/or 2614 keV peak
  - K40 should have been associated with the peak at ~1457 keV when you fit it, if you were showing the reference lines. If not, please associate K40 with the peak by using “Peak Editor”, or ”Peak Manager” tab. Similar for 2614 keV peak
  - Go to the “Energy Calibration” tab, and select to fit only the “Linear” energy calibration coefficient, then hit “Fit Coeffs” button

IN-SITU EXAMPLE – STEP 3: NUCLIDE ID



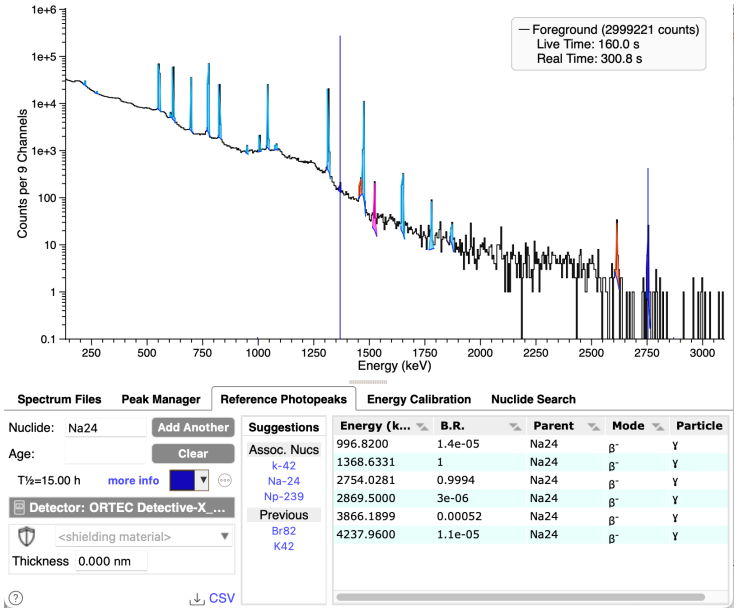
- Select the “Nuclide Search” tab, and then click near the mean of one of the larger non-background peaks – this will fill this energy to search on, and the result table will populate
  - Click the different result rows to find which nuclide is a candidate – shown above the first result of Br82 matches well

IN-SITU EXAMPLE – STEP 3: PEAK FIT

Tip: clicking the “more info” link, and/or checking for the presence of associated nuclides is useful

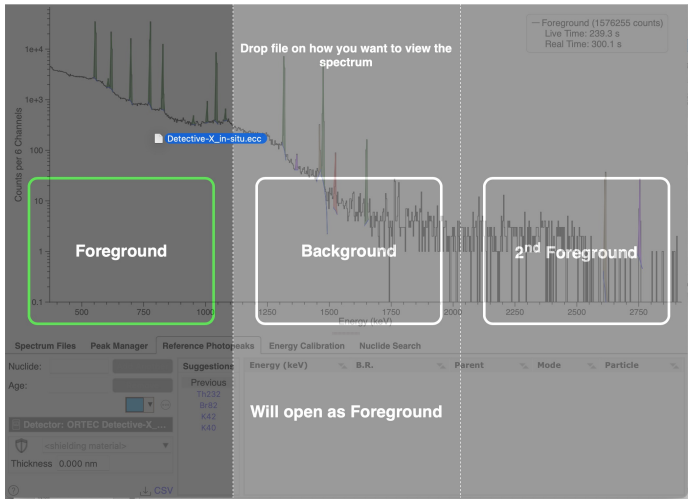
- Fit peaks explained by this nuclide
  - Usually double-clicking on the spectrum near the peak is good enough
  - You can also use the “Search for Peaks” button on the “Peak Manager” tab

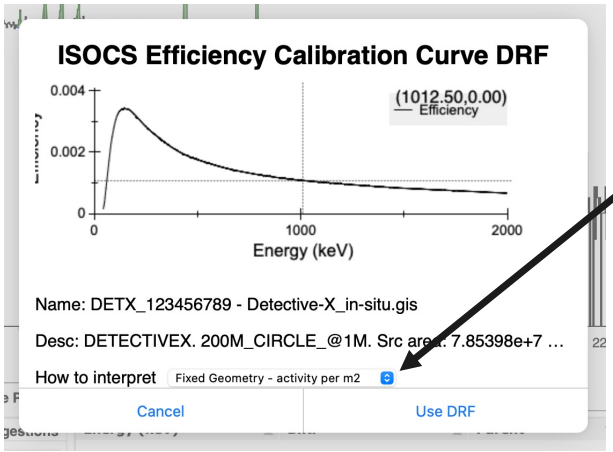
IN-SITU EXAMPLE – STEP 4: REPEAT STEPS 2 AND 3



- For any unidentified, non-background peaks, repeat steps 2 and 3, of performing nuclide ID and fitting the peaks
  - For this example, both K42 and Na24 that were shown as associated with Br82 are present

IN-SITU EXAMPLE – STEP 5: LOAD DETECTOR EFFICIENCY FUNCTION



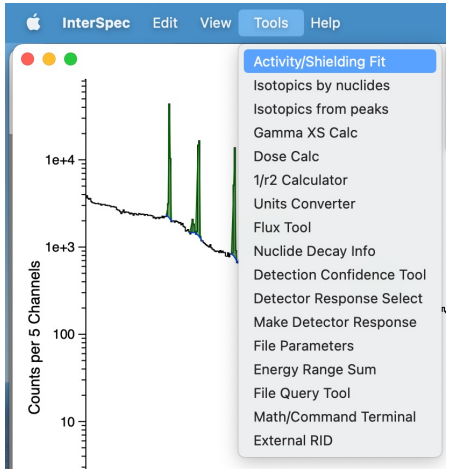


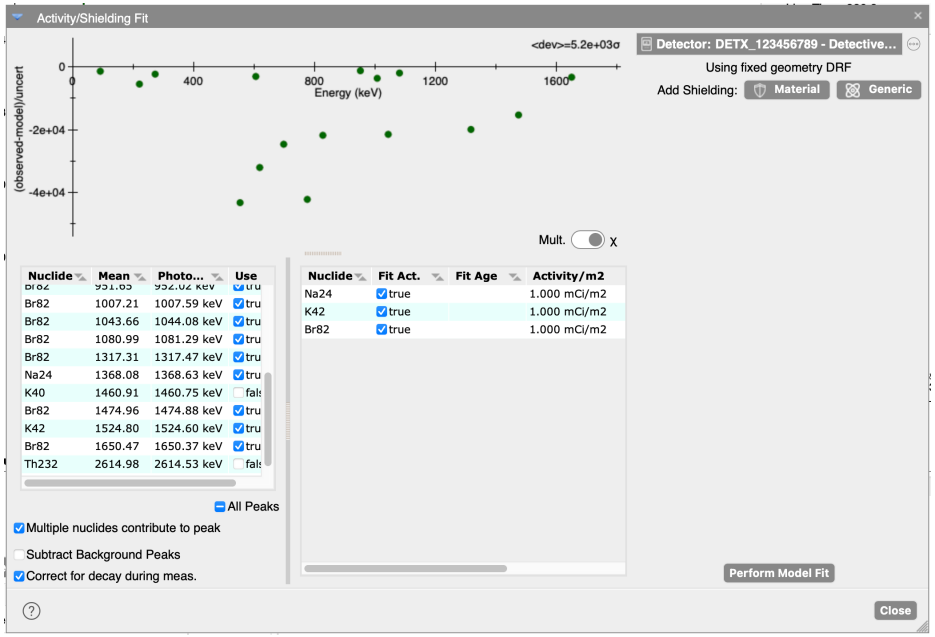
Select this det. efficiency is for activity per m^2

