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GADRAS-DRF Enhancements for Safeguards – Custom Peak Fitting to Enhance Model Fitting and Isotopics

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ABSTRACT

One major software update was accomplished within the Gamma Detector Response and Analysis Software-Detector Response Function (GADRAS-DRF) package. This update allows users to adjust individual peak fits for use in subsequent analysis processes within GADRAS-DRF. A graphical user interface (GUI) was implemented so users can see the effect of their fit adjustments on the spectrum. This new feature will enhance the capability of the previously funded auto-enrichment and peak-based 1D model fit feature that was implemented in FY23 (Fiscal Year). Isotopic analysis was performed using M400 data obtained from uranium standards and the isotopic assessment is given with and without manual peak adjustments.

ACKNOWLEDGEMENTS

This work was funded by the Department of Energy, National Nuclear Security Administration, and Office of International Nuclear Safeguards, NA-241.

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ACRONYMS AND TERMS

Acronym/Term	Definition
SME	Subject Matter Expert
GADRAS	Gamma Detector Response and Analysis Software
DRF	Detector Response Function
GUI	Graphical User Interface
SNM	Special Nuclear Material
RE	Relative Efficiency
DU	Depleted Uranium
HEU	Highly Enriched Uranium
Pu	Plutonium
U	Uranium
HPGe	High Purity Germanium
FY	Fiscal Year
IAEA	International Atomic Energy Agency
FWHM	Full Width at Half Maximum
ORNL	Oak Ridge National Laboratory
LANL	Los Alamos National Laboratory
CZT	CdZnTe (Cadmium Zinc Telluride)

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1. INTRODUCTION

The Gamma Detector Response and Analysis Software – Detector Response Function (GADRAS-DRF) [1] software package is currently being explored as a new tool for the International Atomic Energy Agency (IAEA) to utilize for enrichment/isotopics analysis, automated isotope identification, and large-scale modeling efforts to train machine learning algorithms. GADRAS-DRF applies a detector response function (DRF) to compute the resulting spectra of a radiation detector when it is exposed to radiation [2]. The capabilities of GADRAS-DRF include characterization of detector response parameters, plotting and viewing both measured spectra and spectra generated using this software, creating realistic spectroscopic data, and analyzing spectra. The analysis of measured spectra includes identifying isotopes and estimating source energy distributions [1].

The computed responses generated using GADRAS-DRF can be combined with measured spectra to determine the isotopic enrichment of uranium or plutonium as funded by another NA-241 project called "GADRAS-DRF Enhancements for safeguards" [3]. The GADRAS-DRF addition discussed here allows a subject matter expert (SME) to manually modify the peak fits used in this analysis, as well as the inverse modeling routine in GADRAS-DRF. Having good peak fits are essential for accurate enrichment analysis and will likely be necessary when using an M400 detector due to the skew seen on the low- and high-energy sides of the photopeaks.

1.1. Auto-Enrichment

Auto-enrichment combines the results of four analysis methods to output a combined enrichment estimate. In FY23, NA-241 funded the addition of an advanced user interface for isotopics so that subject matter experts (SME's) can fine tune the inputs to these methods. The custom peak fitting algorithm applies specifically to the relative efficiency (RE) and differential attenuation analysis (DAA) methods. The details of these routines are discussed elsewhere [3]. The custom peak fit tool allows users to save the new peak area from their custom fit for use in subsequent analysis within the isotopics tool.

Since DAA and RE methods are not available for plutonium isotopics, the custom peak fitting capability is only applicable to uranium isotopic analysis. The reason for the exclusion of these methods for plutonium isotopics is because direct peak extraction for Pu-240 is difficult in the general case.

1.2. Fit 1D Model

In FY23, modeling was introduced into GADRAS-DRF. In the full version of GADRAS, the 1D and 3D methodology uses coupled neutron, electron, and photon deterministic transport methods to produce the volumetric photon source terms for a model [4]. In GADRAS-DRF the methodology was altered in FY23 to use non-sensitive gamma-only intrinsic radiation transport so that export-controlled deterministic transport codes are not utilized [3]. Since this alteration only includes intrinsic gamma and x-ray source terms, the GADRAS-DRF model fitting routine was modified to only use photopeak areas when using measurement data to optimize parameters in radiation source models. More details on this can be found elsewhere [3]. Since the routine relies heavily on photopeak areas, allowing users to customize peak fitting will increase the accuracy of analysis. This is especially true for data from the M400 detector where the peaks are skewed and cases where a DRF was not obtained for the exact system used for the measurements.

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2. CUSTOM PEAK FITTING INTERFACE

The custom peak fitting interface can be accessed from the RE and DAA options panels on the isotopics page after an initial analysis has been run. The option is shown below in Figure 1. General usage instructions for the Auto-Enrichment tool can be found elsewhere [3].

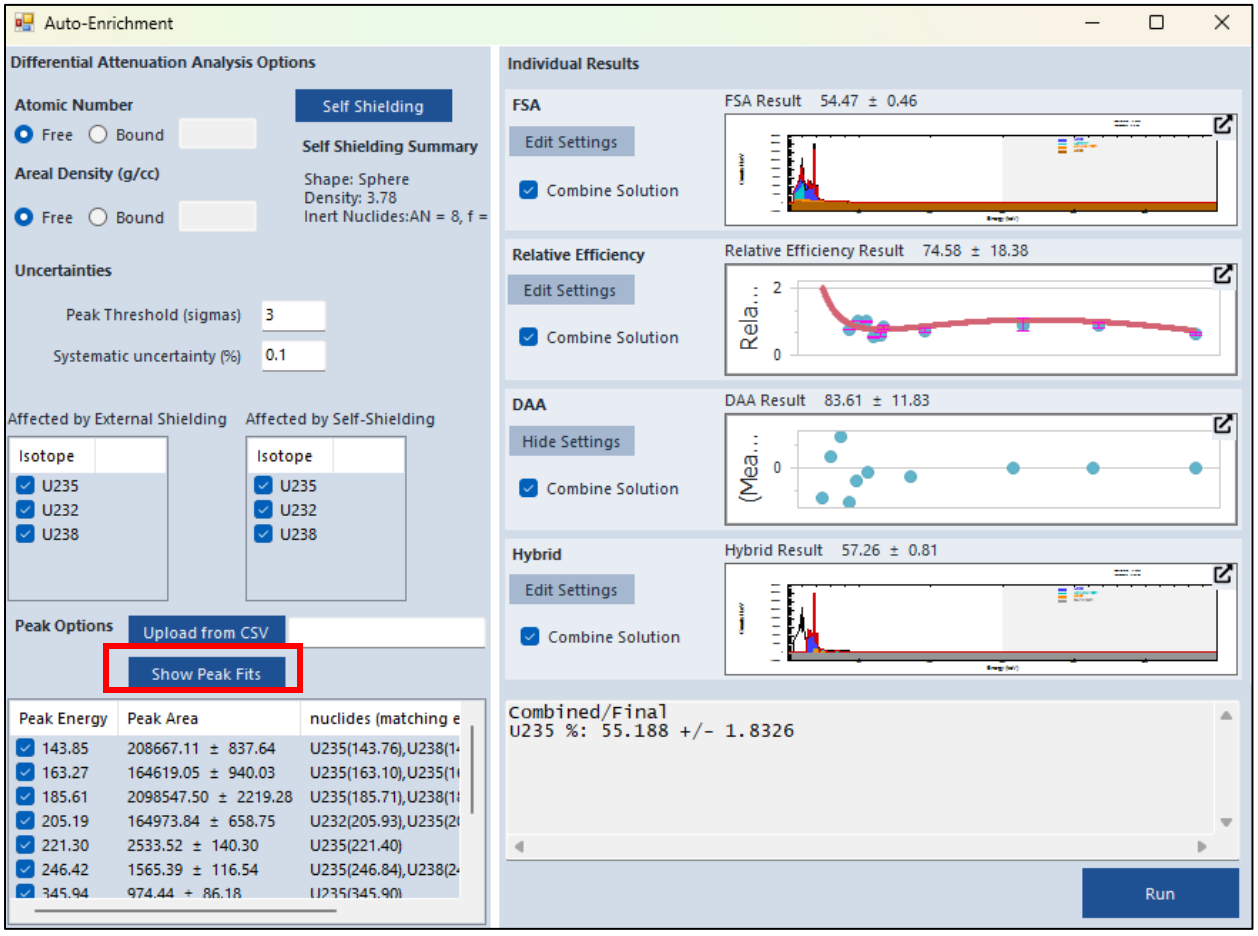


Figure 1. The auto-enrichment analysis page where the option to access the custom peak fitting form is outlined in red.

