

NMR Comparison Analysis

Analysis Overview

Background Subtracted Signals

Overlay Comparison

Normalized Area Comparison

Peak Ration Comparison

Background Subtraction

All runs of a given data set and signal setting were averaged graphed.

Background was defined by wings of data making up 20% of overall data on each side.

Background determined using OLS polynomial regression.

Forth order polynomial used to subtract background of full signal.

Background Subtraction

Two data sets analyzed: Data Set 4 & Data Set 5

Each data set is differentiated by a separate gain setting.

Each data set has four settings.

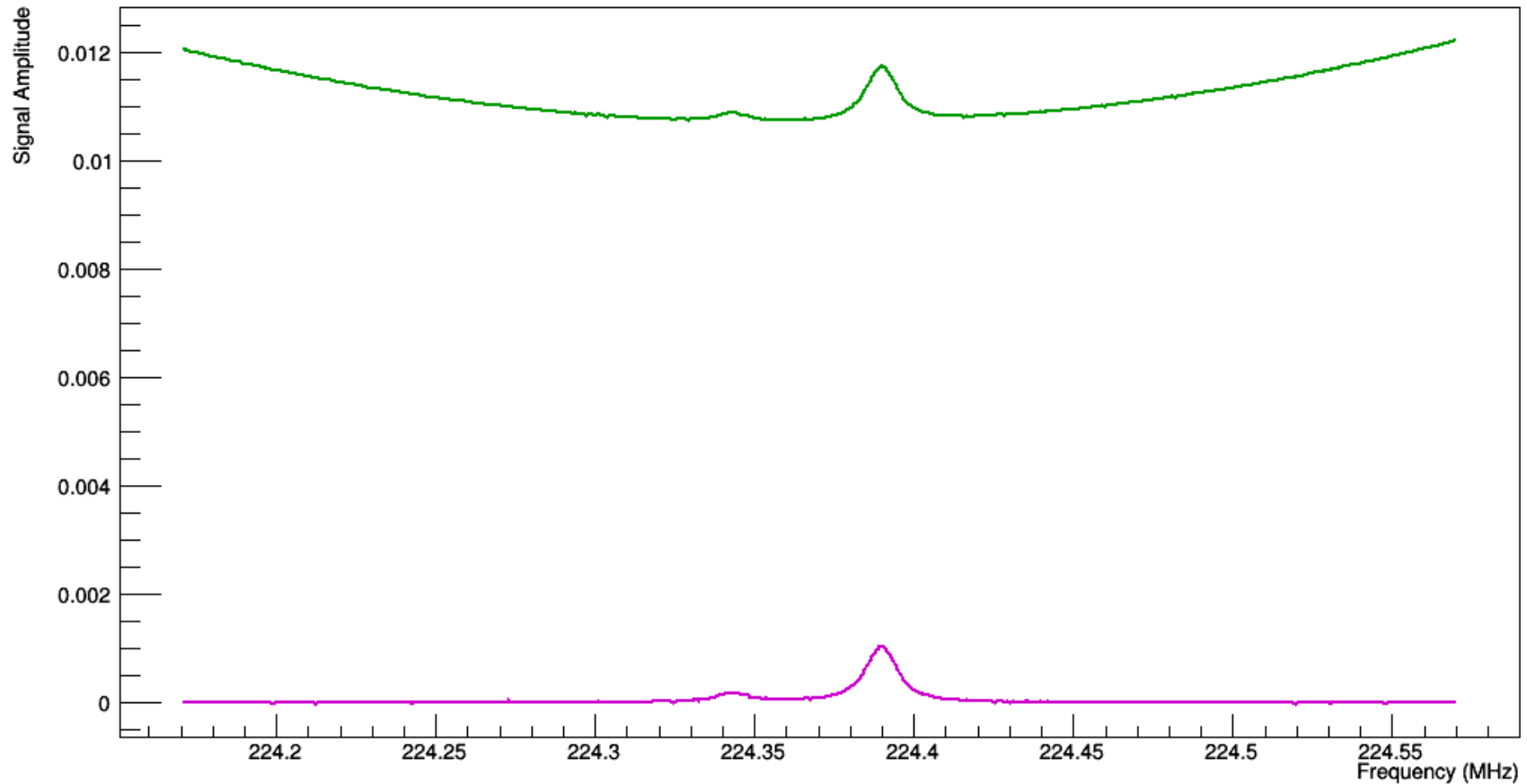
These settings represent different jumper settings on the LRC circuit providing the signal - essentially the jumpers settings change the signal size of the peaks.

PDP - this is the system traditionally used at UVA

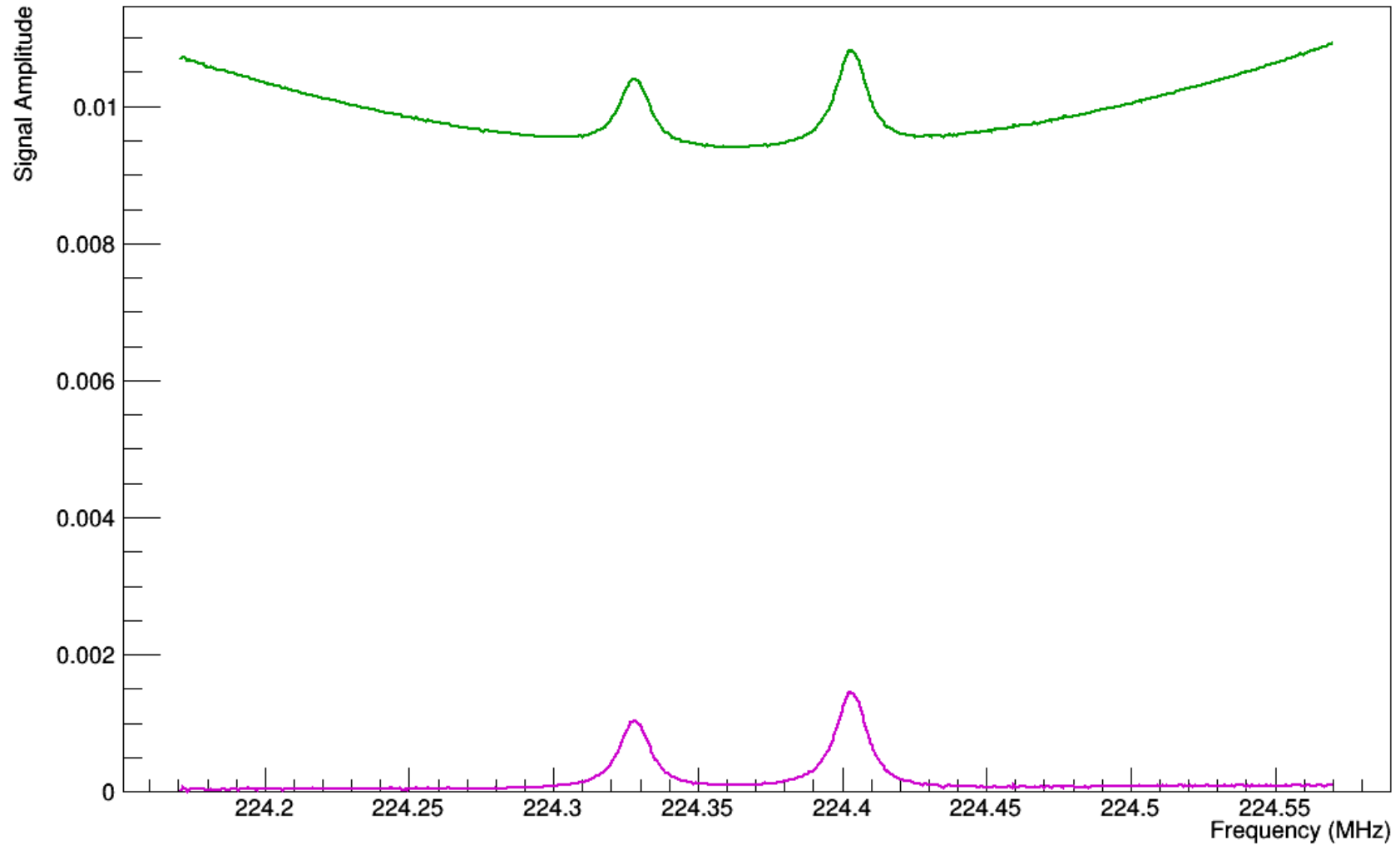
LANL - the new system designed by Los Alamos

Data Set 4

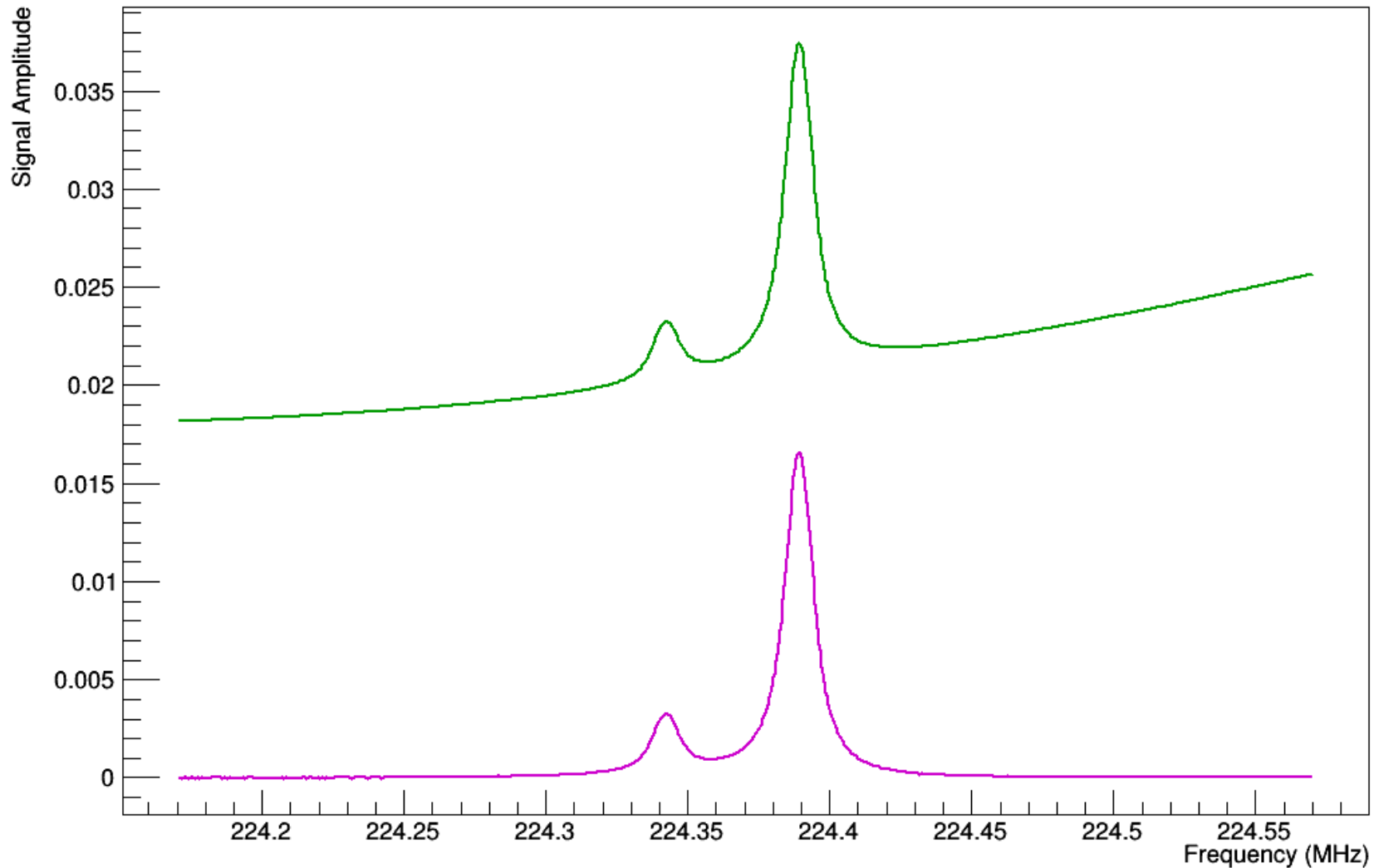
Subtracted Signals: PDP Data 4 Setting 1