- Drag-n-drop the “Detective-X_in-situ.ecc” file onto InterSpec
  - You will then get a dialog asking how to interpret this file
    - This efficiency was made to be in activity meter square meter in ISOCS.
  - Then click the “Use DRF” button

Note: InterSpec comes with many detector efficiency functions, or there are a number of other ways to load, or sources of, detector efficiency functions - this is example is specific to using an ISOCS result

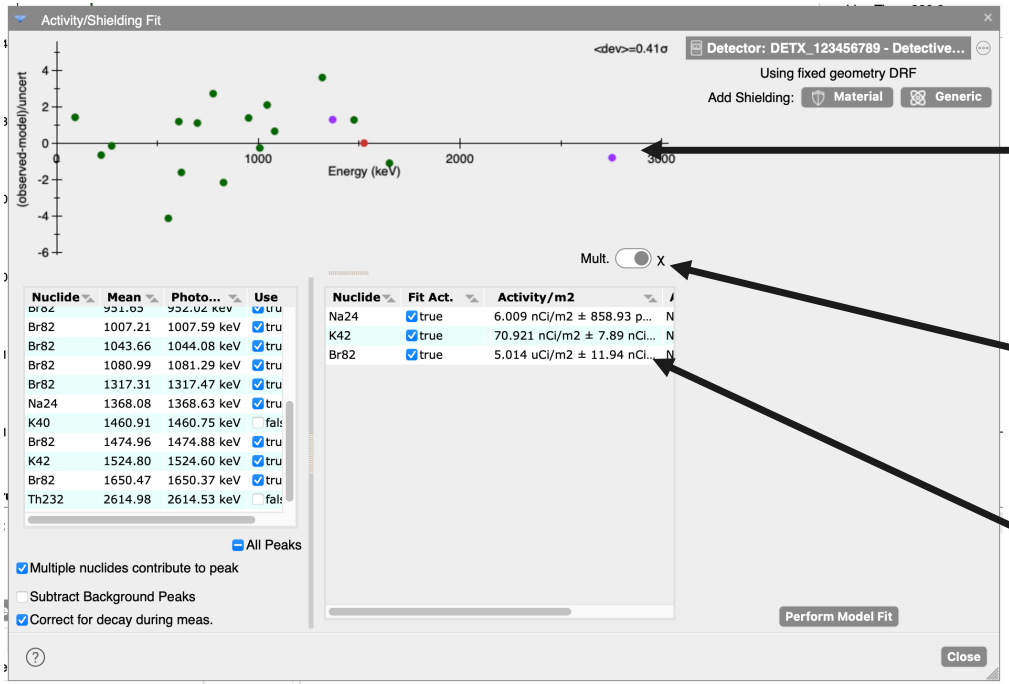
IN-SITU EXAMPLE – STEP 6: FIT ACTIVITIES





- From the tools menu, go to “Activity/Shielding Fit”
- From left-hand side, select which peaks you would like to use
  - If you fit any background peaks, at a minimum, you probably want to de-select those
- We don’t need any shielding, or background subtraction, nuclide ages, or anything else for this simple problem, but if your problem requires these things, you would set them up now

IN-SITU EXAMPLE – STEP 6: FIT ACTIVITIES (CONT)



These dots show within how many statistical sigma each peak is to the final answer – should be scattered between around ±5

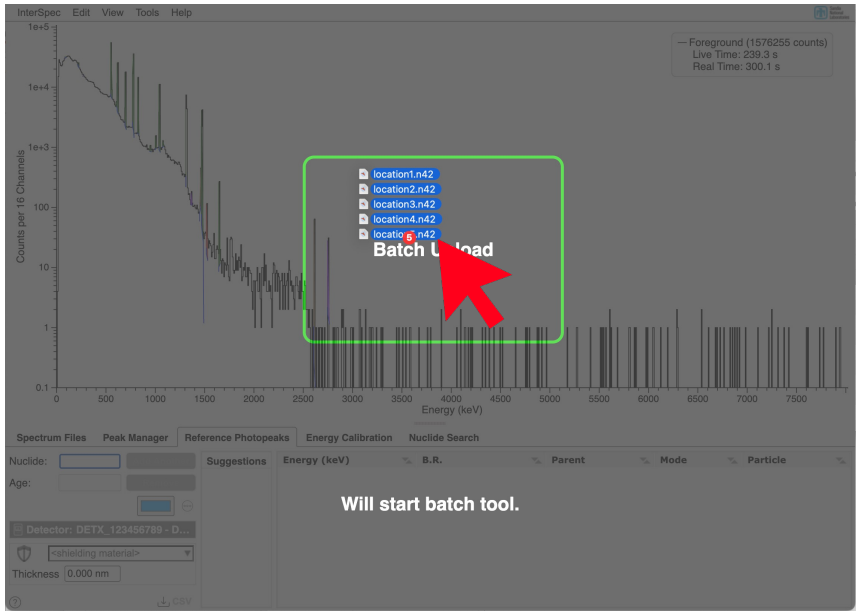
Some people prefer to instead look at the activity multiple of each peak – use this switch here

The fit activities are here

- Click “Perform Model Fit” button, and you should get something like the above
- If you choose, you can use only a single peak for each nuclide, or you can use the weighted mean of more than one
  - The primary InterSpec author prefers to use all peaks, to make sure everything is consistent

THE GUI ROUTE

IN-SITU EXAMPLE – STEP 7: DRAG A BUNCH OF FILES ONTO INTERSPEC

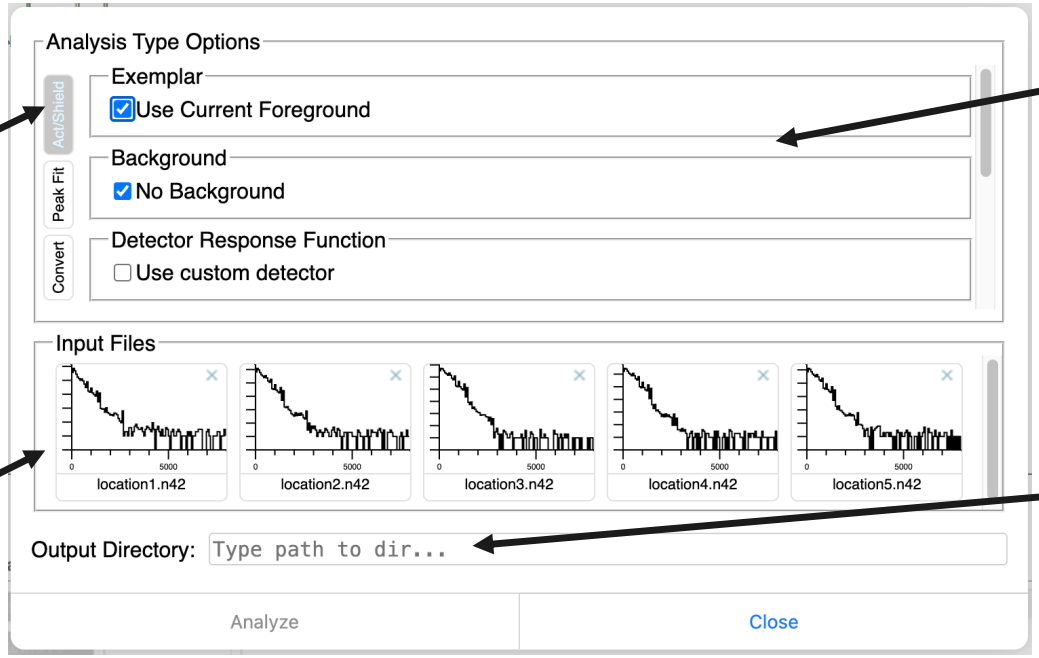


- You might want to save your work by exporting the current file as a N42-2012 file – this will save all your peaks, energy calibration, and Act/Shield fit setup into the N42 file
- From Windows Explorer, macOS Finder, or Linux File manager – drag all the files you want to analyze onto InterSpec, and let go