Selecting the "Show Peak Fits" button, outlined in read above, will bring up the following form in Figure 2. From this form users can view the automatically generated peak fits. Users can left click and drag left or right to zoom in and out, respectively, similar to other displays in GADRAS-DRF.

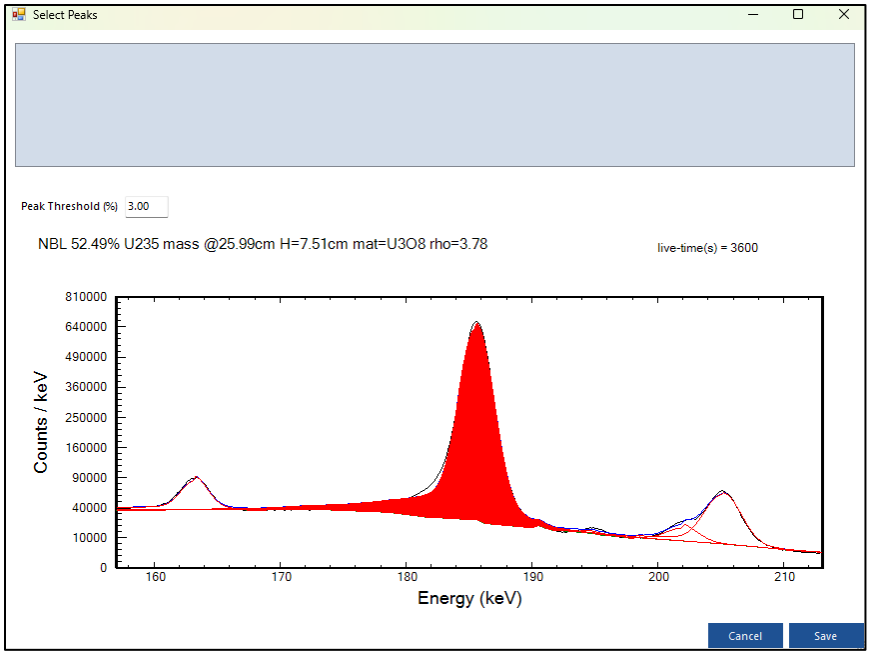


Figure 2. Form where users can view peak fits and select which one to customize.

In Figure 2, left clicking on a peak shown on the plot will bring up a mini form where users can assign a nuclide and energy to the peak as shown below in Figure 3. This form shows the nuclide, energy, and percent yield of that photon so that users can appropriately assign a nuclide.

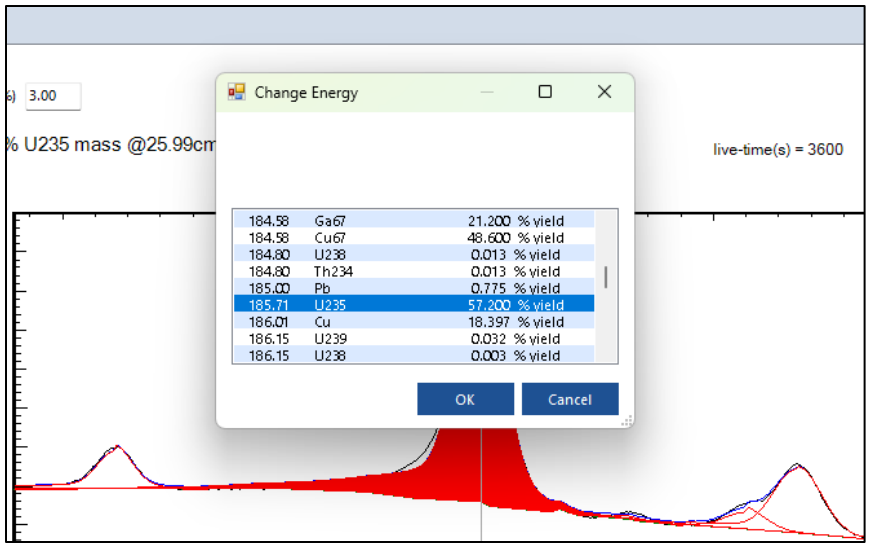


Figure 3. Peak selection form where users can assign a nuclide to the chosen peak.

Once the nuclide has been selected, the energy and nuclide will be displayed as a list in the blue area above the plot. Users can then right click on the energy outlined below Figure 4 in red to bring up the option to open the custom peak fitting form.

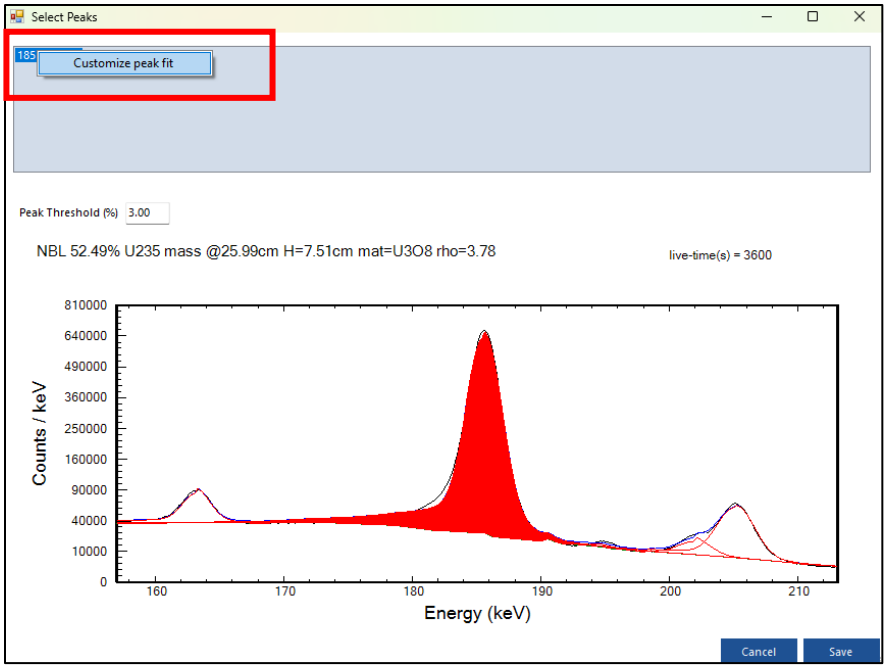


Figure 4. Peak selection form where users can right click on an energy in the table to pull up the option, outlined in red, to access the custom peak fit form.

The custom peak fit form shown below in Figure 5 has several features. It displays a plot showing the peak fits (always shown as a dotted line), the continuum (red), the total computed spectrum that is the continuum plus the peaks (black) and the measured spectrum (green). Displayed will be the energy on the x-axis, and channel number is displayed as a secondary axis. The number of peaks available at once for customization are based on the initial peak selected from the previous form. Any peak with an overlapping region with the selected peak will be displayed and can have the fits customized.