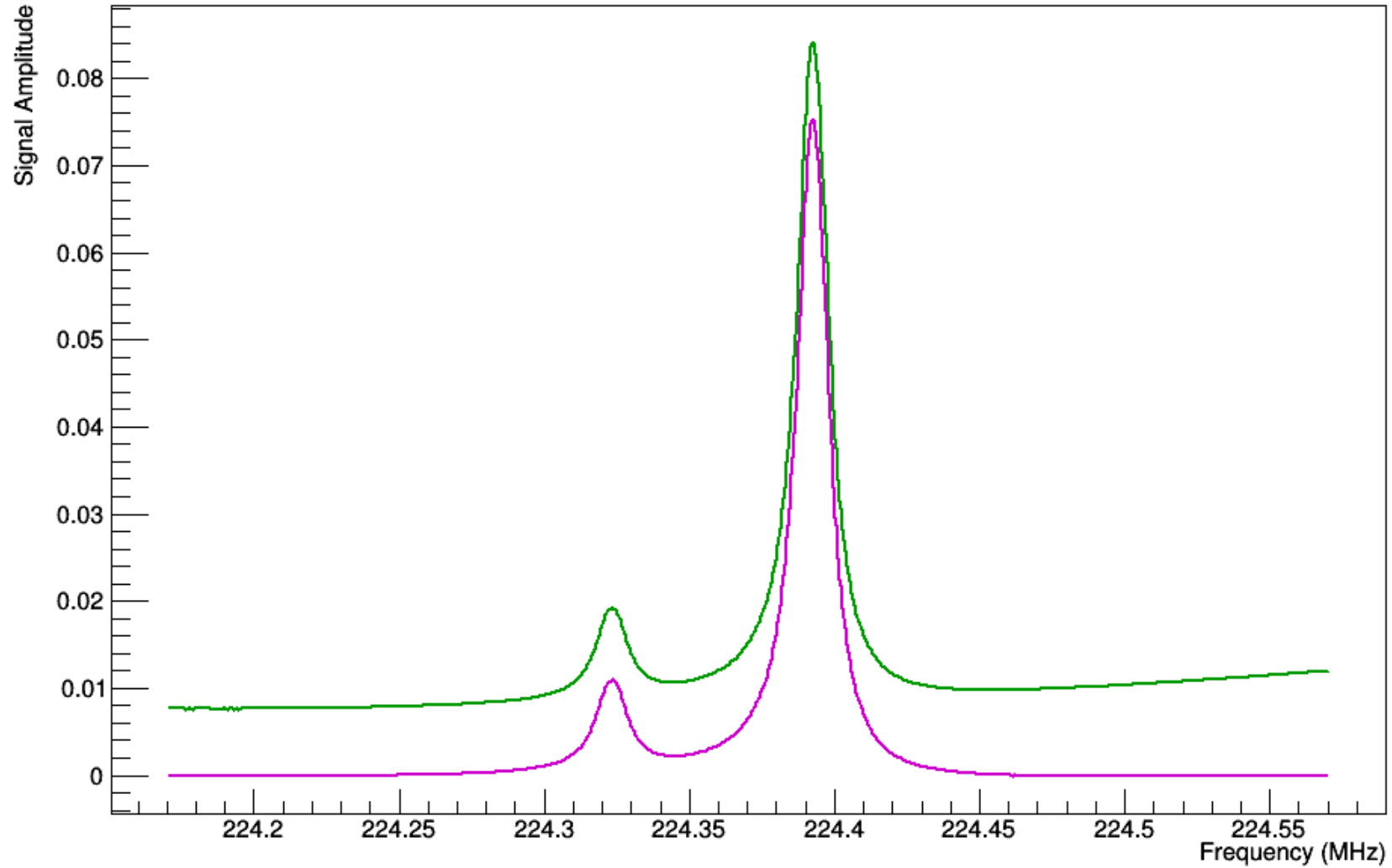
Subtracted Signals: PDP Data 4 Setting 2



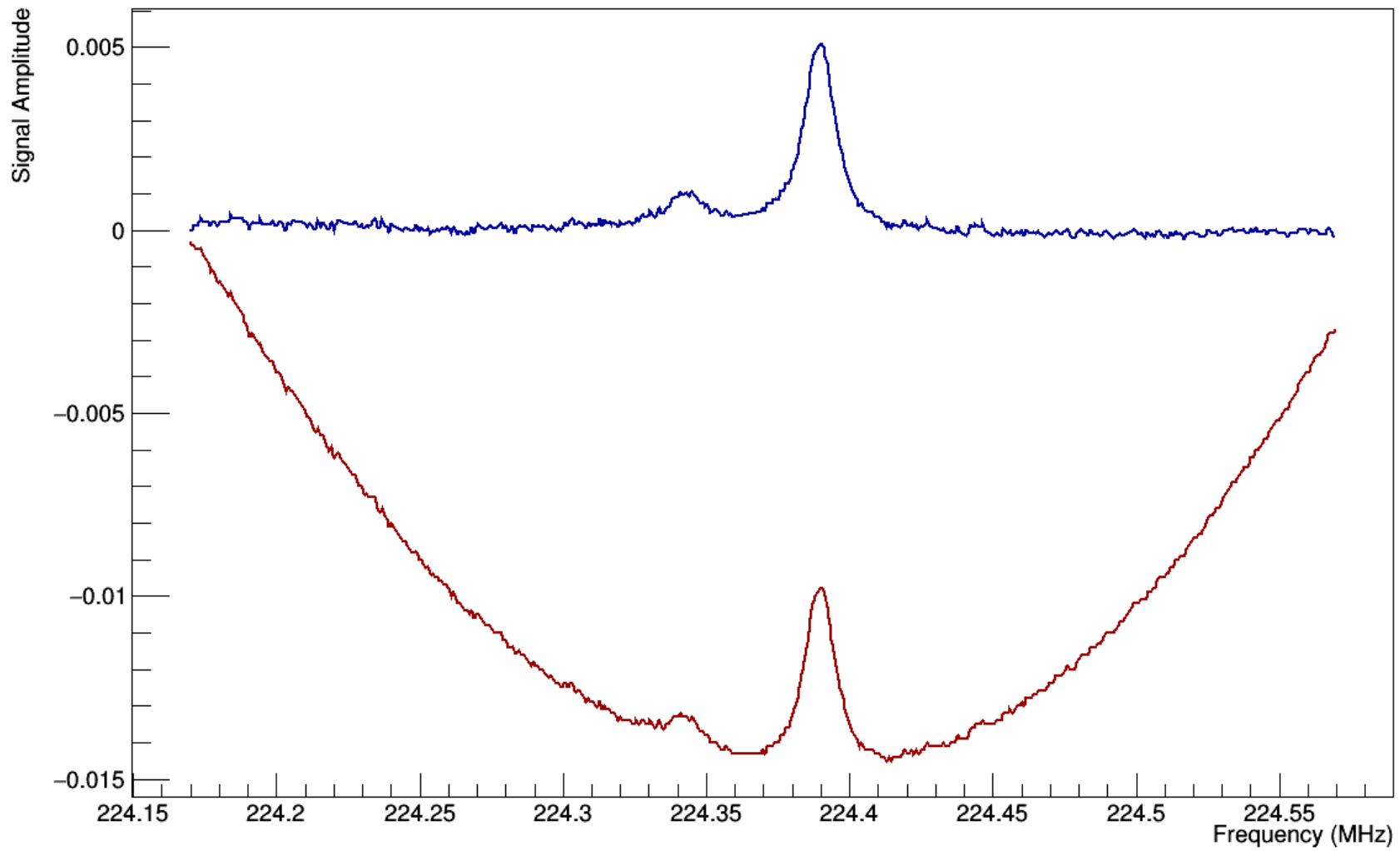
Subtracted Signals: PDP Data 4 Setting 3