IN-SITU EXAMPLE – STEP 8: SELECT OPTIONS

Make sure "Act/Shield" analysis type is selected here

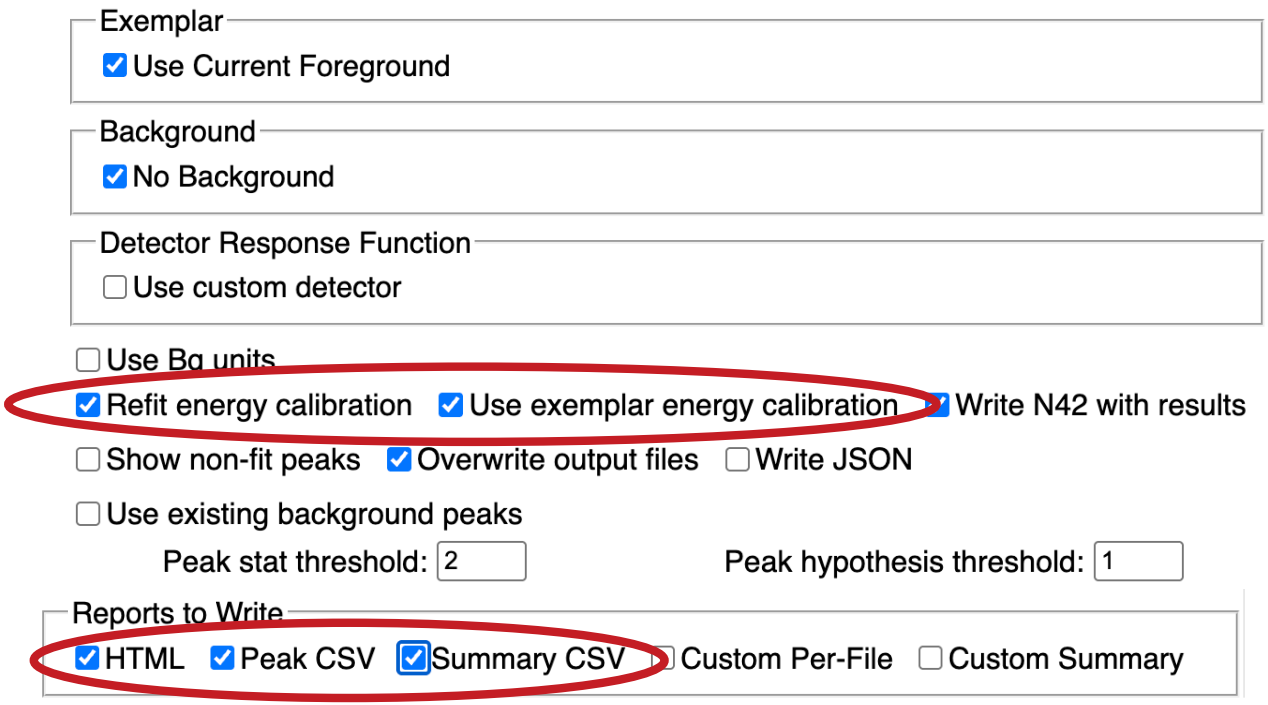
You can drag more files to analyze into this area



There is a bunch of options here, so scroll down

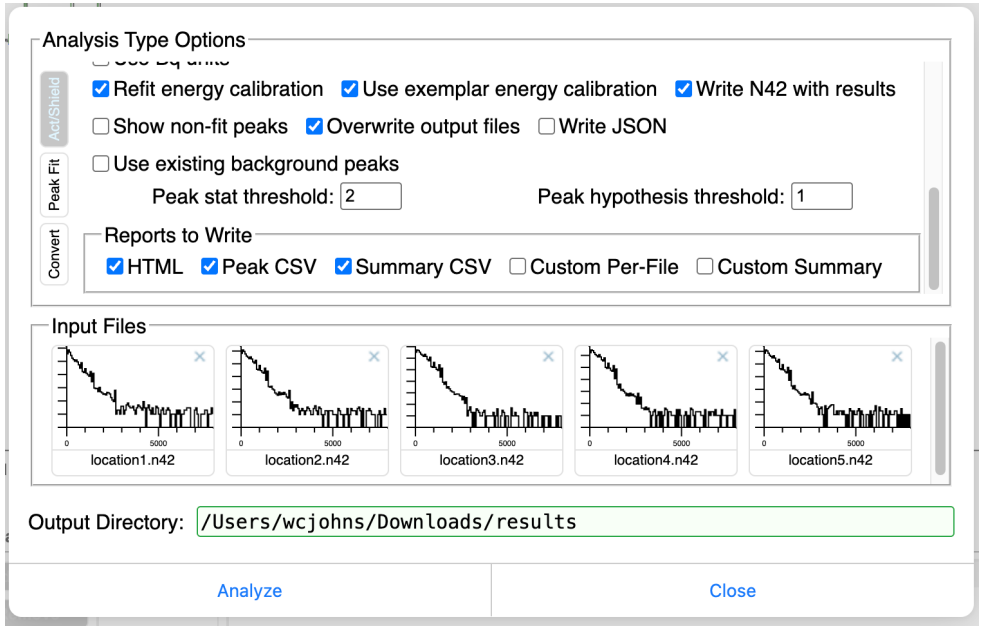
You need to select an output directory to save here (some OS will have a directory chooser)

IN-SITU EXAMPLE – STEP 8: OPTIONS TO SELECT



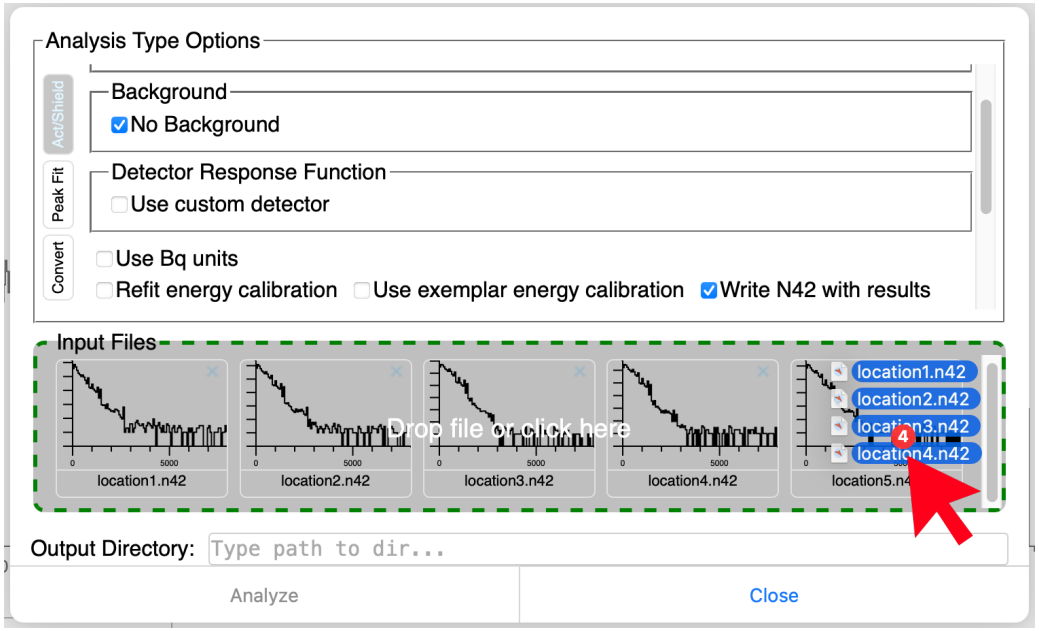
- If you hover your mouse over each of the options, a tool tip will show with further explanation
- These are the same options available from the command line
- For the example problem, choose these options