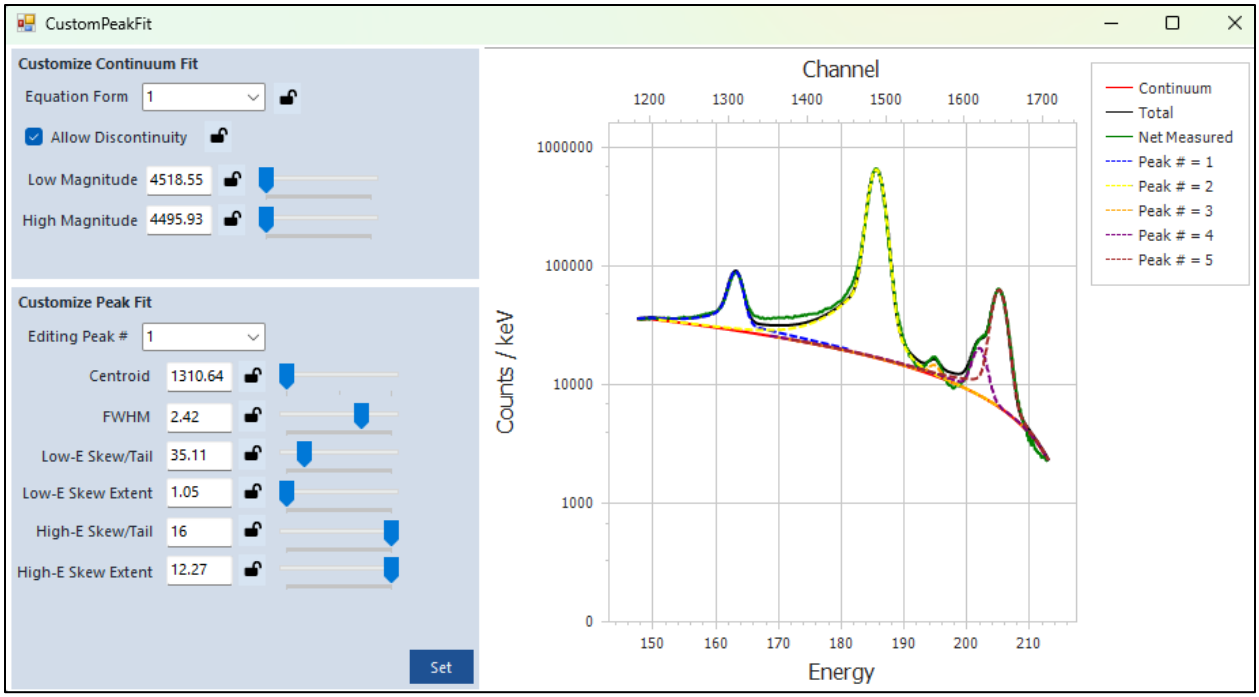


Figure 5. Custom peak fit form.

On the above form, users have the option to change the centroid, full width at half max (FWHM), and skew parameters of the peak selected from the drop down outlined in red below in Figure 6. These parameters mean the same as those on the detector page found within GADRAS. Descriptions and use of these parameters can be found elsewhere [1][2]. For M400 detectors, adjusting the skew parameters and the FWHM will likely result in increased accuracy of isotopic estimates.

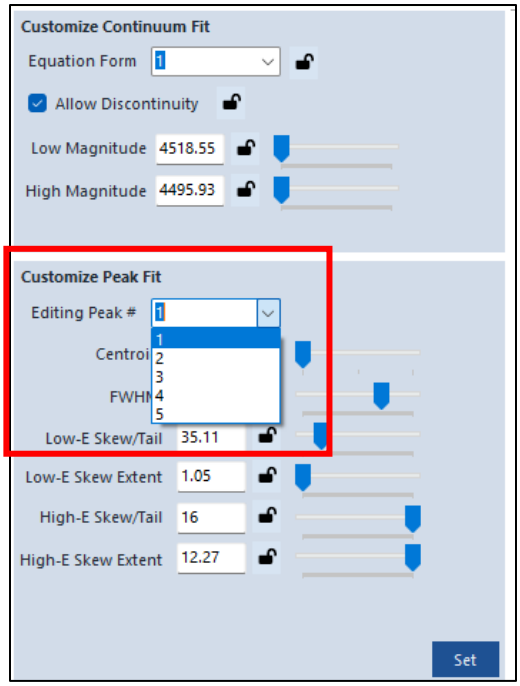
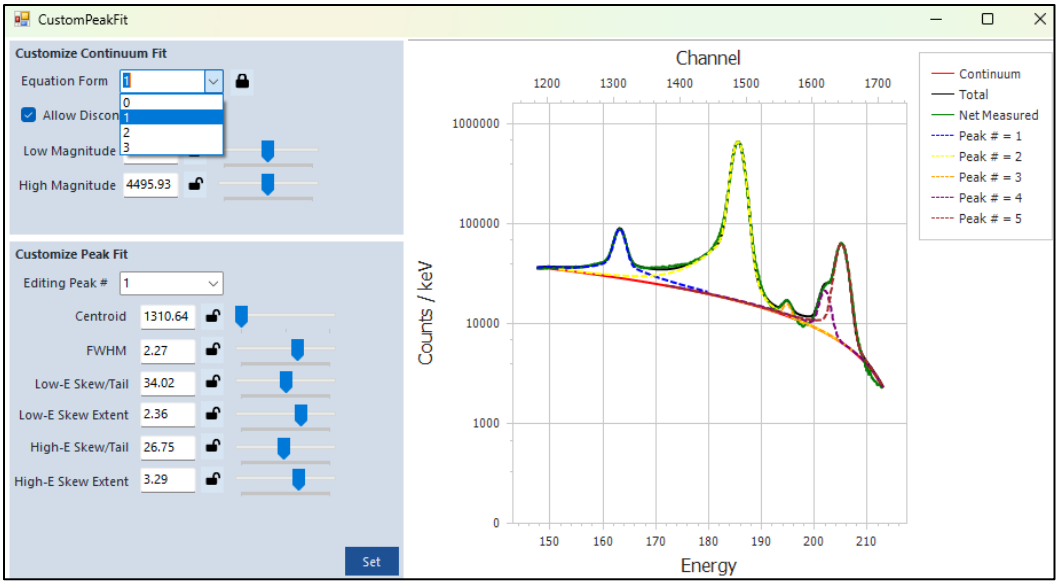


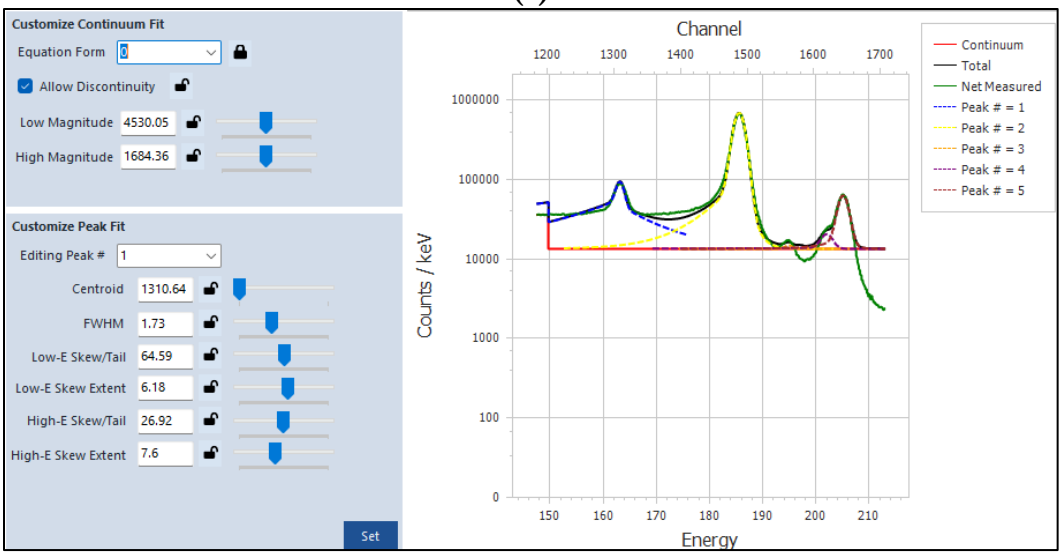
Figure 6. Custom peak fit options form. The peak to edit can be changed by selecting a peak from the list outlined in red. The peak numbers correspond to those displayed on the plot.