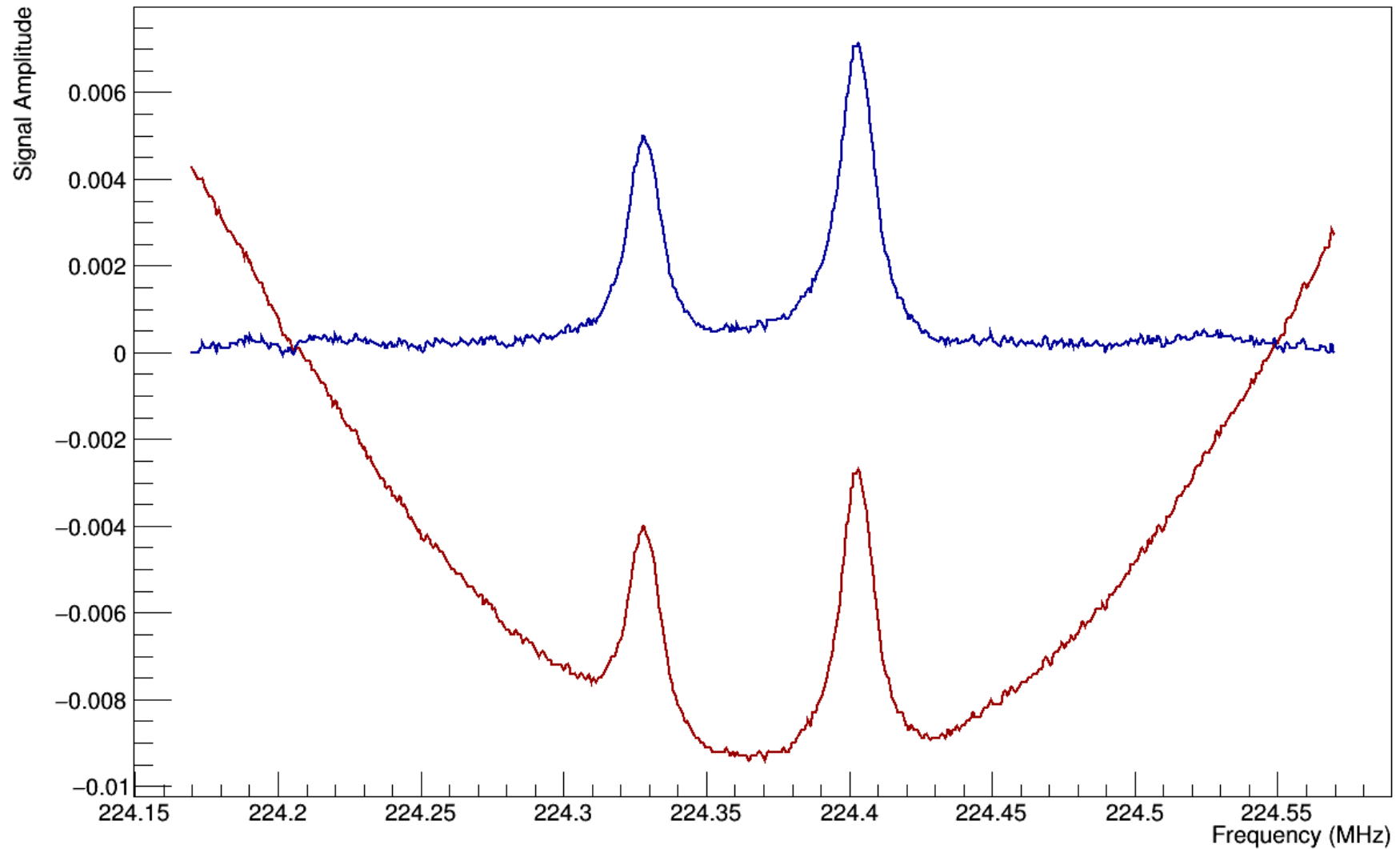
Subtracted Signals: PDP Data 4 Setting 4



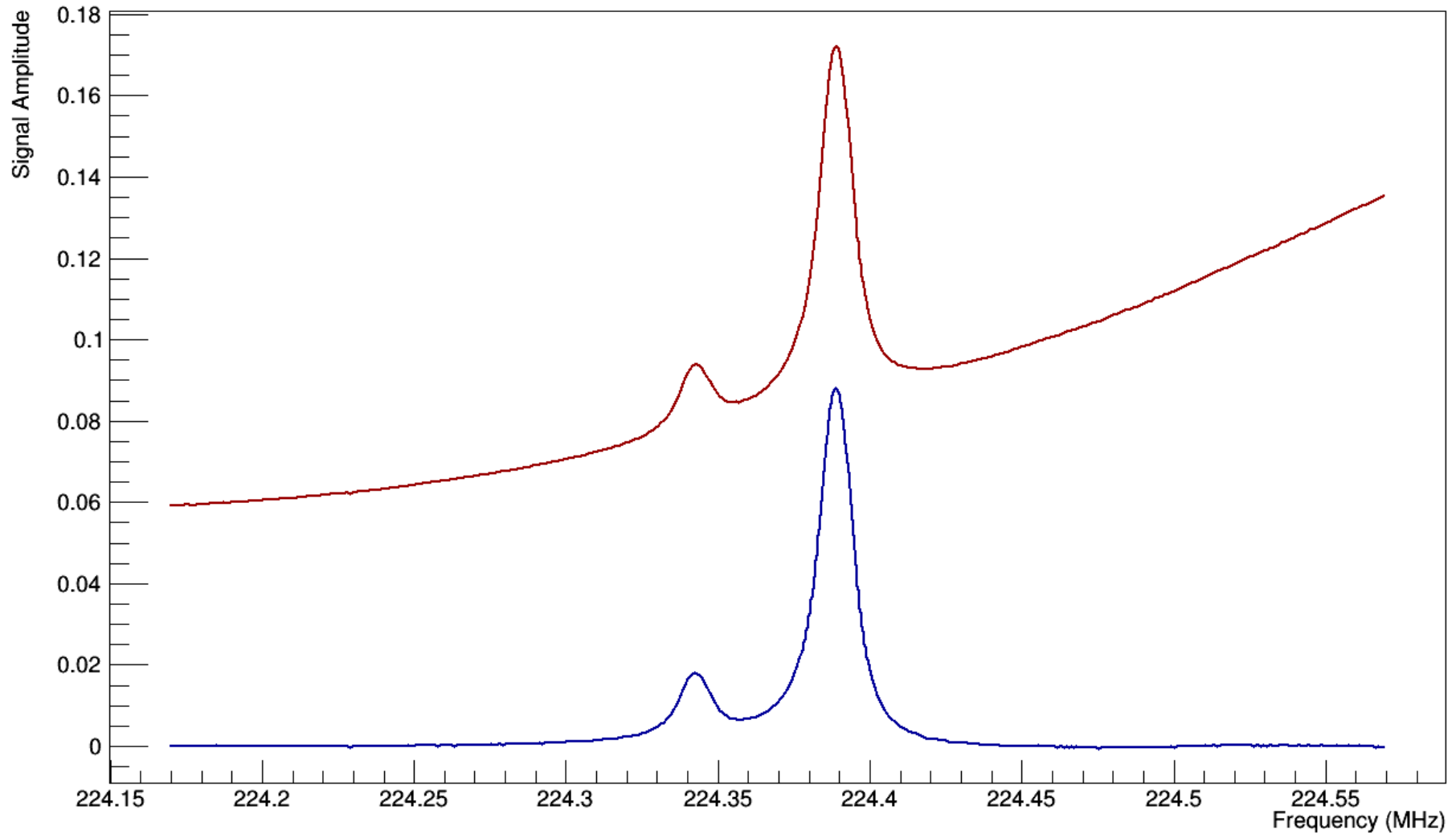
Subtracted Signals: LANL Data 4 Setting 1



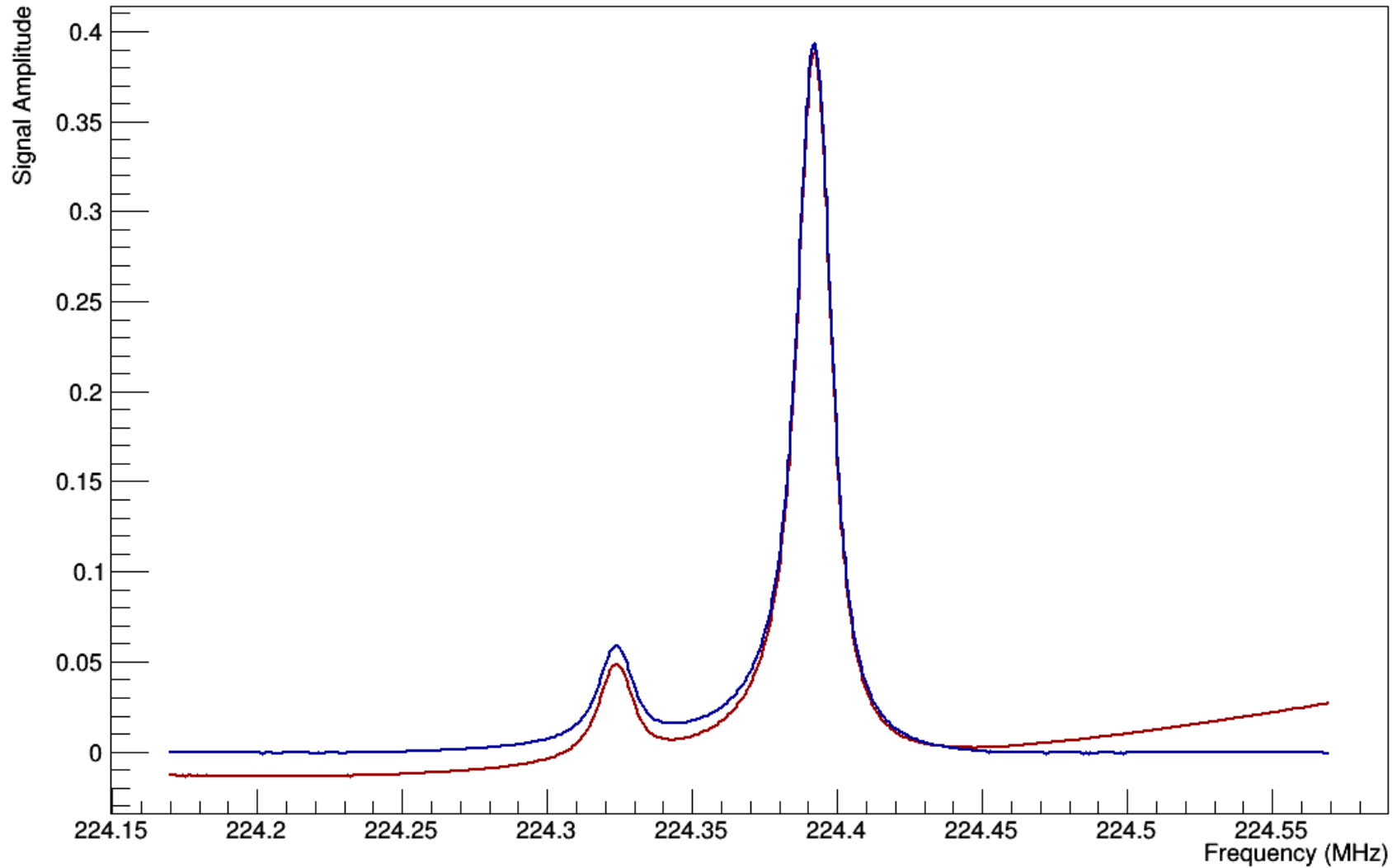
Subtracted Signals: LANL Data 4 Setting 2