IN-SITU EXAMPLE – STEP 8: SELECT OUTPUT DIRECTORY



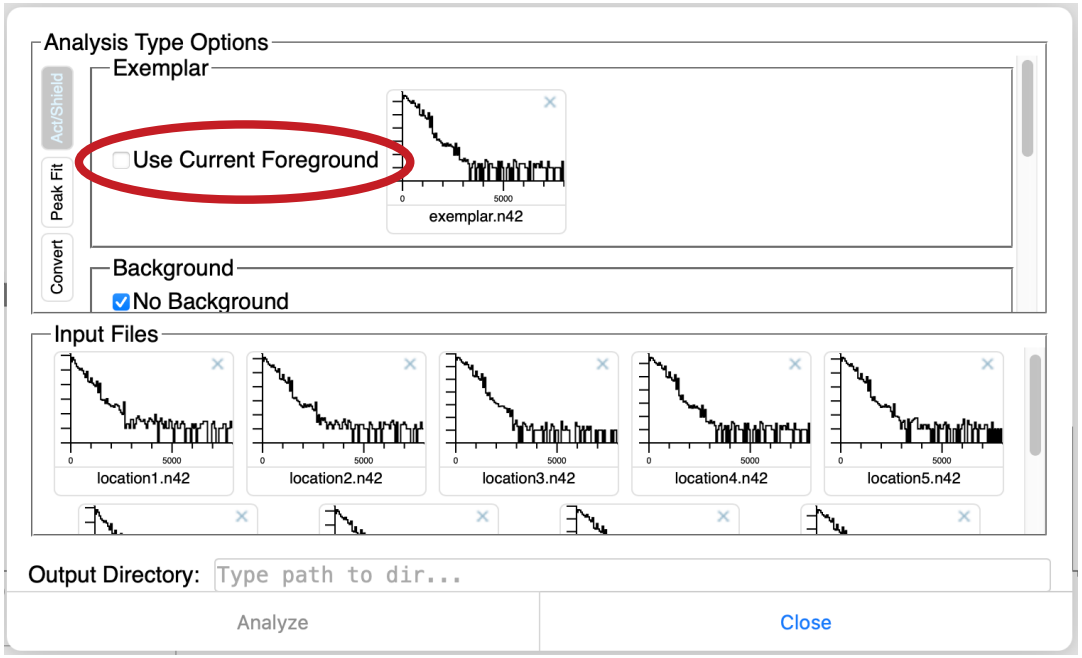
- Depending on the OS/build of InterSpec, you may need to either select the directory, or copy/paste/type in the full path
- If you re-use an output directory from a previous analysis – the results will not be overwritten by default, unless you select the “Overwrite output files” checkbox.

SIDE NOTE:



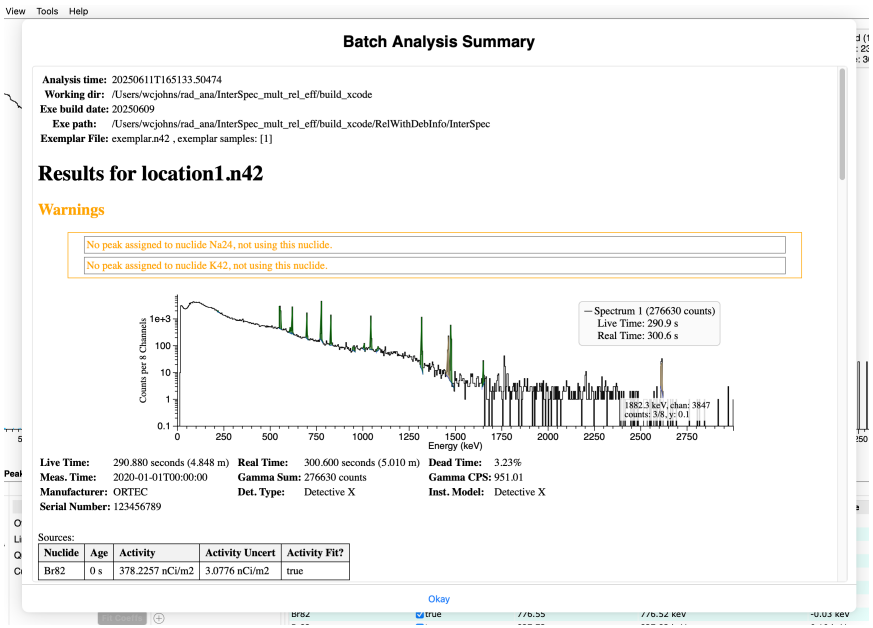
- You can drag-n-drop more input files to the input-files area (or click in an empty space in the area to bring up file browser)
- Same thing for selecting background file, or custom detector efficiency

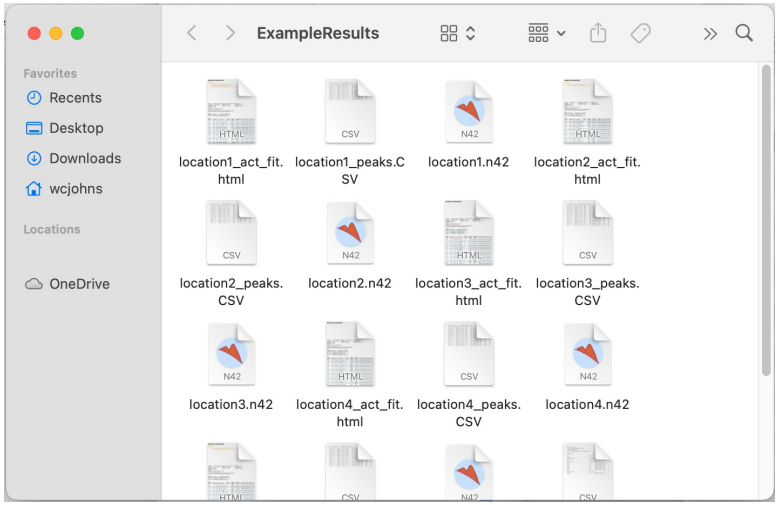
ANOTHER SIDE NOTE



- You don't have to use the currently loaded foreground for your exemplar – you can use a N42 file you exported from InterSpec, that has the exemplar peaks or Act/Shield setup
- Same thing applies to detector efficiency function and background spectrum

STEP 8: RESULTS (MORE DETAILS LATER)