Users can either type in a number or use the trackbars to the right of the textboxes to adjust the parameters. As the user moves a trackbar, the plot will update in real time. Once a parameter has been changed, the icon by the textbox will change from an open lock to a closed lock. This means that the fitting algorithm cannot change these values. To let these values be optimized by the fit routine again, simply click on a lock to open it.

As for the continuum options, the magnitude of the continuum, the polynomial order (labeled as Equation Form), and whether the continuum is discontinuous, can all be changed. The continuum parameter changes the continuum for all peaks shown on the plot at once as demonstrated in Figure 7 when the "Equation Form" is changed from 1 to 0.



(a)



(b)

Figure 7. Demonstration on how changing the polynomial order (Equation Form) of the continuum alters the continuum below all photopeaks plotted. Figure 7a is using a polynomial order of 1, and Figure 7b shows a polynomial order of 0.

Notice that in Figure 7 "Allow Discontinuity" is checked. This enabled users to specify different magnitudes above and below the centroid of a photopeak. When multiple photopeaks are present, the discontinuity is placed at the highest peak centroid. If "Allow Discontinuity" is unchecked, then there is no discontinuity and only one magnitude parameter is available for adjustment as shown in Figure 8.

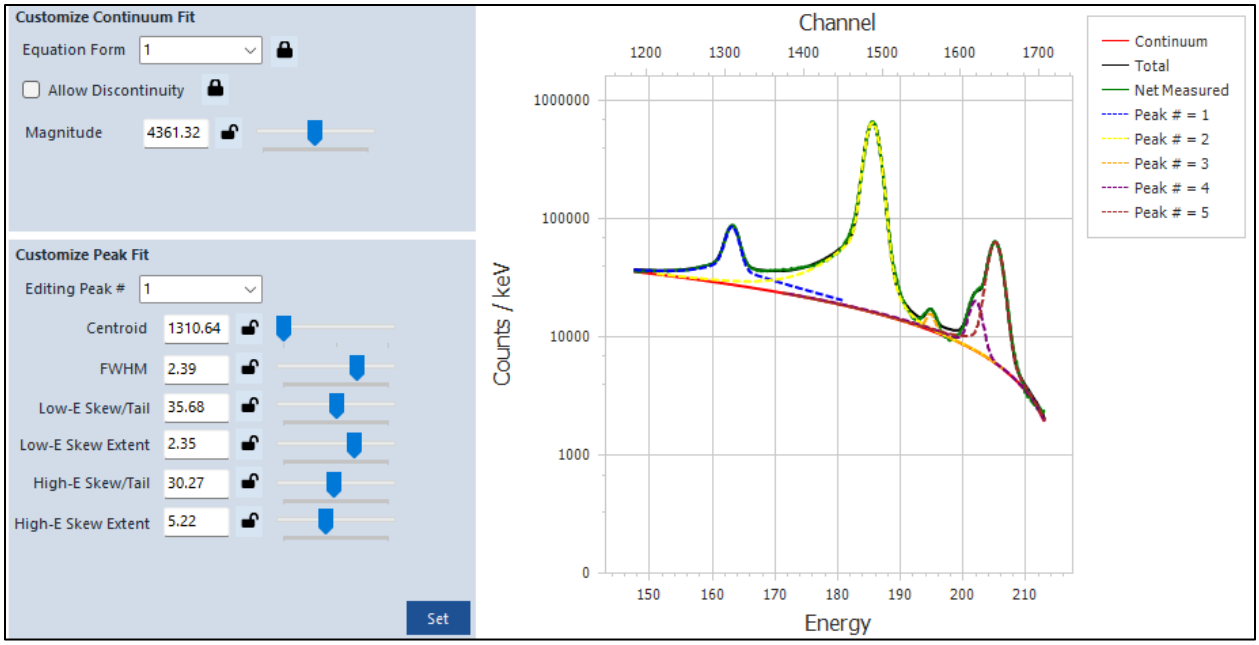


Figure 8. The custom peak fit form with no discontinuity allowed.

Once users have the desired fit, they can select the "Set" option at the bottom of the form. This saves the new peak areas for use in the analysis routine. Customizing peak fits can be applied to Model Fit or to Isotopics. To access the custom peak fit form for use with model fitting, users need to select "Add", outlined in red in Figure 9, and add gamma measurements with peaks only selected as in Figure 10. Selecting "OK" in Figure 10, will then bring up the form shown previously in Figure 2. From here the process is the same for customizing peaks as discussed previously.

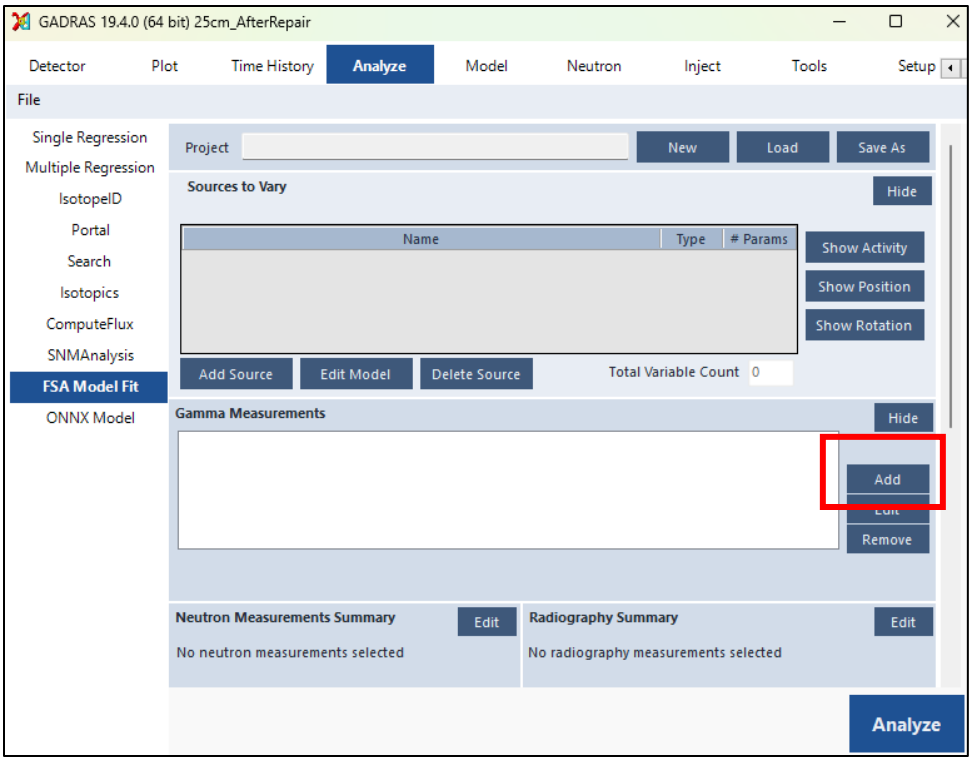


Figure 9. FSA model fit analysis form.