Subtracted Signals: LANL Data 4 Setting 3

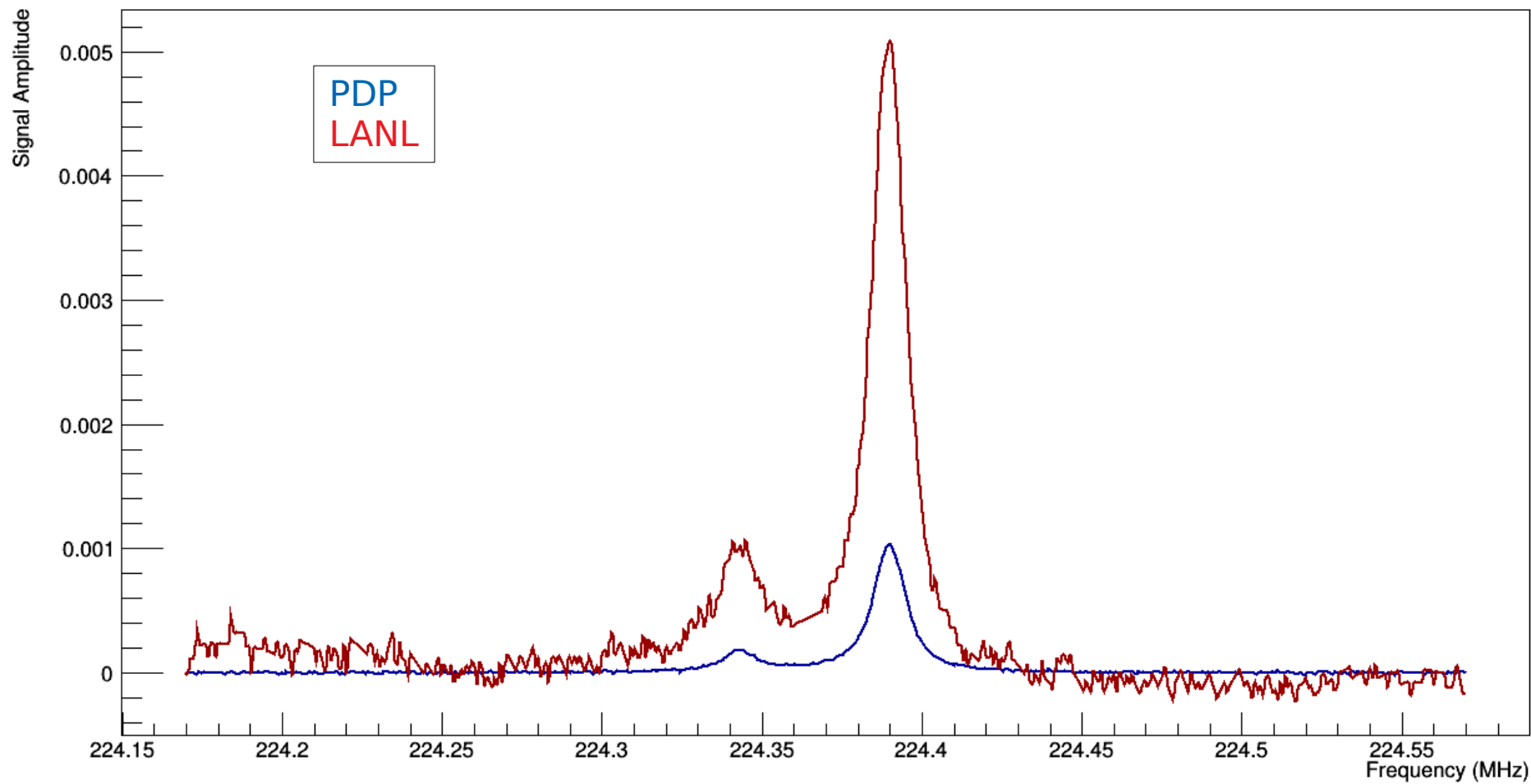


Subtracted Signals: LANL Data 4 Setting 4

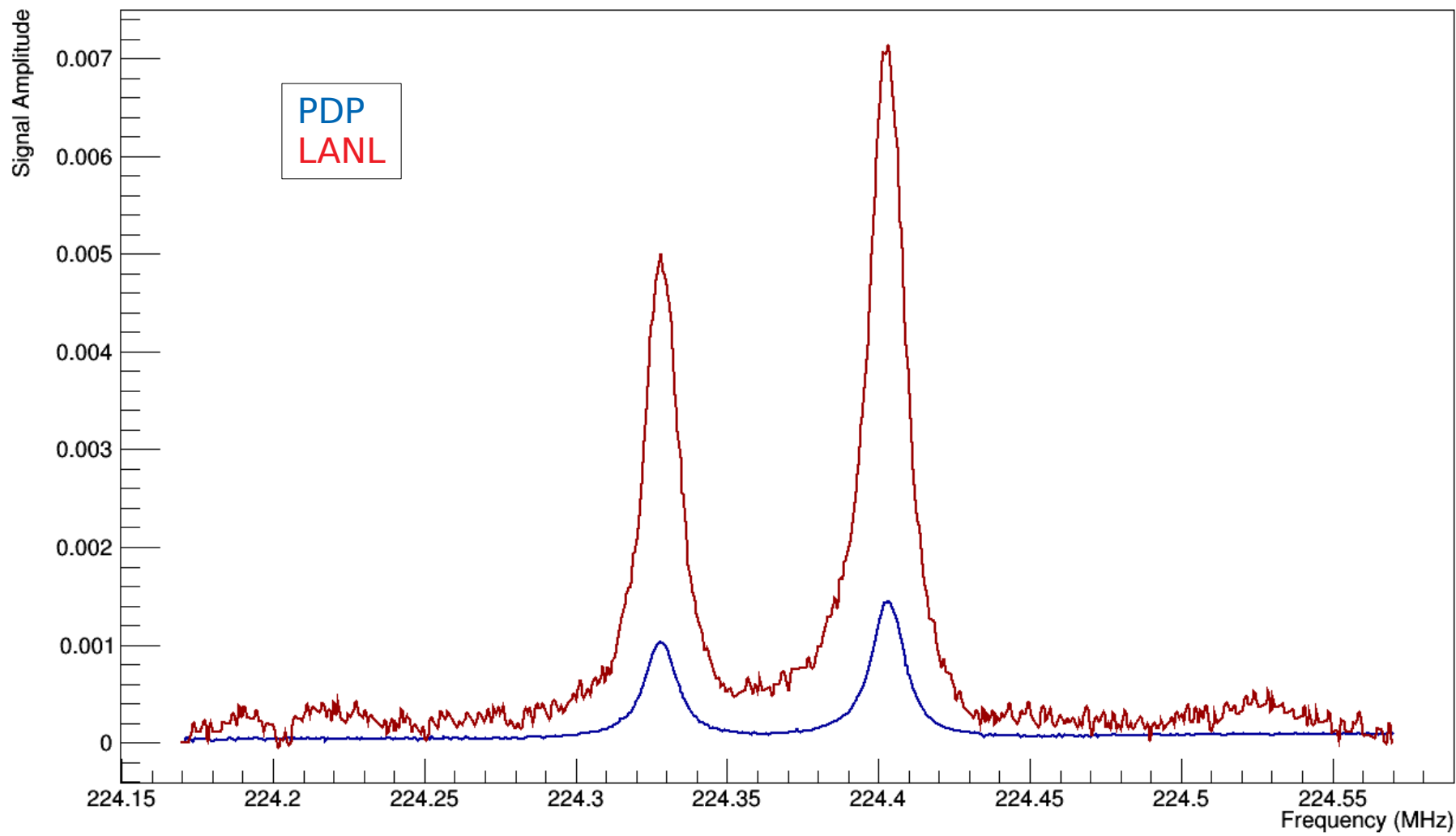


Signal Overlay

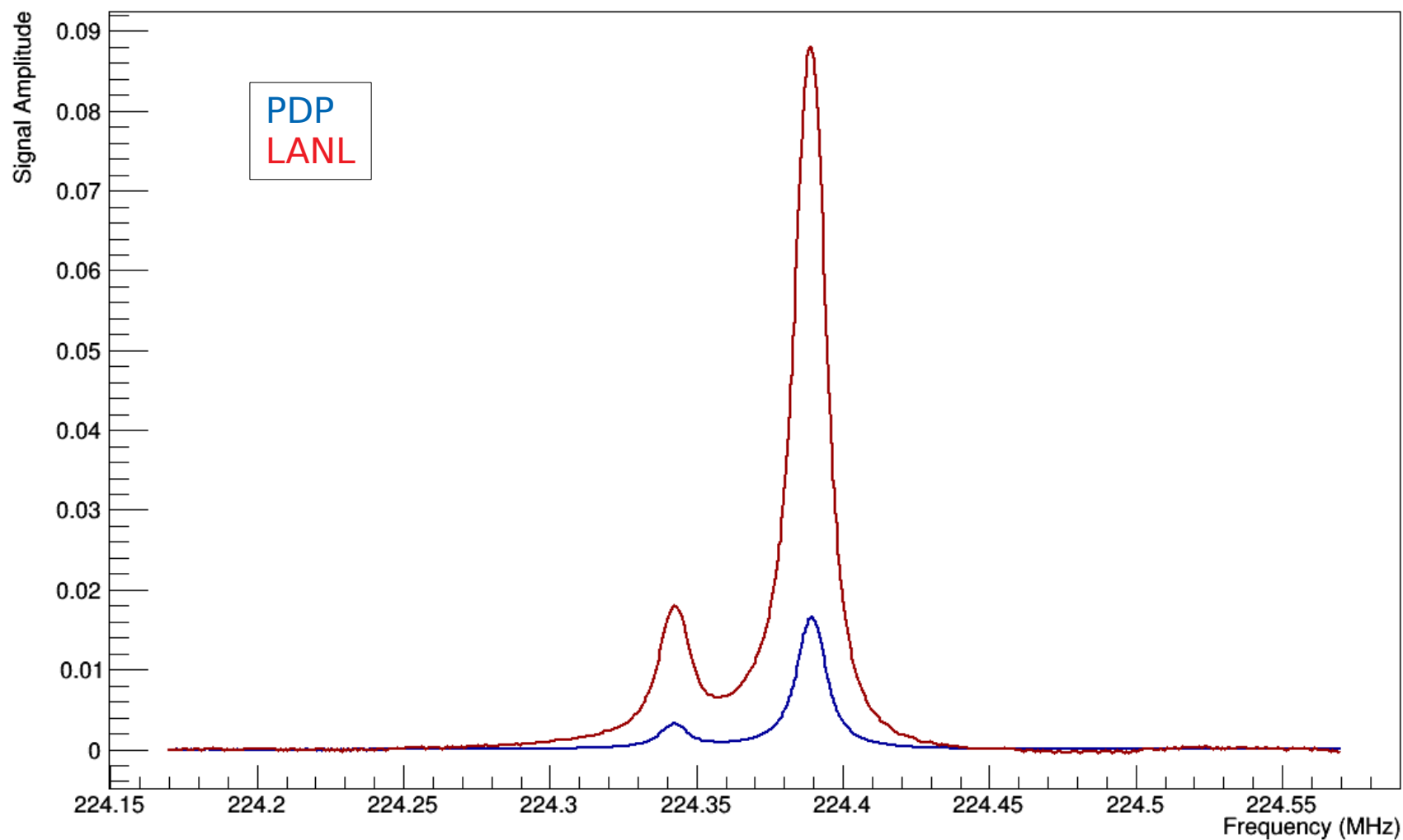
Total Signal: NMR Comparison Setting 1



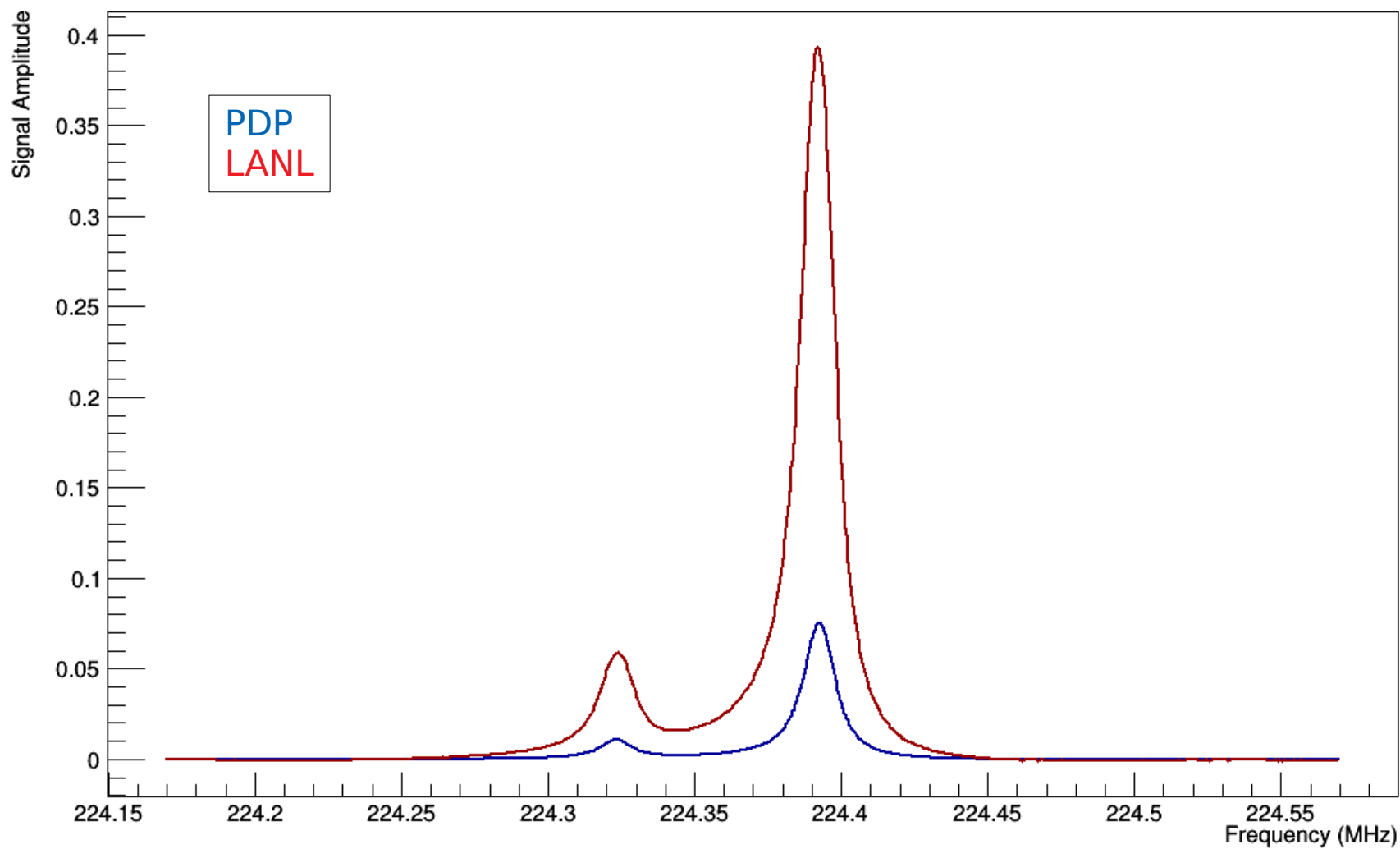
Total Signal: NMR Comparison Setting 2



Total Signal: NMR Comparison Setting 3



Total Signal: NMR Comparison Setting 4



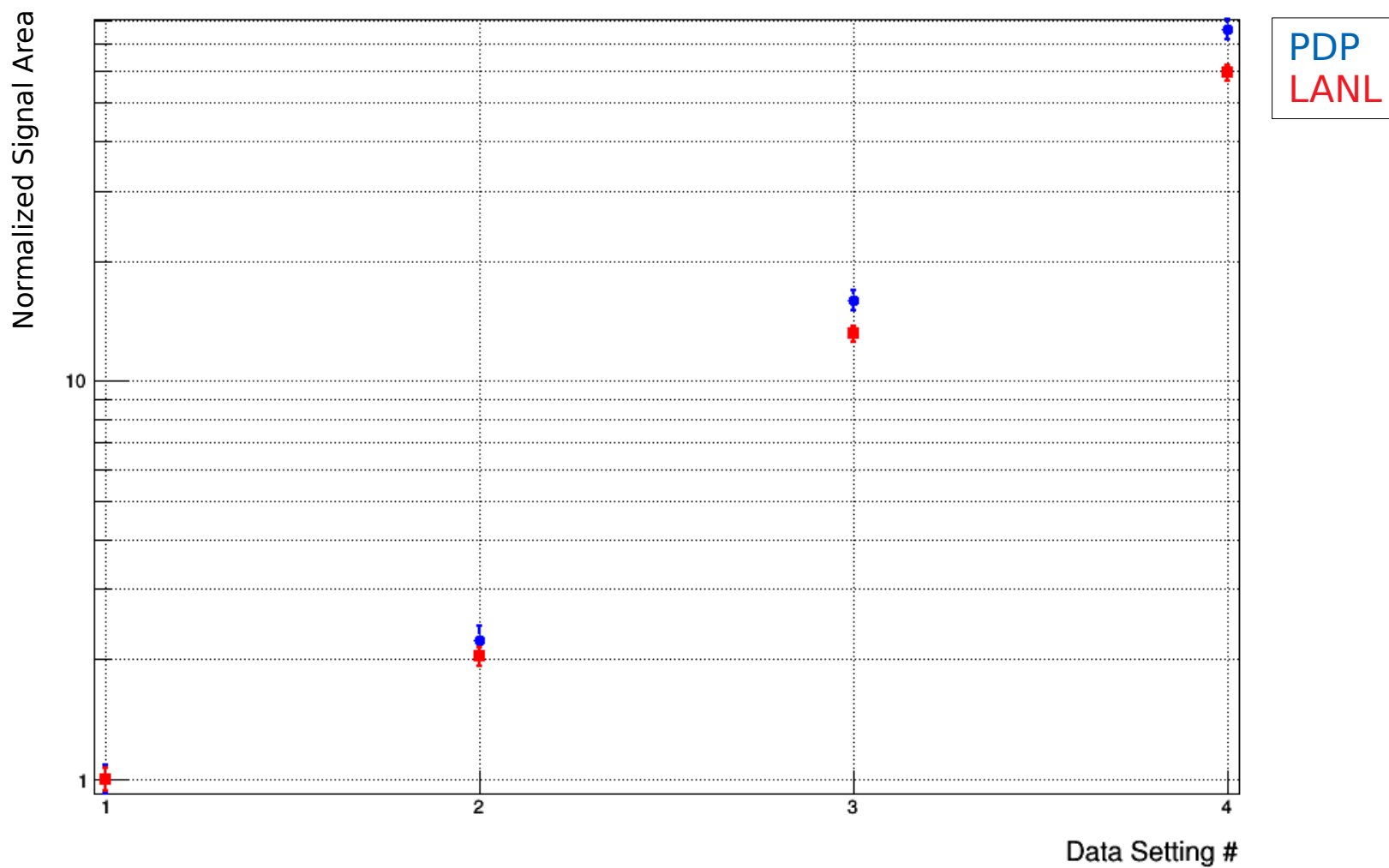