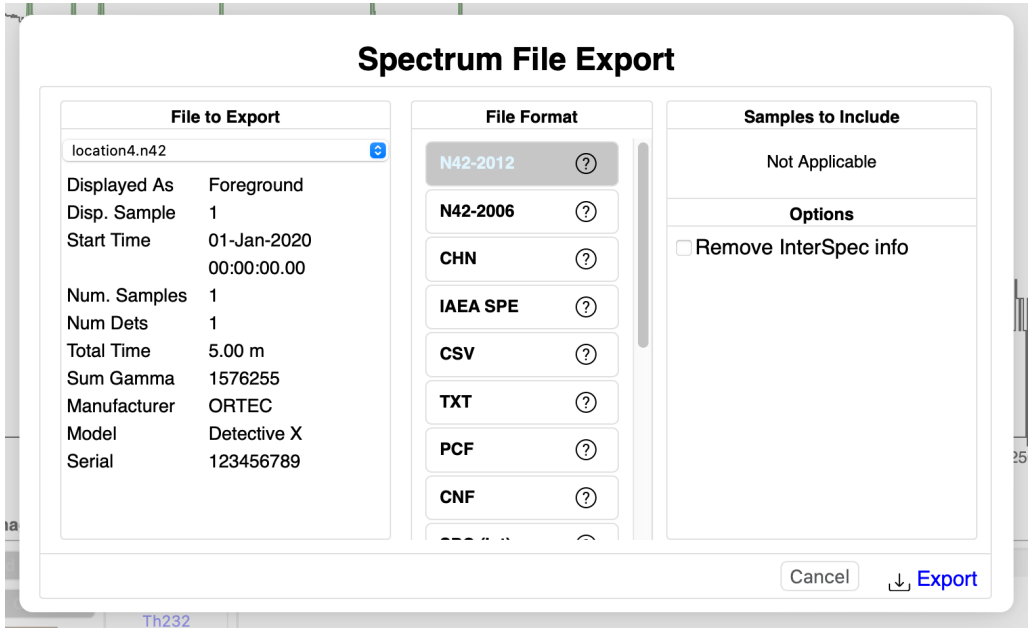




- After the analysis you will get pop-ups with any warnings/errors, as well as a summary of results, that you can scroll through
- You will get a bunch of files in the output directory – some will contain summaries/info from all the files, and some will be for each individual file

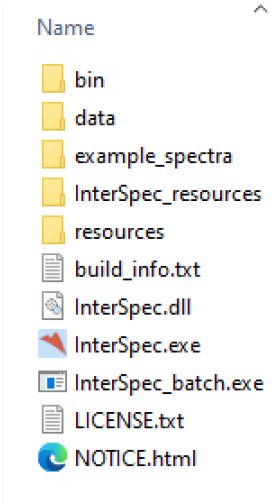
THE COMMAND-LINE ROUTE

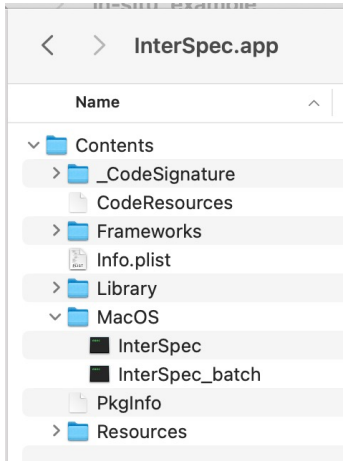
IN-SITU EXAMPLE - COMMAND LINE - STEP 7: EXPORT N42 FILE



- Close the “Activity/Shielding Fit” tool, and go to **InterSpec → Export File…**
- Select N42-2012 format (default), and then click the “Export” button
  - You may want to save the file with something like “exemplar” as the file name

IN-SITU EXAMPLE - COMMAND LINE - STEP 8: RUN BATCH ANALYSIS

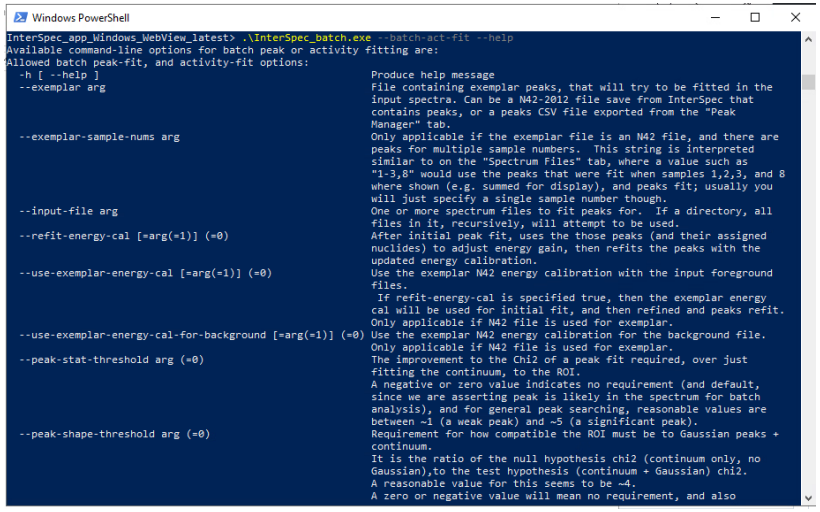




- Starting with InterSpec v1.0.13, or "bleeding edge" builds in September of 2024, InterSpec comes with two executables, the normal GUI application, and "`InterSpec_batch`" to be used from the command line
  - "bleeding edge" build at https://github.com/sandialabs/InterSpec/releases/tag/bleeding-edge
  - On Windows "`InterSpec_batch.exe`" is right next to normal `InterSpec.exe`
  - On macOS, you would access it at `/Applications/InterSpec.app/Contents/MacOS/InterSpec_batch`
  - As of Sep. 2024, the Linux, or "Electron" build for Windows doesn't support batch, but it is expected to just be the same executable as launches the GUI

IN-SITU EXAMPLE - COMMAND LINE - STEP 8: RUN BATCH ANALYSIS (CONT)

- You will need to open up a terminal (Power Shell, or CMD on Windows, and Terminal.app or iTerm on macOS), and all following commands assume Windows, and you have cd'd to the same directory as the InterSpec_batch executable (but this isn't required – just for brevity)
- There are a lot of options, and you can type "InterSpec_batch.exe --help" to get a list of options, and the specific one we are interested in is "--batch-act-fit", so we can get help on this sub-option using:
  InterSpec_batch.exe --batch-act-fit --help



IN-SITU EXAMPLE - COMMAND LINE - STEP 8: RUN BATCH ANALYSIS (CONT)

```
InterSpec_app_Windows_WebView_latest> .\InterSpec_batch.exe --batch-act-fit `
>>     --exemplar .\in-situ_example\exemplar.n42 `
>>     --use-exemplar-energy-cal `
>>     --input-file .\in-situ_example\location*.n42 `
>>     --out-dir in-situ-results
```