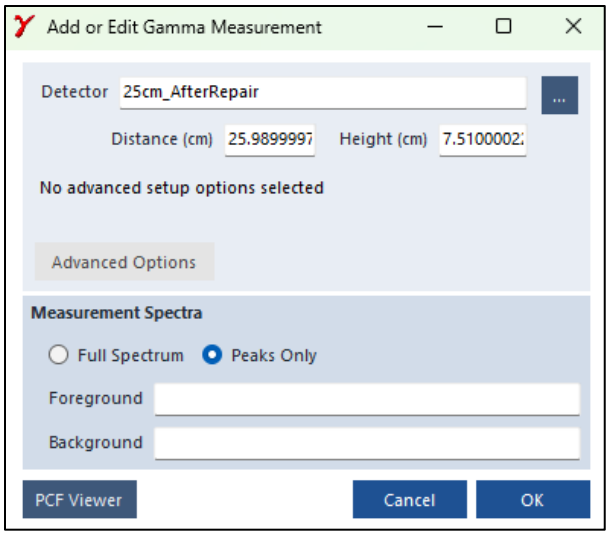


Figure 10. Gamma measurements form.

3. RESULTS

3.1. Improvement to Isotopic Analysis using Uranium Standards

To demonstrate how customizing peak fits can change the isotopics solution, this section shows isotopic results for measurements of Uranium standards using an M400 with and without customizing the peak fits. In 2021 Oak Ridge National Laboratory (ORNL) and Los Alamos National Laboratory (LANL) used an H3D M400 CZT detector to collect uranium spectra [5][6][7]. The detector has four 2-cm x 2-cm x 1-cm crystals. The standards were aligned with the cross hairs on the detector face as shown in Figure 11. The energy resolution is approximately 0.65% FWHM at 661 keV. However, there is substantial high and low energy tailing as with all CZT detectors. Thus, making the overlapping peaks challenging to fit.

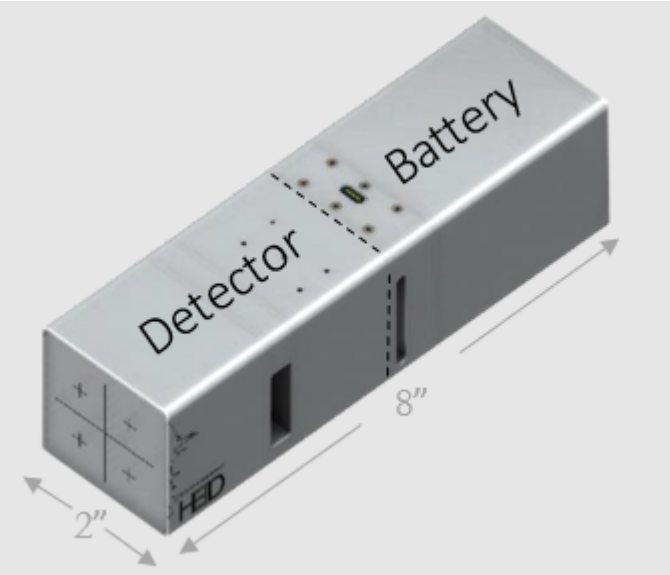


Figure 11. H3D M400 detector with battery.

The NBL standards measured were U3O8 with a density of 2.50 g/cc. The measured uranium standard properties used in this report for analysis are shown below in Table 1.

Table 1. CZT measured uranium standards properties.

Standard	U-235 (%)	U_3O_8 Mass (g)	U_3O_8 Diameter (cm)	U_3O_8 Thickness (cm)	U_3O_8 Bulk Density (g/cc)	Aluminum Window Thickness (mm)
CRM 146 NBL 0021	0.31	230	7.00	1.58	2.50	1.994
CRM 146 NBL 0022	0.71	230	7.00	1.58	2.50	1.994

The following analysis was done with this material selected and the density. The custom fit form was used to adjust the peak areas in both RE and DAA analysis routines. For the initial estimates, self-

shielding was taken into account. The results are below in Table 2 and are the combined estimates from both RE and DAA.

Table 2. Result of adjusting peaks for isotopic estimations on NBL standards that are 0.31% and 0.71% enriched.

Ground Truth U-235 (%)	Initial Estimate U-235 (%)	Adjusted Estimate U-235 (%)	Photopeak customized (keV)
0.31	0.209 +/- 0.291	0.265 +/- 0.3404	163, 185, 258, 1001
0.71	0.738 +/- 0.7563	0.707 +/ - 0.6492	163, 185, 205, 258, 1001

The following Figures Figure 13 Figure 20 show the initial peak fits and peak fit adjustments for the 0.31% enrichment case. For this case, the initial estimate from only RE was 0.18 +/- 0.04 % and the RE plot is show below in Figure 12.

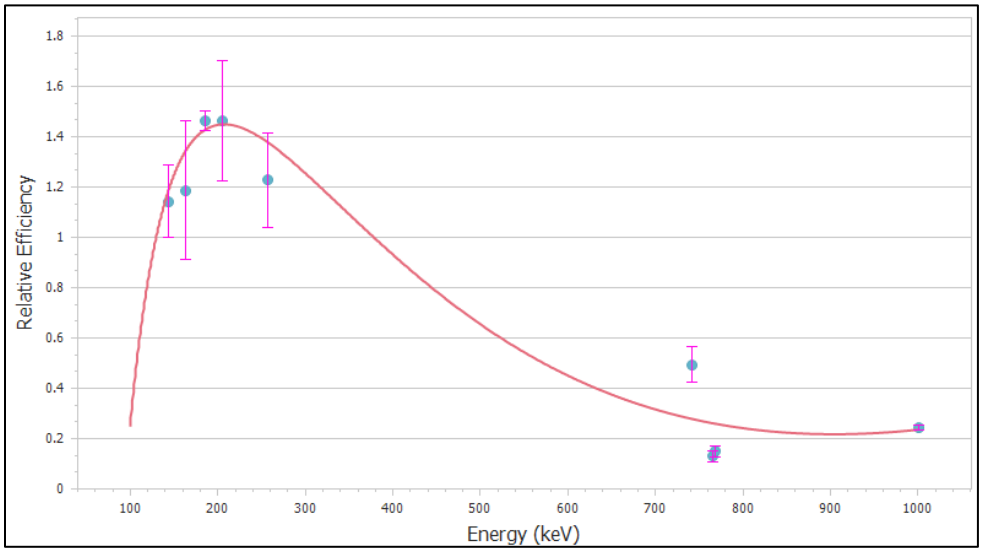


Figure 12. Relative Efficiency curve using the initial peak fits. The equation form is Ln(x) of order 3.

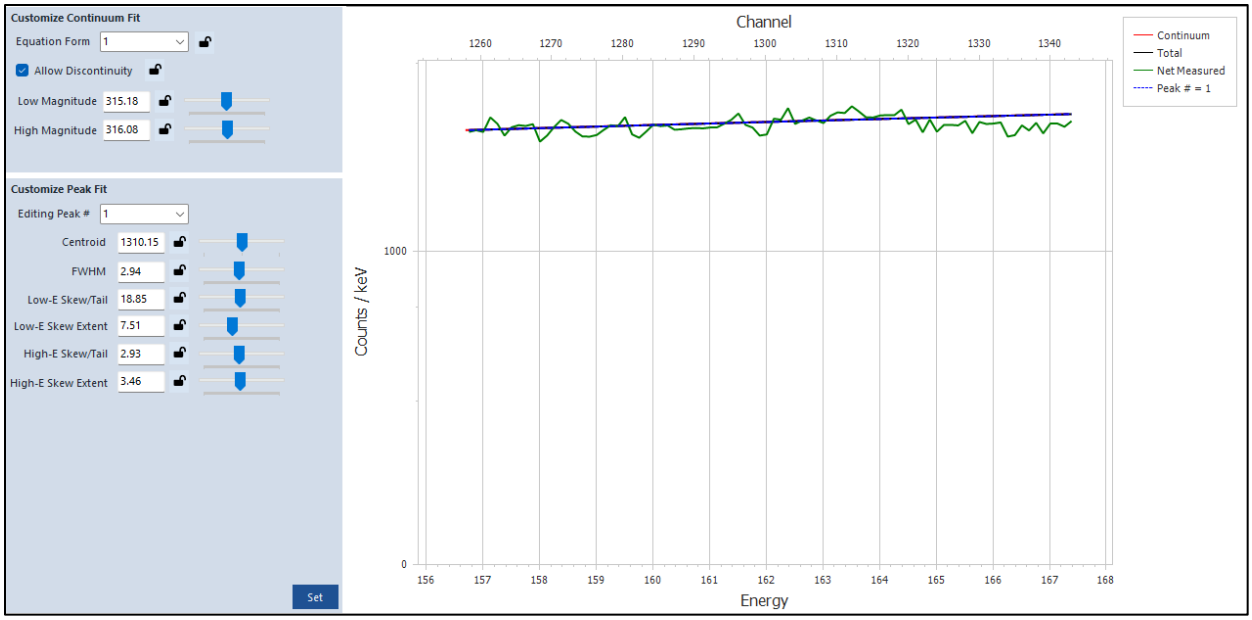


Figure 13. Initial peak fit of the 163 keV peak.