Normalized Area Comparison

For each signal setting the integrated area under the signal was normalized by the integrated signal of the first setting.

Ratios were then plotted versus signal setting.

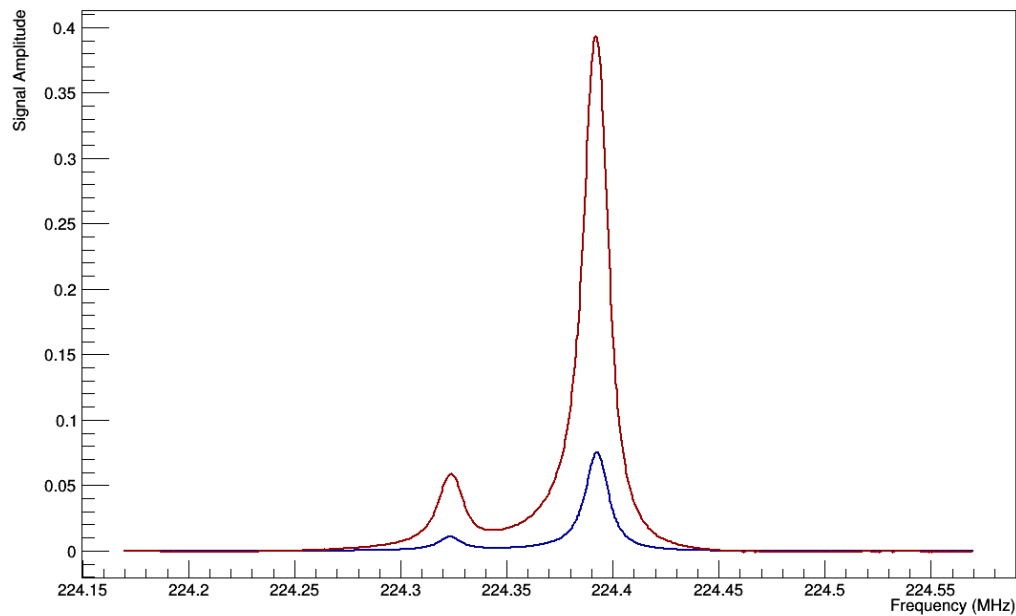
Lower bound errors were estimated by calculating the average standard error of the background fit and then scaling to accommodate the full signal spectrum. This error was then propagated into the area calculation.