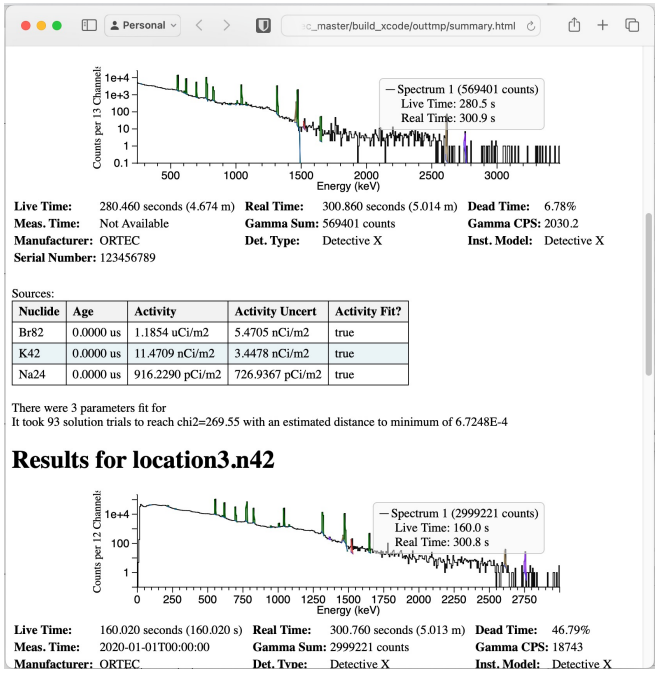
- If you read through the options, the options we want to specify are:
  - --exemplar “\Path\To\Exemplar.n42”
    - This is the N42 file we exported in step 7
  - --use-exemplar-energy-cal
    - This says to use the energy cal we fit in the exemplar, for each of the input foreground files
  - --input-file \Path\To\Input\location*.n42
    - This uses a wildcard (*) to specify all the input files to be analyzed. You could instead type out each one individually
  - --out-dir \Path\To\Results\Output
    - This is the directory to place the results in – it **must** already exist

IN-SITU EXAMPLE - RESULTS

Name	Date modified	Type	Size
location1_act_fit.html	9/27/2024 4:20 PM	Microsoft Edge H...	622 KB
location1_act_fit.txt	9/27/2024 4:20 PM	Text Document	10 KB
location1_peaks.CSV	9/27/2024 4:20 PM	Microsoft Excel C...	5 KB
location2_act_fit.html	9/27/2024 4:20 PM	Microsoft Edge H...	623 KB
location2_act_fit.txt	9/27/2024 4:20 PM	Text Document	10 KB
location2_peaks.CSV	9/27/2024 4:20 PM	Microsoft Excel C...	5 KB
location3_act_fit.html	9/27/2024 4:20 PM	Microsoft Edge H...	625 KB
location3_act_fit.txt	9/27/2024 4:20 PM	Text Document	10 KB
location3_peaks.CSV	9/27/2024 4:20 PM	Microsoft Excel C...	5 KB
location4_act_fit.html	9/27/2024 4:20 PM	Microsoft Edge H...	624 KB
location4_act_fit.txt	9/27/2024 4:20 PM	Text Document	10 KB
location4_peaks.CSV	9/27/2024 4:20 PM	Microsoft Excel C...	5 KB
location5_act_fit.html	9/27/2024 4:20 PM	Microsoft Edge H...	623 KB
location5_act_fit.txt	9/27/2024 4:20 PM	Text Document	10 KB
location5_peaks.CSV	9/27/2024 4:20 PM	Microsoft Excel C...	5 KB
summary.csv	9/27/2024 4:20 PM	Microsoft Excel C...	5 KB
summary.html	9/27/2024 4:20 PM	Microsoft Edge H...	813 KB

- After running the command, you should see contents similar to the above in your specified output directory.
- There is both a HTML and TXT result for each input file
- And there is a summary HTML and CSV file
- What gets output can be customized – will briefly cover later

IN-SITU EXAMPLE – INITIAL RESULTS



	A	B	C	D	E	F	G	H
1	Setup							
2	Analysis time : 20240930T191236.64523							
3	Working dir : /Users/wcjohns/rad_ana/InterSpec_master/build_xcode							
4	Exe build date : InterSpec build date: Sep 28 2024							
5	Exe build date : InterSpec build date: 20240922							
6	Exe path : /Users/wcjohns/rad_ana/InterSpec_master/build_xcode/Debug/InterSpec							
7								
8	Exemplar File : in-situ_example/ex_exemplar.n42							
9								
10								
11								
12	Filename	Nuclide	Activity	ActivityUncertainty	ActivityUncertainty (%)	Activity (uCi)	ActivityUncertainty (uCi)	Activity
13	Warnings:							
14	No peak ass	not using this nuclide.						
15	No peak ass	not using this nuclide.						
16	location1.n4	Br82	378.2924 nC	3.0787 nCi/m2	0.81%	0.378292435	0.003078711	378292
17	location2.n4	Br82	1.1854 uCi/r	5.4705 nCi/m2	0.46%	1.18535712	0.00547053	118535
18	location2.n4	K42	11.4709 nCi/	3.4478 nCi/m2	30.06%	0.011470867	0.00344783	11470.8
19	location2.n4	Na24	916.2290 pC	726.9367 pCi/m2	79.34%	0.000916229	0.000726937	916.229
20	location3.n4	Br82	14.3761 uCi/	25.0019 nCi/m2	0.17%	14.37607905	0.025001861	1437(
21	location3.n4	K42	221.7385 nC	17.8173 nCi/m2	8.04%	0.221738536	0.017817321	221738
22	location3.n4	Na24	7.6880 nCi/r	1.3658 nCi/m2	17.76%	0.00768796	0.001365839	7687.96
23	location4.n4	Br82	5.0143 uCi/r	12.0511 nCi/m2	0.24%	5.01433975	0.012051082	501433
24	location4.n4	K42	70.9220 nCi/	8.1356 nCi/m2	11.47%	0.070922035	0.008135566	70922.(
25	location4.n4	Na24	5.8791 nCi/r	908.8983 pCi/m2	15.46%	0.005879103	0.000908898	5879.1(
26	Warnings:							
27	No peak ass	not using this nuclide.						
28	location5.n4	Br82	1.6434 uCi/r	6.4303 nCi/m2	0.39%	1.643423499	0.006430256	16434
29	location5.n4	K42	16.8760 nCi/	3.7722 nCi/m2	22.35%	0.016876015	0.00377218	16876.(

- The HTML files all contain interactive spectra (you can zoom in/out), showing peak fits, and some basic summary information
- CSV summary file contains just activities
- HTML/TXT files for individual files contain more information than the summary files

IN-SITU EXAMPLE – COMPARISON TO GENIE2K

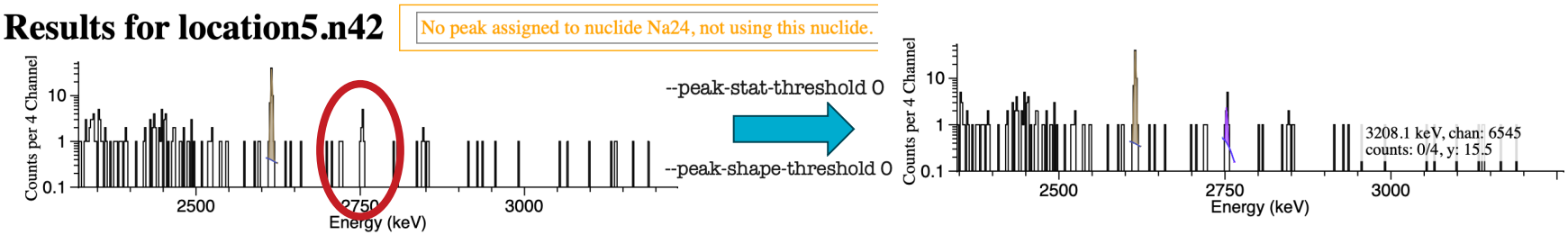
Location	Nuclide	InterSpec Act. (μCi/m²)	Genie2k Act. (μCi/m²)
1	Br82	0.378292	0.383800
3	Br82	14.376079	14.270000
	K42	0.221739	0.205800
4	Br82	5.014340	5.038000
	K42	0.070922	0.067150
5	Br82	1.643423	1.641000