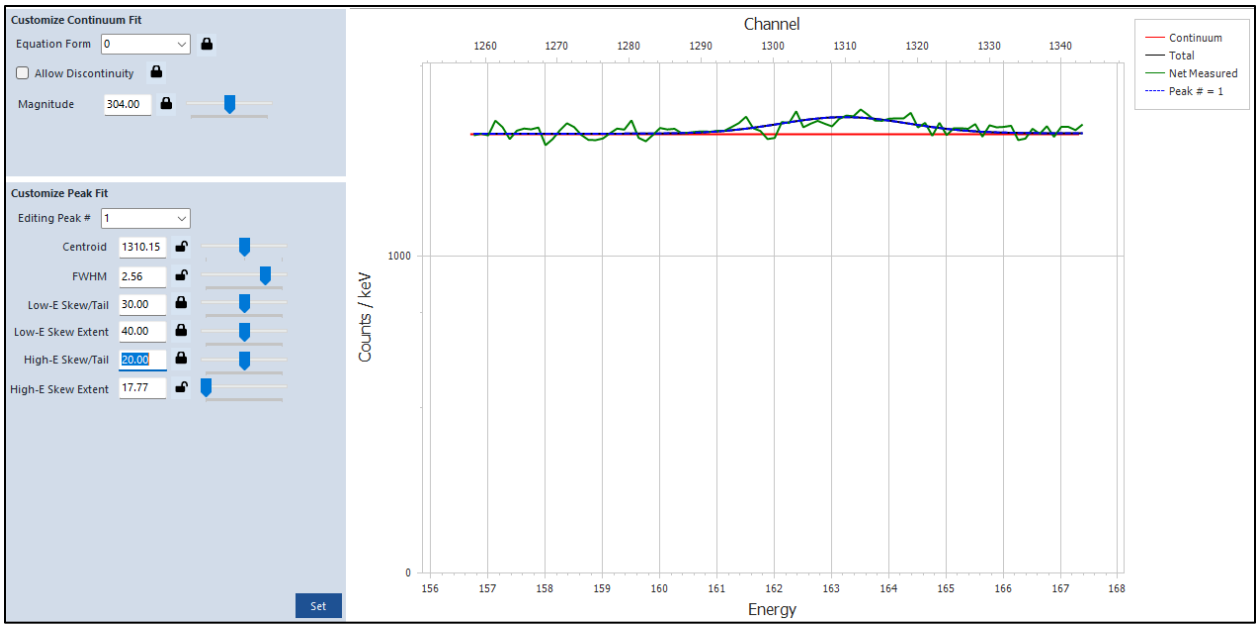


Figure 14. Adjustment of the 163 keV peak.

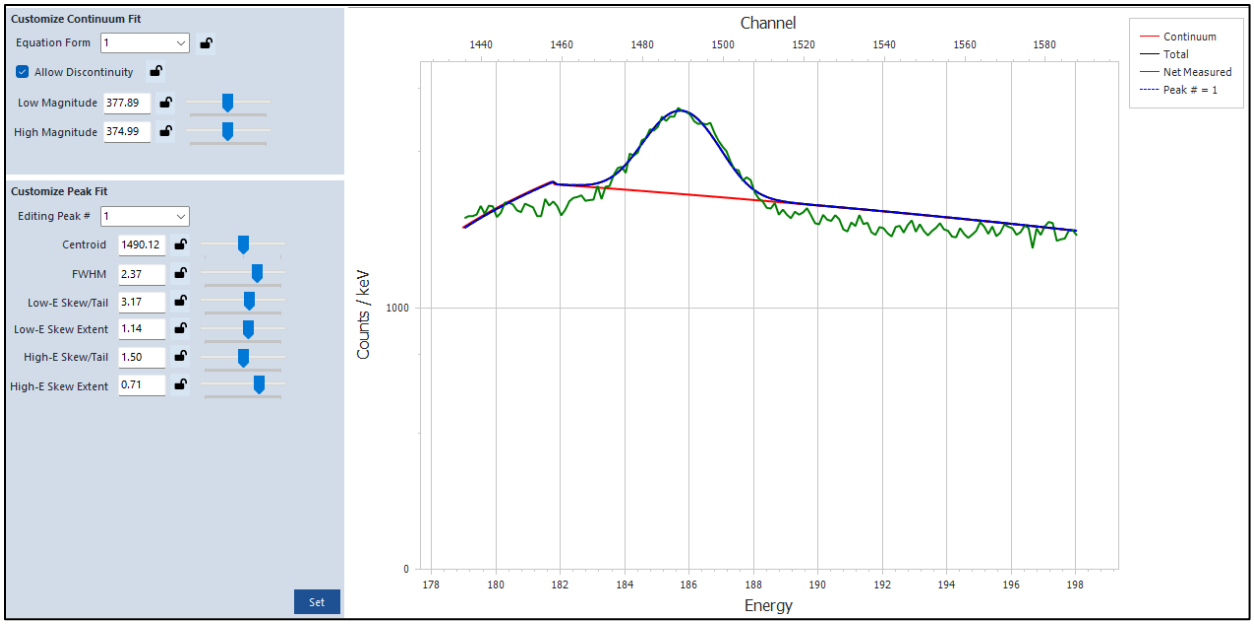


Figure 15. Initial peak fit of the 185 keV peak.

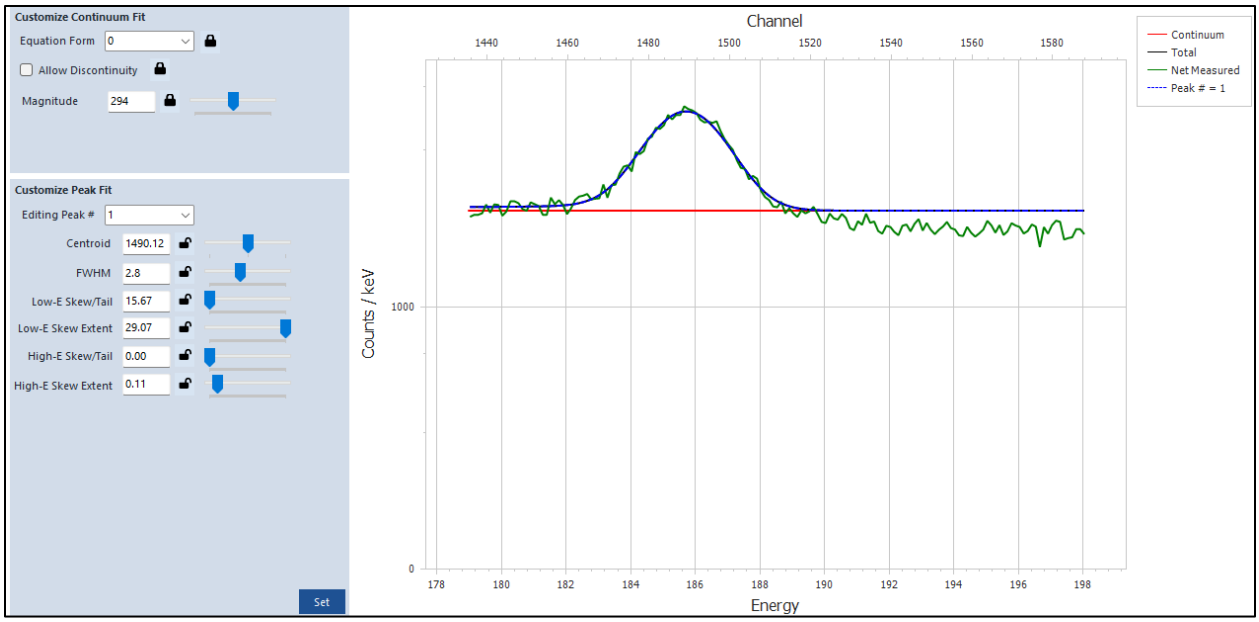


Figure 16. Adjustment of the 185 keV peak.