Normalized Signal: NMR Comparison

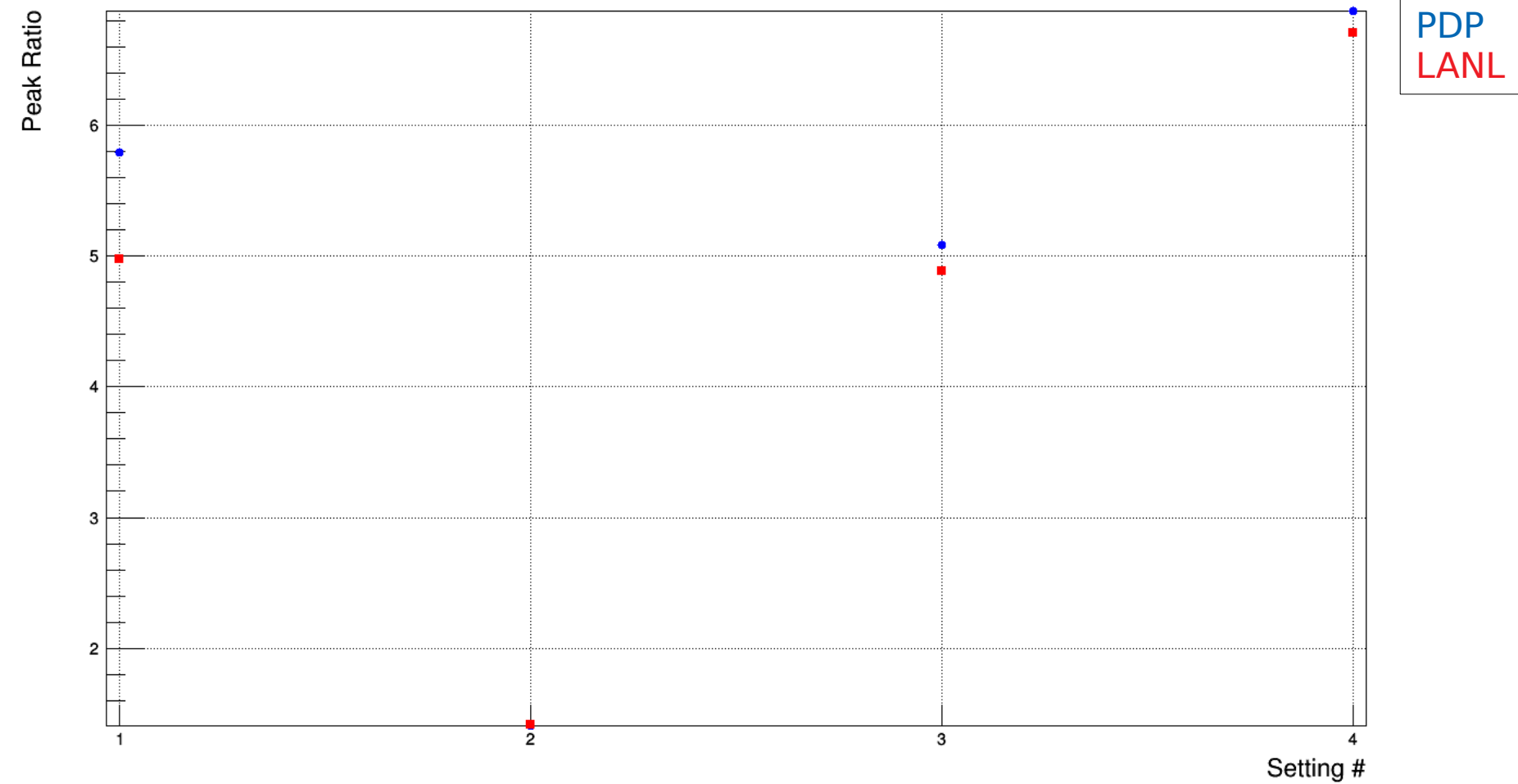


Peak Ratio

For each data set the amplitude of each peak in the subtracted spectrum was determined and the ration of the higher peak to the lower peak was calculated. This was plotted versus signal setting.