- A standard FRMAC analysis sequence was used with Genie2k, using the same detector efficiency, to compare activities
  - Activities below a pre-set detection threshold not shown
  - There was an error analyzing location 2 in Genie2k, so it is not shown
  - Key lines were used in G2K, but weighted average of peak used in InterSpec
- Results the same, within expectations

ADDITIONAL COMMAND LINE OPTIONS

- Command-line options you can read about if you "InterSpec_batch.exe --batch-act-fit --help"
  - help,
    ini-file,
    exemplar, exemplar-sample-nums,
    refit-energy-cal, use-exemplar-energy-cal, use-exemplar-energy-cal-for-background,
    peak-stat-threshold, peak-shape-threshold,
    back-sub-file, background-sample-nums, hard-background-subtract,
    use-existing-background-peaks,
    include-nonfit-peaks,
    out-dir, overwrite-output-files,
    write-n42-with-results, peak-csv-output, result-json-output, print,
    file-report-template, summary-report-template, report-template-include-dir
    drf-file, drf-name,
    distance,
    use-bq
- The more notable options will be explained in the next few slides

COMMAND LINE OPTIONS – PEAK THRESHOLDS



The default peak threshold settings cause the 2754 keV Na24 peak of "location 5" file to not be fit

--peak-stat-threshold arg (=0)	The improvement to the Chi2 of a peak fit required, over just fitting the continuum, to the ROI. A negative or zero value indicates no requirement (and default, since we are asserting peak is likely in the spectrum for batch analysis), and for general peak searching, reasonable values are between ~1 (a weak peak) and ~5 (a significant peak).
--peak-shape-threshold arg (=0)	Requirement for how compatible the ROI must be to Gaussian peaks + continuum. It is the ratio of the null hypothesis chi2 (continuum only, no Gaussian),to the test hypothesis (continuum + Gaussian) chi2. A reasonable value for this seems to be ~4. A zero or negative value will mean no requirement, and also no'peak-stat-threshold' requirement.

- By default, InterSpec requires peaks to be *something like* 2 sigma significant, and to match the data better than just a continuum, but we can adjust these settings
- --peak-stat-threshold
  - This is roughly stat significance improvement over just a flat continuum – but if you think of it as number of sigma significant the peak is, it is close-enough
- --peak-shape-threshold
  - Ratio of null-hypothesis χ^2 (i.e., continuum only) to χ^2 of continuum + Gaussian

COMMAND LINE OPTIONS – MORE USEFUL OPTIONS

- --overwrite-output-files
  - By default the output files wont be overwritten, if you run the analysis again, this option lets you overwrite them, in case you are running many times
- --peak-csv-output
  - Write CSVs of the peaks fit for each input file – these are same CSV file you can download from the "Peak Manager" tab, or that can be saved from Peak Easy
- --write-n42-with-results
  - Will write N42 files, with the fit peaks in them, for each input file; will eventually include the Act/Shield Fit setup
- --use-exemplar-energy-cal, --use-exemplar-energy-cal-for-background
  - Use the exemplars energy calibration for the input foreground, and/or background
- --refit-energy-cal
  - If specified, after fitting peaks (and if specified using exemplar energy cal), will fit the energy calibration coefficients - will then re-fit the peaks. Useful for small energy cal drifts during measurements, because the ROIs are defined by energy, so this helps in getting consistent ROI extents
- --back-sub-file, --hard-background-subtract
  - If signal peaks overlap background peaks, you can account for this by specifying a background spectrum file. By default InterSpec will try to fit peaks in the background, and then do a peak-by-peak subtraction, unless you specify a "hard" background subtraction, then the background will be subtracted on a channel-by-channel basis

USING A INI FILE TO SPECIFY COMMAND-LINE ARGUMENTS

- Typing everything can be tedious, so you can instead use a combination of a INI file, and command-line options
- Any option specified in the INI file, will be overruled if the option is specified on the command-line
- If you save this file as "InterSpec_batch.ini" in your current working directory, it will automatically be used.
  Or you can specify the INI file explicitly like:
  "InterSpec_batch.exe --batch-act-fit --ini-file config.ini ..."
  - You still need to specify "--batch-act-fit" on the command-line
  - You also probably want to specify "--input-file" on the command line, so you can use wildcard (*) to list many files easily

Using the INI file shown, the command would then be:

```
InterSpec_batch.exe --batch-act-fit --ini-file config.ini
```

```
# A example default batch activity INI file

# the out-dir must exist, or you will get an error
out-dir = result_dir

# Allow overwriting previous results in case we need
# to run multiple times to get options right
overwrite-output-files = true

# Use the corrected energy cal in the exemplar for the input files
use-exemplar-energy-cal = true

# Dont use exemplar energy cal for background - it was corrected
# manually already
use-exemplar-energy-cal-for-background = false

# Require the peaks to be reasonable shape and significance
peak-stat-threshold = 3
peak-shape-threshold = 2

# Lets not bother refiting energy cal for each input file, the
# calibration looks stable for all input files
refit-energy-cal = false

# Exemplar file to use
exemplar = in-situ_example/exemplar.n42

# If you want to specify input foreground files, you can specify
#  'input-file' multiple times - but you can not use wildcards.
input-file = in-situ_example/location1.n42
input-file = in-situ_example/location2.n42
input-file = in-situ_example/location3.n42
input-file = in-situ_example/location4.n42
```

Example config.ini file contents

CUSTOMIZING OUTPUT REPORTS

- The output of the analysis can be highly customized
- InterSpec uses the wonderful {{ inja }} templating library to create the output files; you can specify for InterSpec to use a template file that you choose.
  - For example, a simple template to make a CSV of the activity, of all files could be:

```
## for file in Files
## if existsIn(file,"Sources")
## for src in file.Sources
{{ file.Filename }}, {{ src.Nuclide }}, {{ src.Activity_uCi }}, {{ src.ActivityUncert_uCi }}
## endfor
## endif
## endfor
```

  - This loops over all input files, and prints a line for each fit nuclide, giving its activity and uncertainty, in uCi.
  - If you saved the above as my_summary.tmplt.csv, then you would specify to use it as:

    InterSpec_batch.exe --batch-act-fit --summary-report-template my_summary.tmplt.csv ...