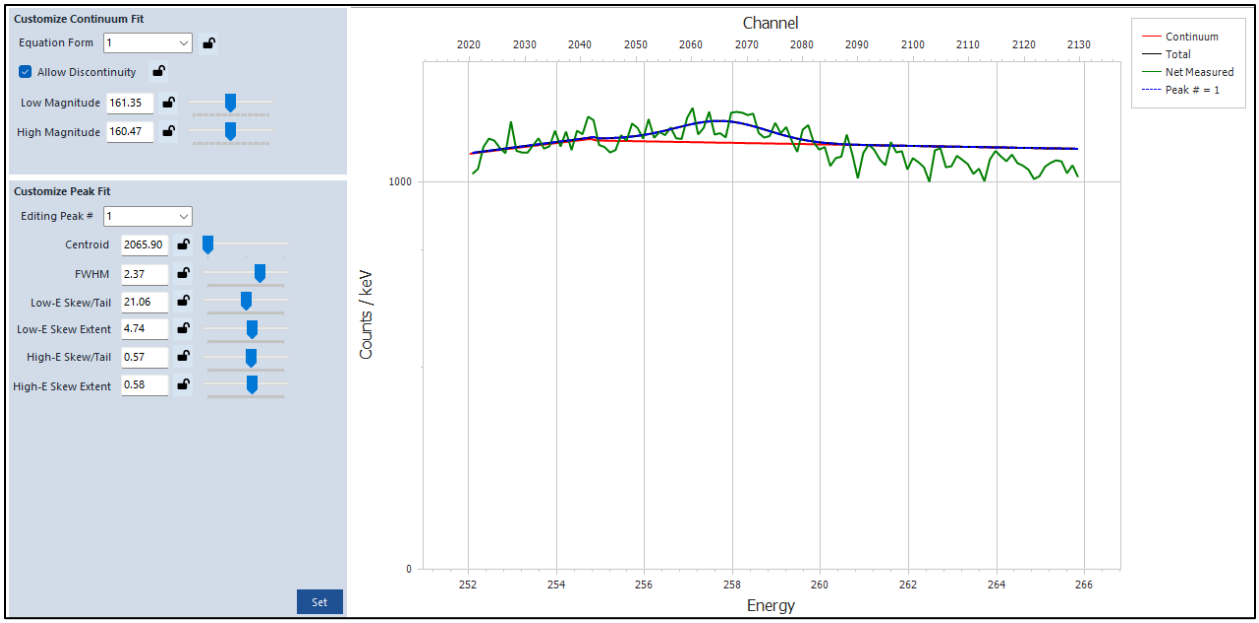


Figure 17. Initial peak fit of the 258 keV peak.

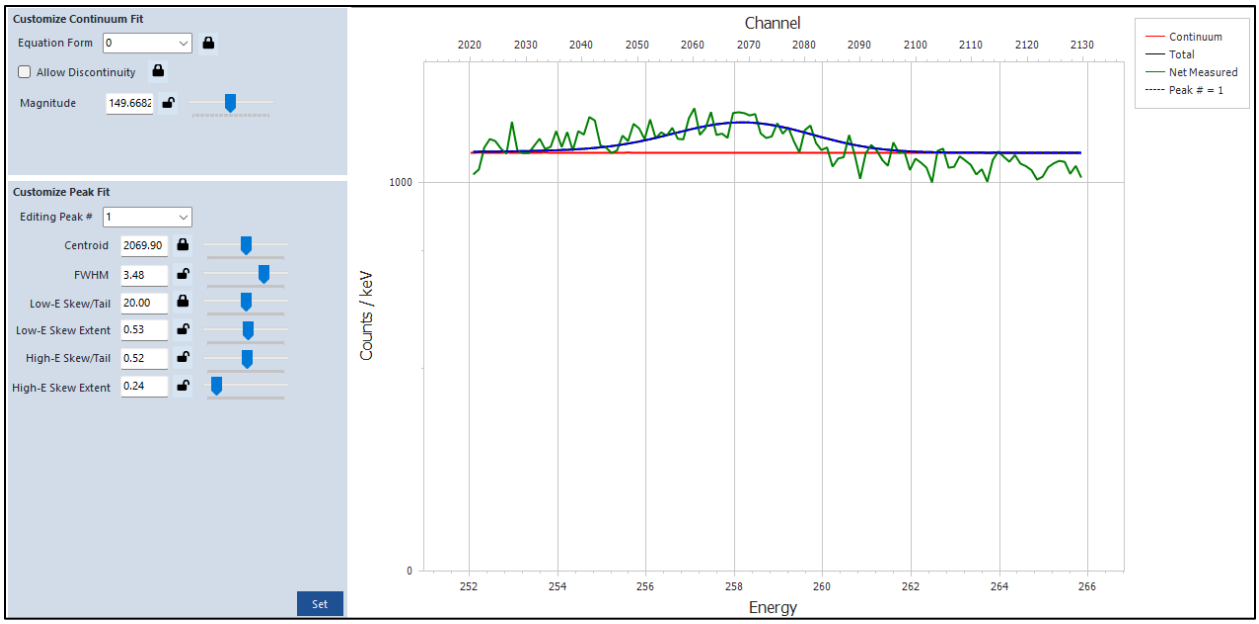


Figure 18. Adjustment of the 258 keV peak.