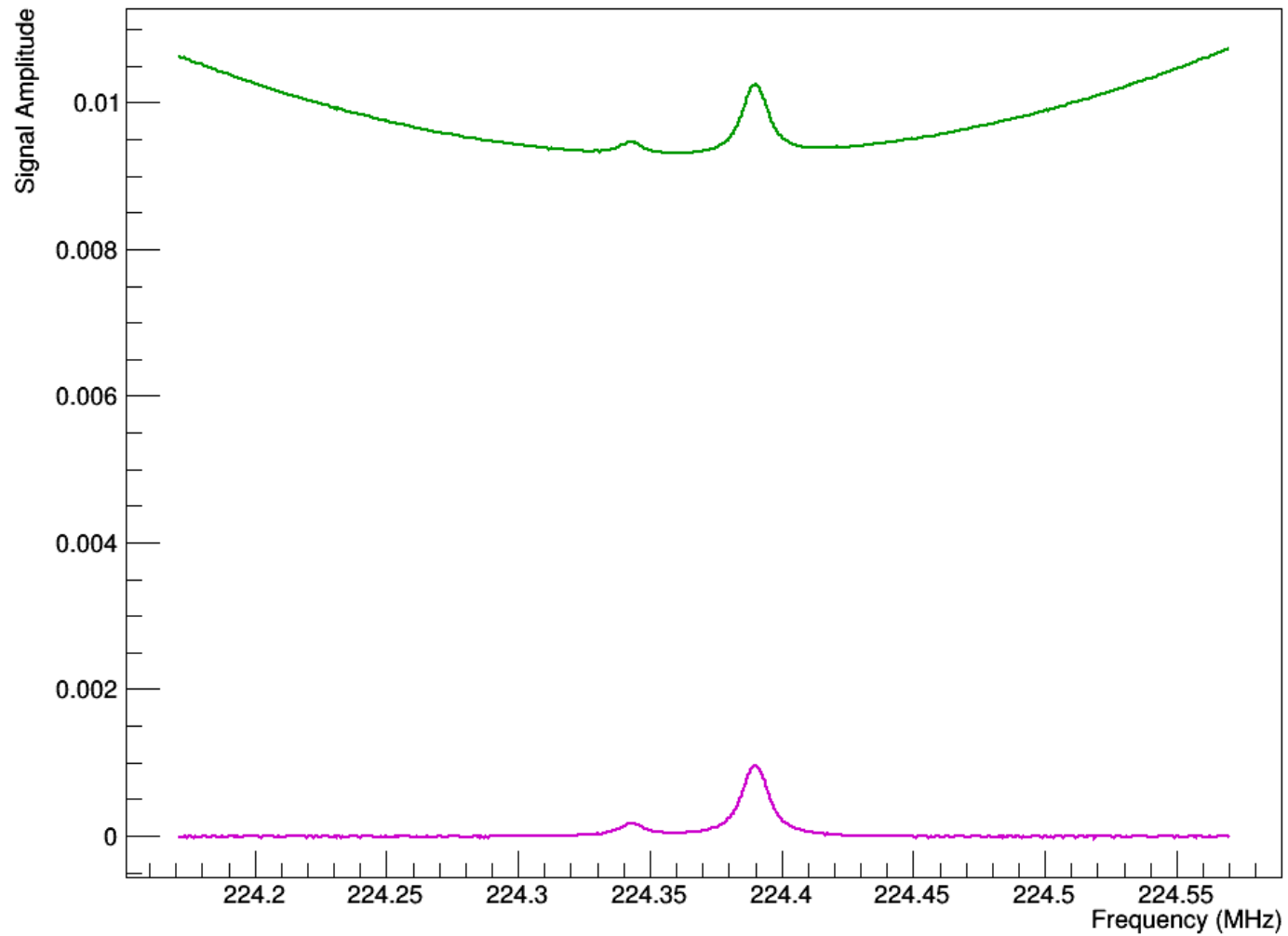


Normalized Signal: NMR Peak Comparison

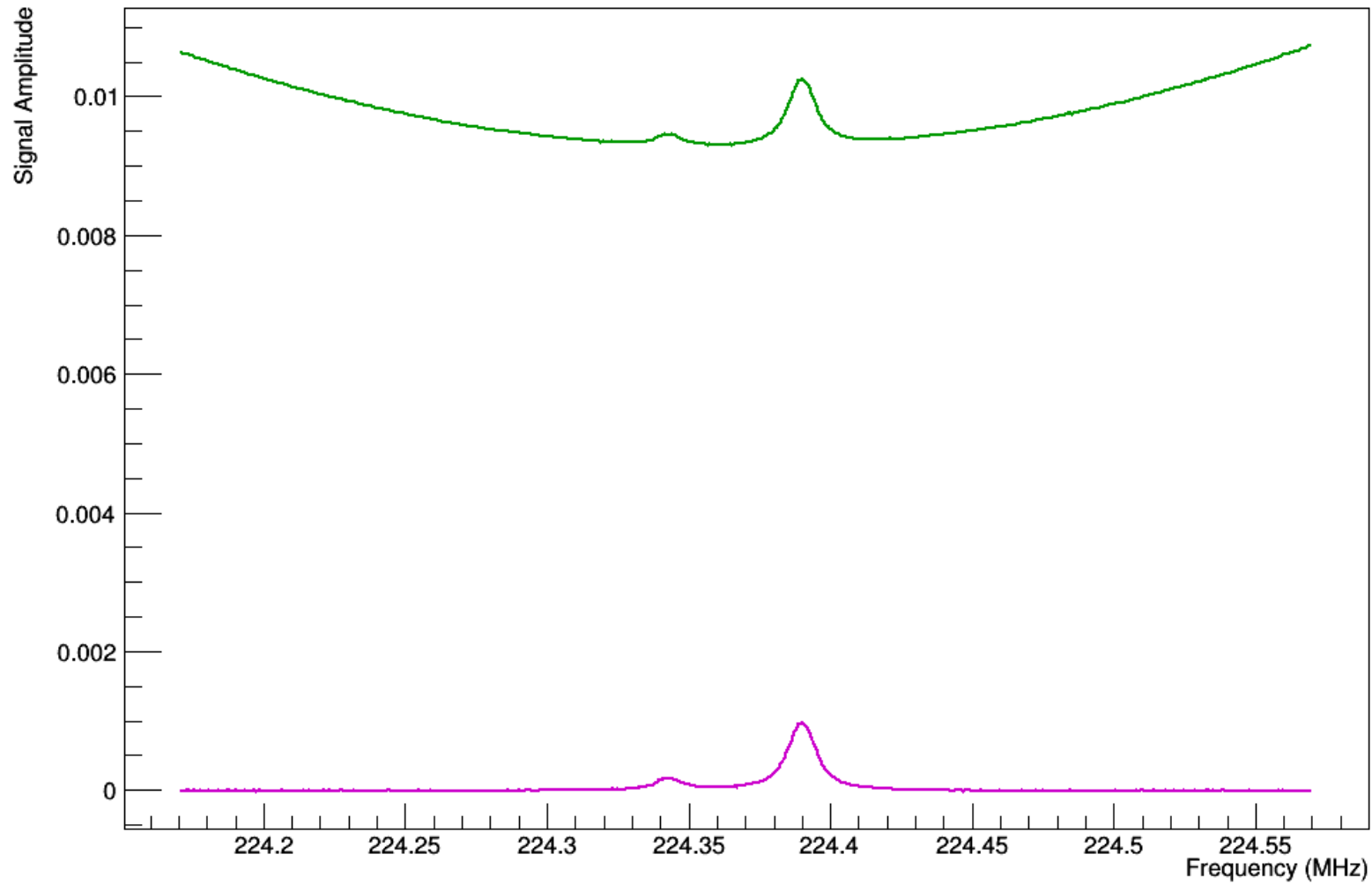


Data Set 5

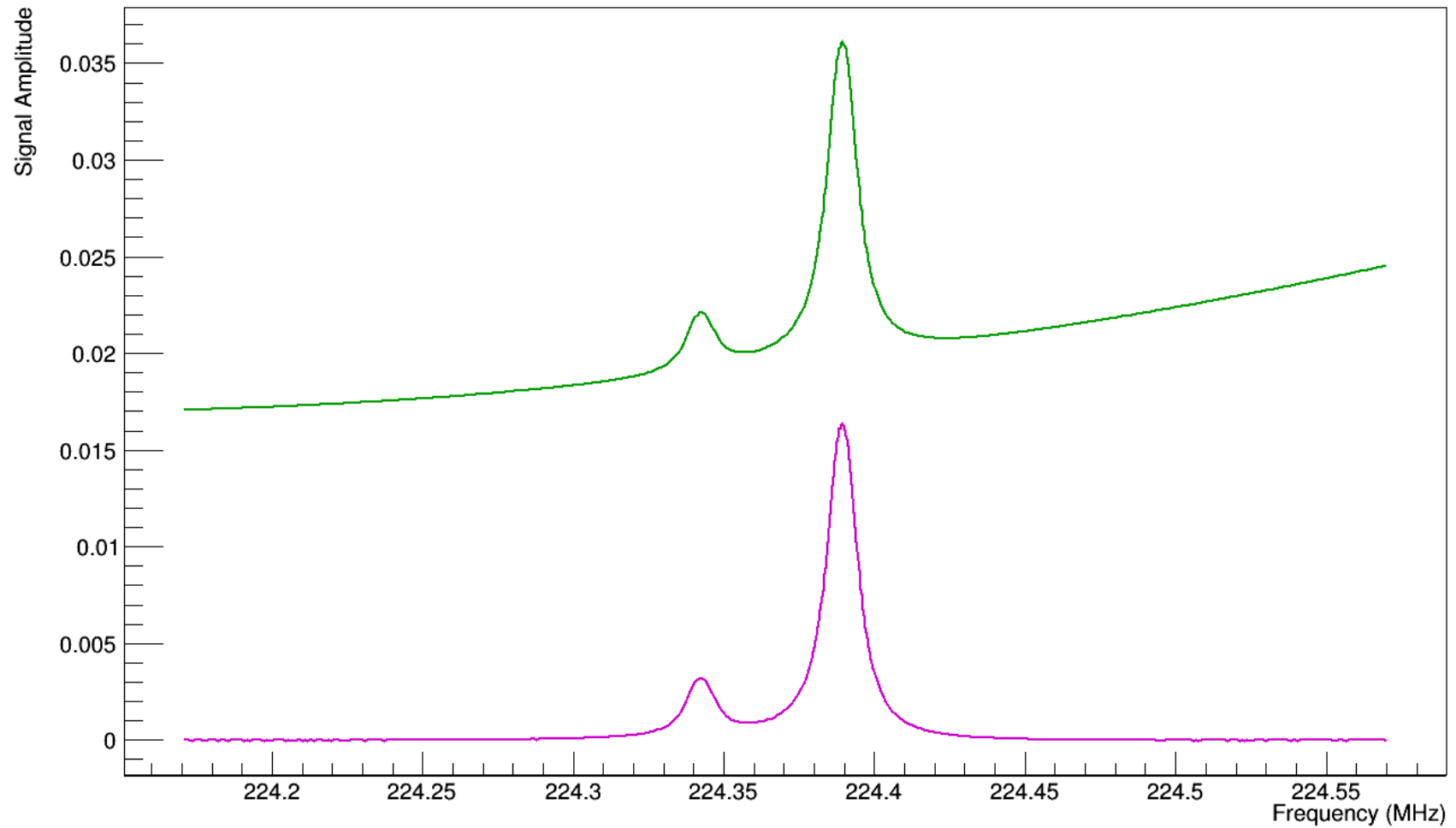
Subtracted Signals: PDP Data 5 Setting 1



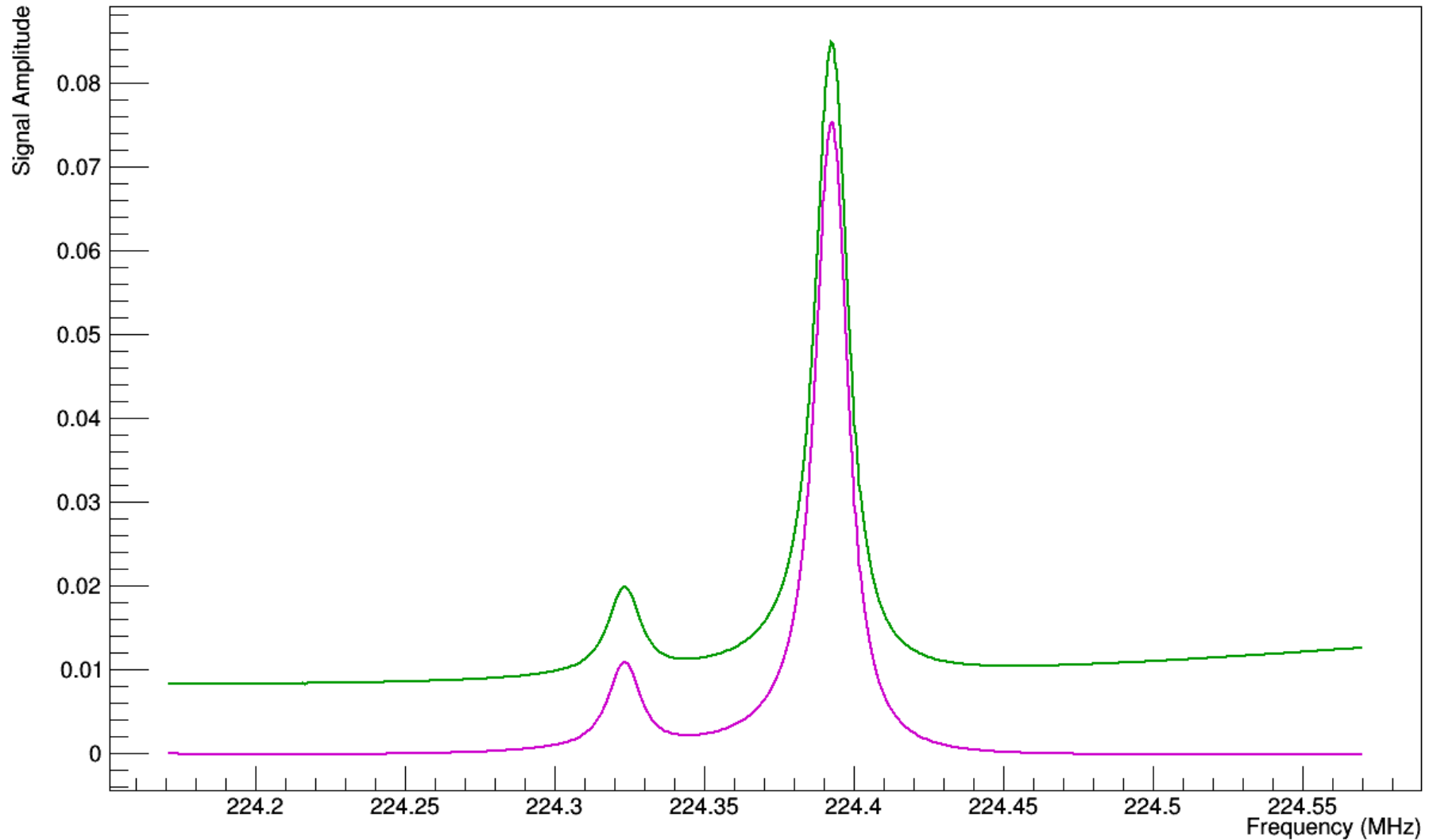
Subtracted Signals: PDP Data 5 Setting 2