    And the output would be my_summary.csv in the specified output directory

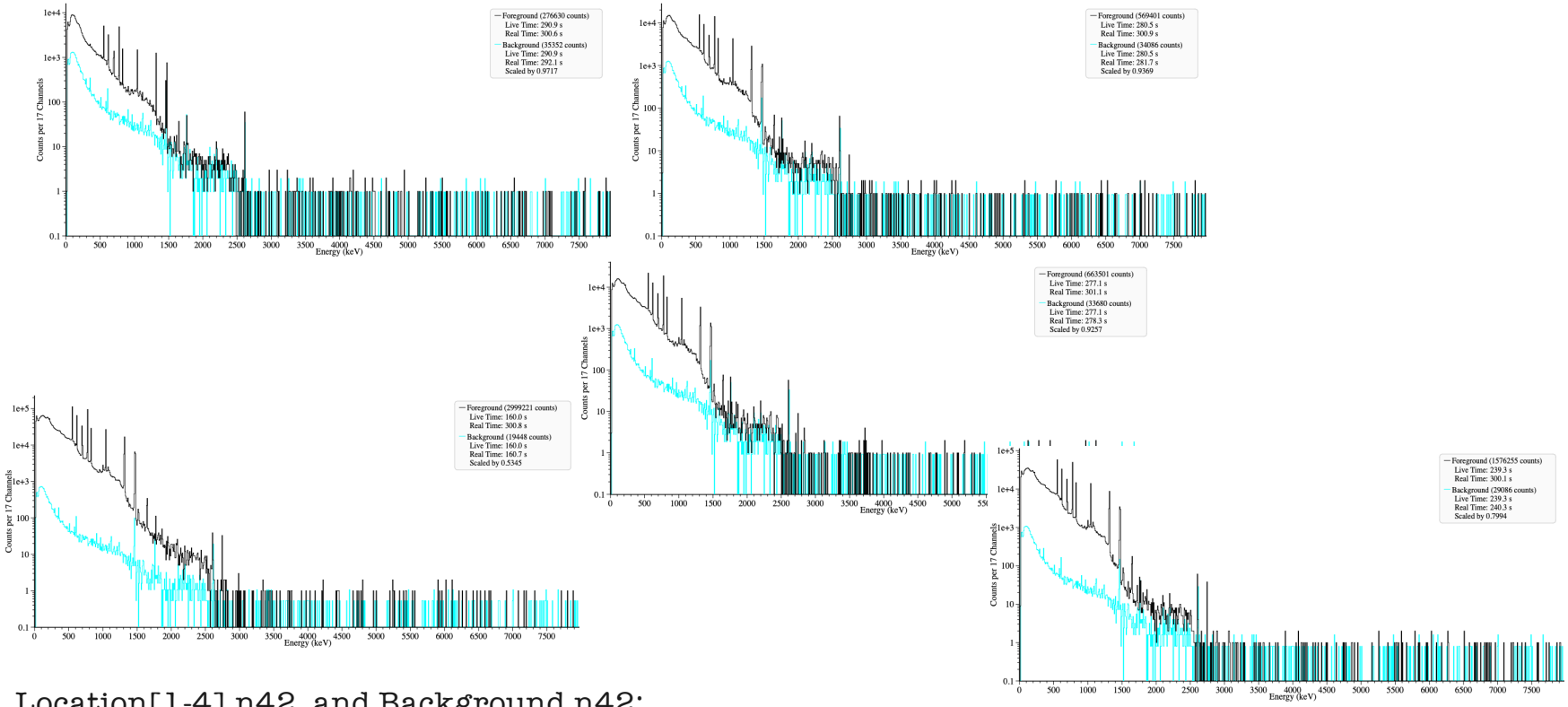
CUSTOMIZING OUTPUT REPORTS (CONT)

- Full documentation of the templating language can be found at:
  https://github.com/pantor/inja
- The input to `{{ inja }}` is JSON, that InterSpec creates during the calculation, and with the results.
  - You can save this JSON by specifying the `--result-json-output` argument, so you can then open up the JSON file, and see variables you want to use in the report template
    - Its then fairly straightforward to look for what you want in the JSON file, and use it within your custom template file
    - An absolute ton of information is saved into the JSON – but if anything has been missed you would like, please email InterSpec@sandia.gov
- The default output from batch processing is created from the templates in
  `InterSpec\InterSpec_resources\static_text\ShieldSourceFitLog\`
  You can probably start from these and just edit them to what you want

SUMMARY

- The “batch” version of InterSpec hopefully makes repetitive peak-fitting, or Activity/Shielding fitting less mundane.
- As of October 2024, the feature should be considered to be in an “alpha” or preview state
  - We would greatly appreciate feedback, suggestions, or to hear your use-case to improve things – as well as any bugs or short-comings
  - The batch feature was implemented with a very minimal amount of resources, so there is likely some rough edges, bugs, and obvious omissions – please let us know about these
  - In the future, if support for implementation is found, we would like to:
    - Add a graphical interface, so if you drag a bunch of spectrum files into the InterSpec app, a batch tool will pop-up to perform the batch analysis in a little more user friendly way
    - Adding support the Isotopics from peaks/nuclide tools, as well as the flux, and detection limits
    - Add options to fit peaks of nuclides specified from the command line, as well as vary more options from the command line

SPECTRA INCLUDED WITH THIS PRESENTATION



Location[1-4].n42, and Background.n42:
Spectra collected from ground contaminated with Br82 and K42, using a Detective-X, facing down, 1-meter from the ground

DETECTIVE-X_IN-SITU.ECC

```
SGI_template: CIRCULAR_PLANE
ISOCS_file_name: Detective-X_in-situ.gis
Detector_name: DETX_123456789
Collimator_name: no_collimator

Convrgence_[%]: 1.0000
Test_description: 200M_CIRCLE_@1M
Comment: DETECTIVEX
Date_Time: Thu_Oct_12_11:48:16_2023
Source_area_cm2:  7.85398e+7
Source_grams:  7.85398e+4
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:    45.00    2.19261e-8   15.0    1.72207e-3     0.191039   -0.160151    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:    50.00    4.60361e-8   12.0    3.61567e-3     0.186583   -0.153196    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:    60.00    1.24465e-7   10.0    9.77543e-3     0.186925   -0.143154    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:    70.00    2.01979e-7   10.0    1.58634e-2     0.186660   -0.138756    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:    80.00    2.76918e-7   10.0    2.17491e-2     0.184463   -0.135942    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:    90.00    3.30226e-7   10.0    2.59359e-2     0.185093   -0.134321    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   100.00    3.73344e-7   10.0    2.93223e-2     0.184142   -0.133496    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   125.00    4.26117e-7   10.0    3.34672e-2     0.184060   -0.132741    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   150.00    4.34106e-7   10.0    3.40946e-2     0.183269   -0.132145    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   175.00    4.27406e-7   10.0    3.35684e-2     0.182102   -0.132157    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   200.00    4.06607e-7    8.0    3.19349e-2     0.180679   -0.131995    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   250.00    3.60431e-7    8.0    2.83082e-2     0.180972   -0.131577    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   300.00    3.23407e-7    8.0    2.54003e-2     0.180076   -0.131384    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   400.00    2.61612e-7    6.0    2.05470e-2     0.176911   -0.131033    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   500.00    2.23522e-7    6.0    1.75554e-2     0.177270   -0.130608    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   661.00    1.83227e-7    6.0    1.43906e-2     0.175880   -0.129957    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   700.00    1.75999e-7    6.0    1.38230e-2     0.177072   -0.129848    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:   800.00    1.60378e-7    5.0    1.25961e-2     0.177247   -0.129722    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:  1000.00    1.37836e-7    4.0    1.08256e-2     0.178356   -0.129079    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:  1400.00    1.10116e-7    4.0    8.64851e-3     0.177544   -0.128761    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:  1500.00    1.04736e-7    4.0    8.22596e-3     0.178501   -0.128680    11119
keV_eff_%err_effw_%cnvrg(i)_%cnvrg(i-1)_pntsN:  2000.00    8.44439e-8    4.0    6.63221e-3     0.173937   -0.127951    11119
```

The efficiency, as a function of energy, computed by Mirion ISOCS, for a Detective-X in-situ measurement