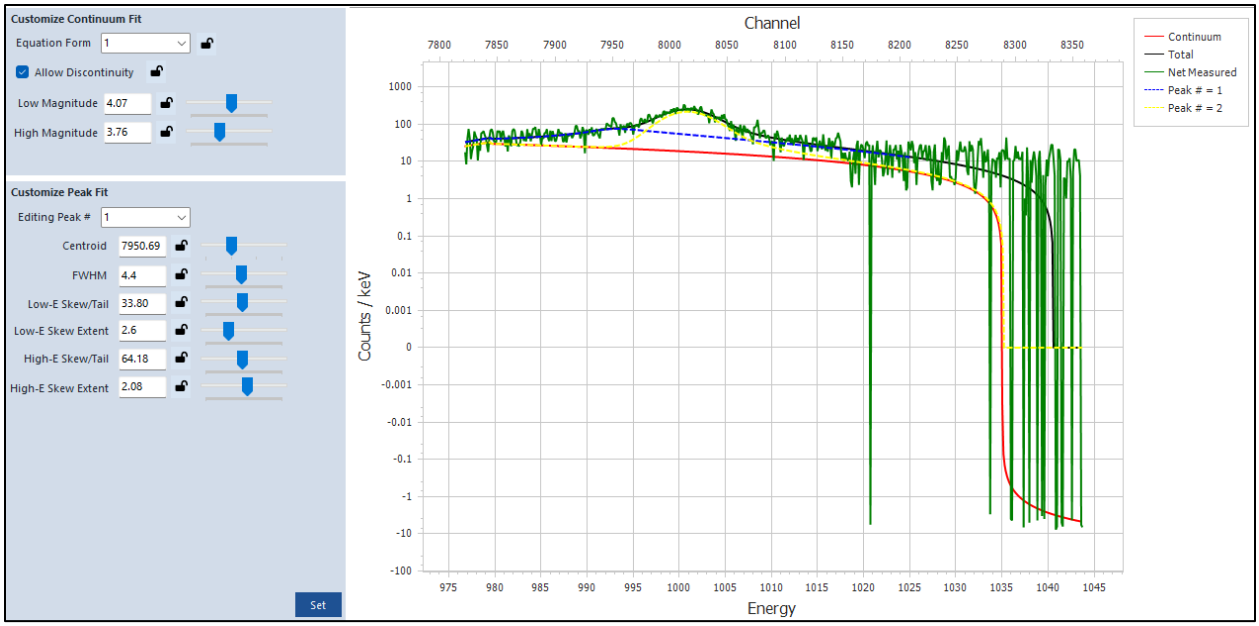


Figure 19. Initial peak fit of the 1001 keV peak.

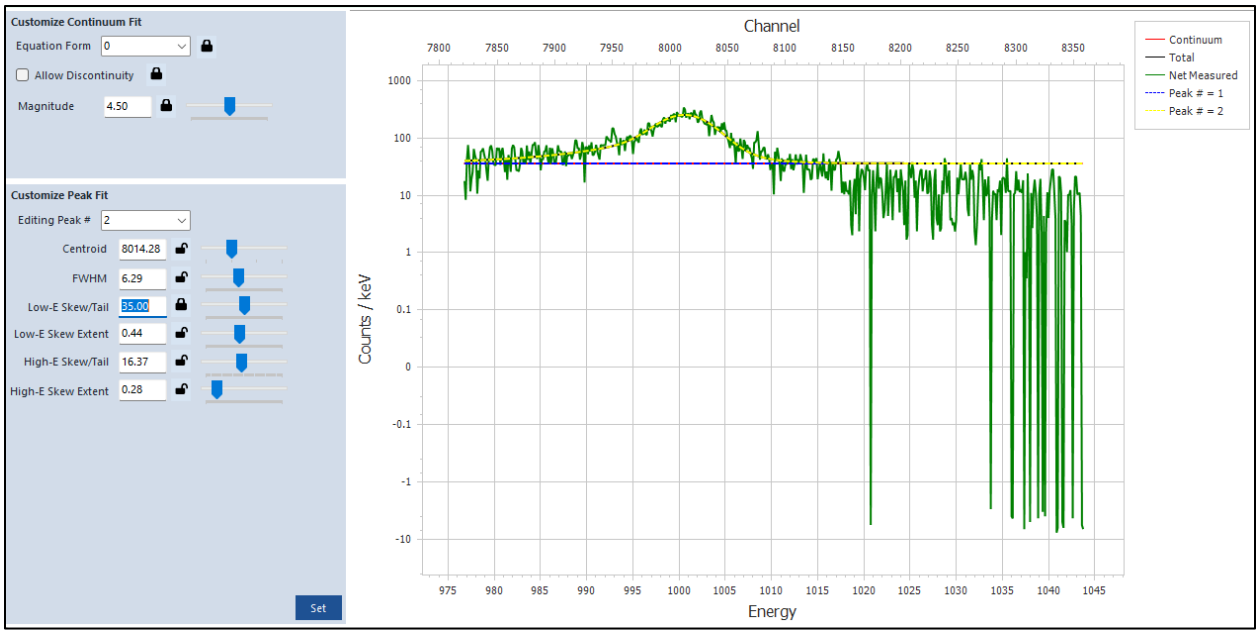


Figure 20. Adjustment of the 1001 keV peak.

The new relative efficiency curve, after making the peak adjustments shown, is found below in Figure 21 and the new peak areas are displayed below in Table 3.

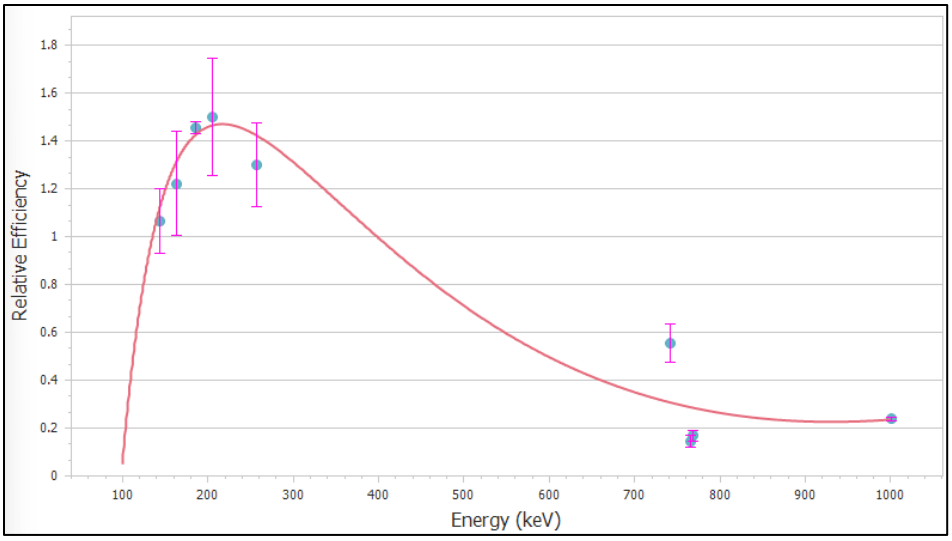


Figure 21. Relative Efficiency curve using the adjusted peak areas. The equation form is Ln(x) of order 3.

Table 3. Peak energies and the corresponding peak areas used for estimating enrichment.

Energy (keV)	Peak Area
143.93	1638.51 +/- 205.43
163.40	894.51 +/- 159.45
185.72	11879.89 +/- 190.67
205.03	1128.19 +/- 183.83
257.65	943.77 +/- 127.51
742.22	527.05 +/- 75.77
765.61	429.06 +/- 72.97
767.81	491.50 +/- 68.96
1000.96	1984.45 +/- 59.57

Eliminating the 765 keV peak from the RE analysis gives a result of 0.23 +/- 0.05 % and a combined estimate of RE and DAA of 0.265 +/- 0.3404 % as shown previously in Table 2. Prior to eliminating the 765 keV peak, the RE analysis gave a result of 0.22% enriched. Adjusting the peak areas resulted in a 26.1% difference in the isotopics estimate for the 0.31% enriched NBL standard. The large uncertainty shown in Table 2 implies that improvements need to be made to how uncertainty is estimated within GADRAS-DRF.

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4. CONCLUSION

For this project, the main enhancement is the ability to customize individual peak fits. A GUI was developed for this feature, and the GADRAS-DRF peak fitting routine was modified to allow users to set specific parameters. Users can adjust both peak and continuum parameters, while seeing the peak fits update in real time. Once users have their desired fit, they can save the new peak areas for use in two different analysis routines. The first routine is 1D model fitting, also known as FSA model, fit on the analysis page of GADRAS-DRF. This routine will use the newly updated peak information when adjusting model parameters. The second is the isotopic analysis routine. Users can customize peaks and the isotopics routine will use the new peak areas when determining enrichment.

Using NBL standard measurements obtained by ORNL and LANL, peak fits were customized, and the results are found in Section 3.1. For the 0.31% enriched case, the peak adjustments resulted in a 26.1% improvement to the estimated enrichment. The DRF for this detector was representative of the one used for measurements, so only slight peak adjustments were made. It should also be noted that improvements could be made to the isotopic uncertainty estimate in GADRAS-DRF.

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