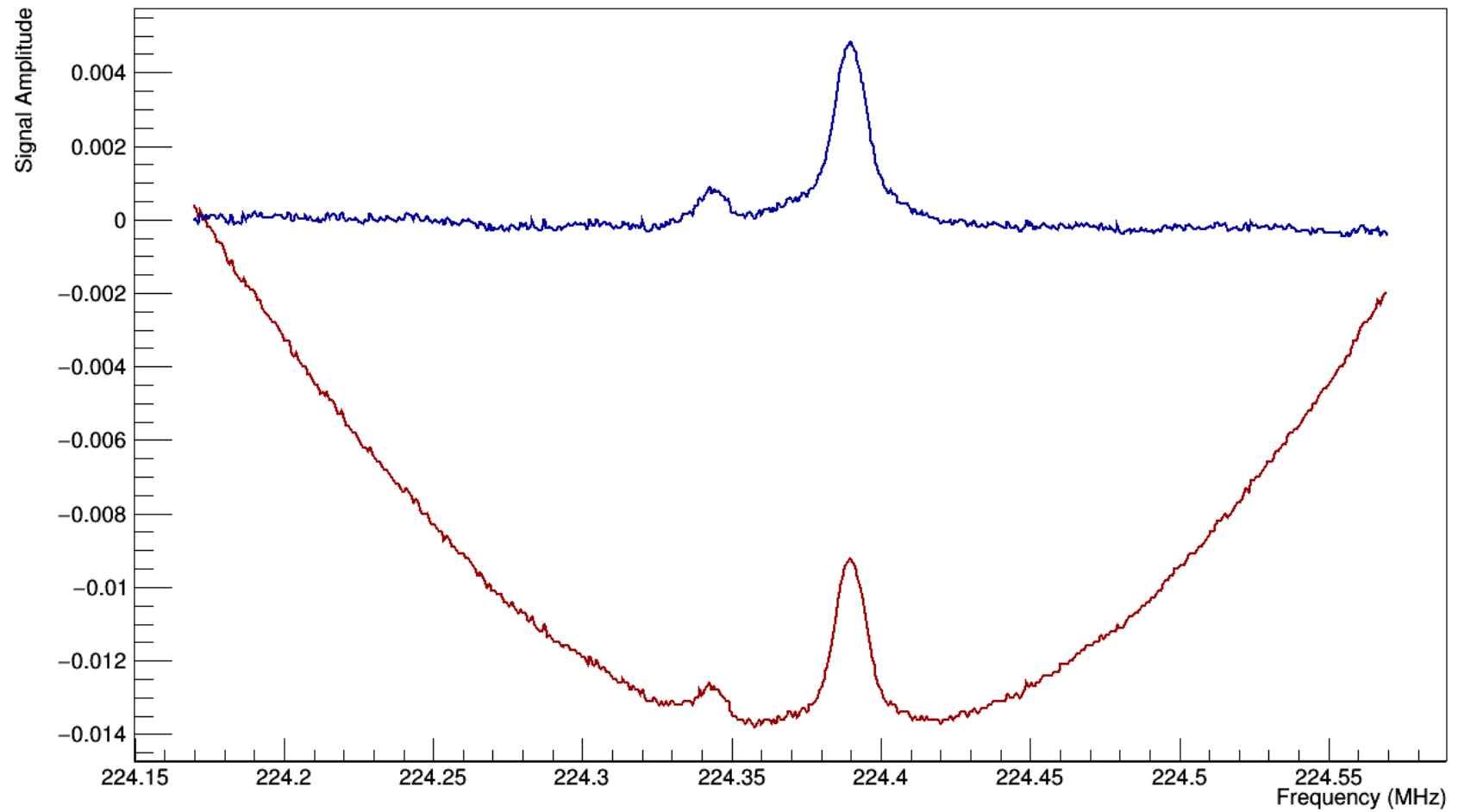
Subtracted Signals: PDP Data 5 Setting 3



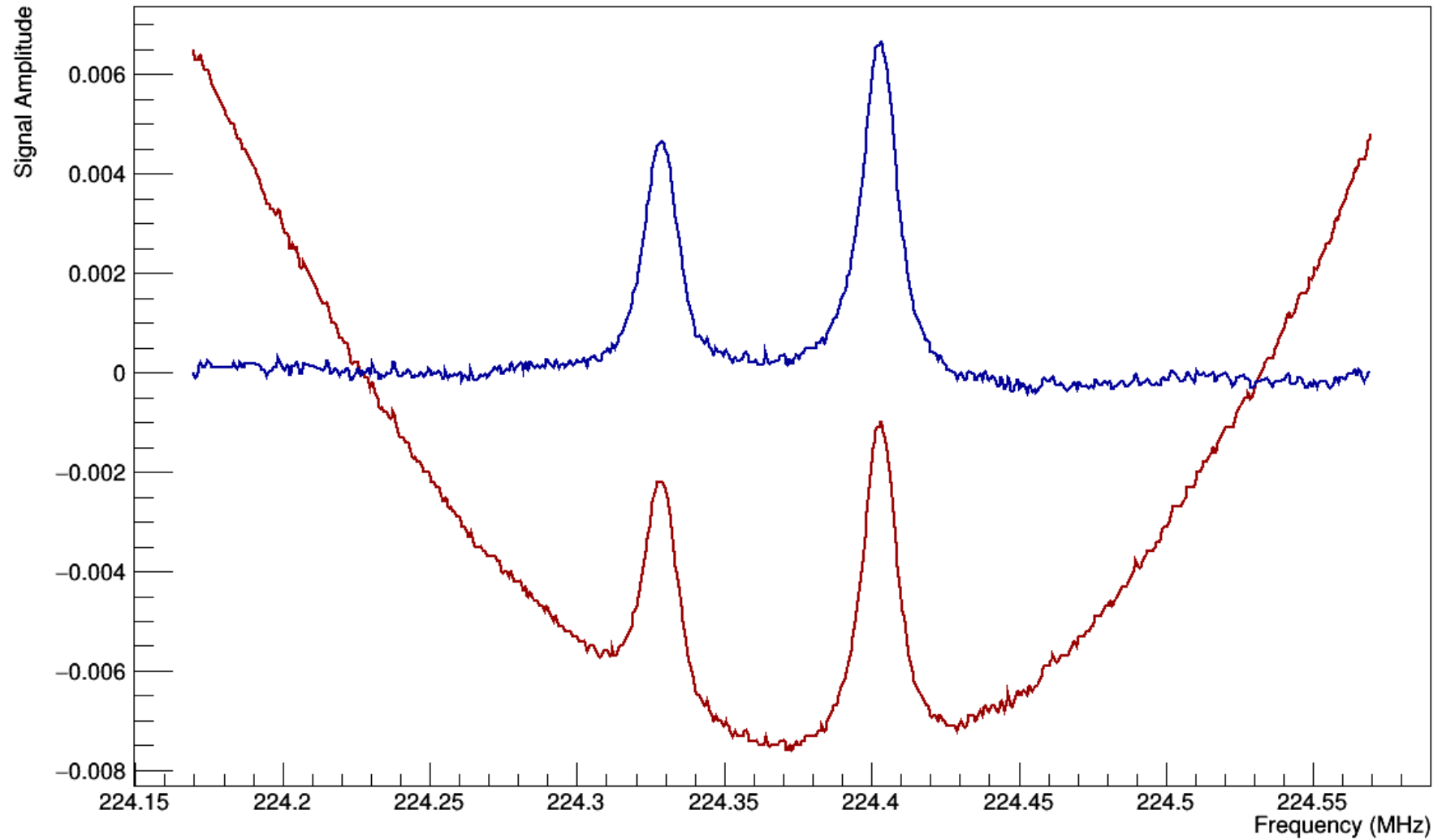
Subtracted Signals: PDP Data 5 Setting 4



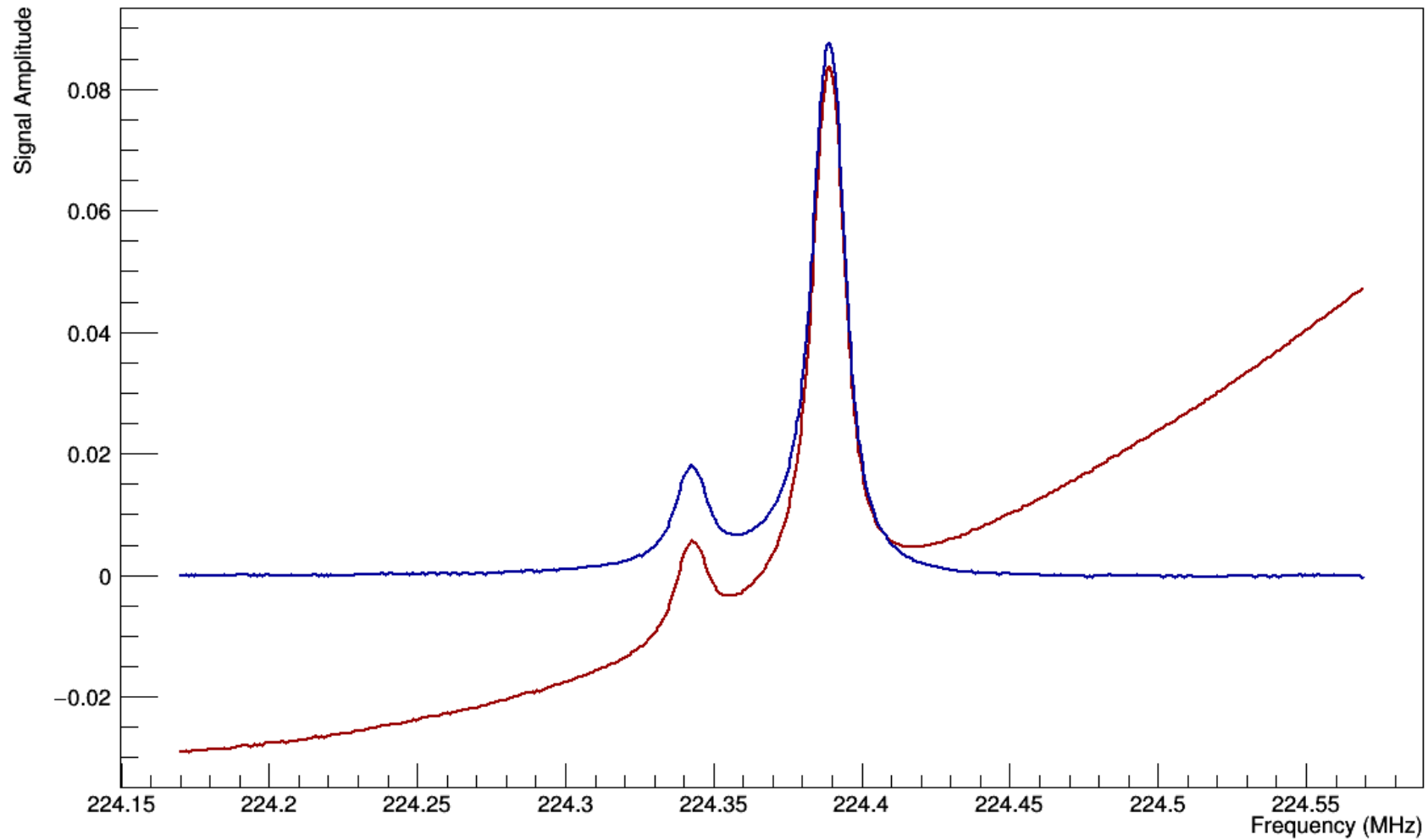
Subtracted Signals: LANL Data 5 Setting 1



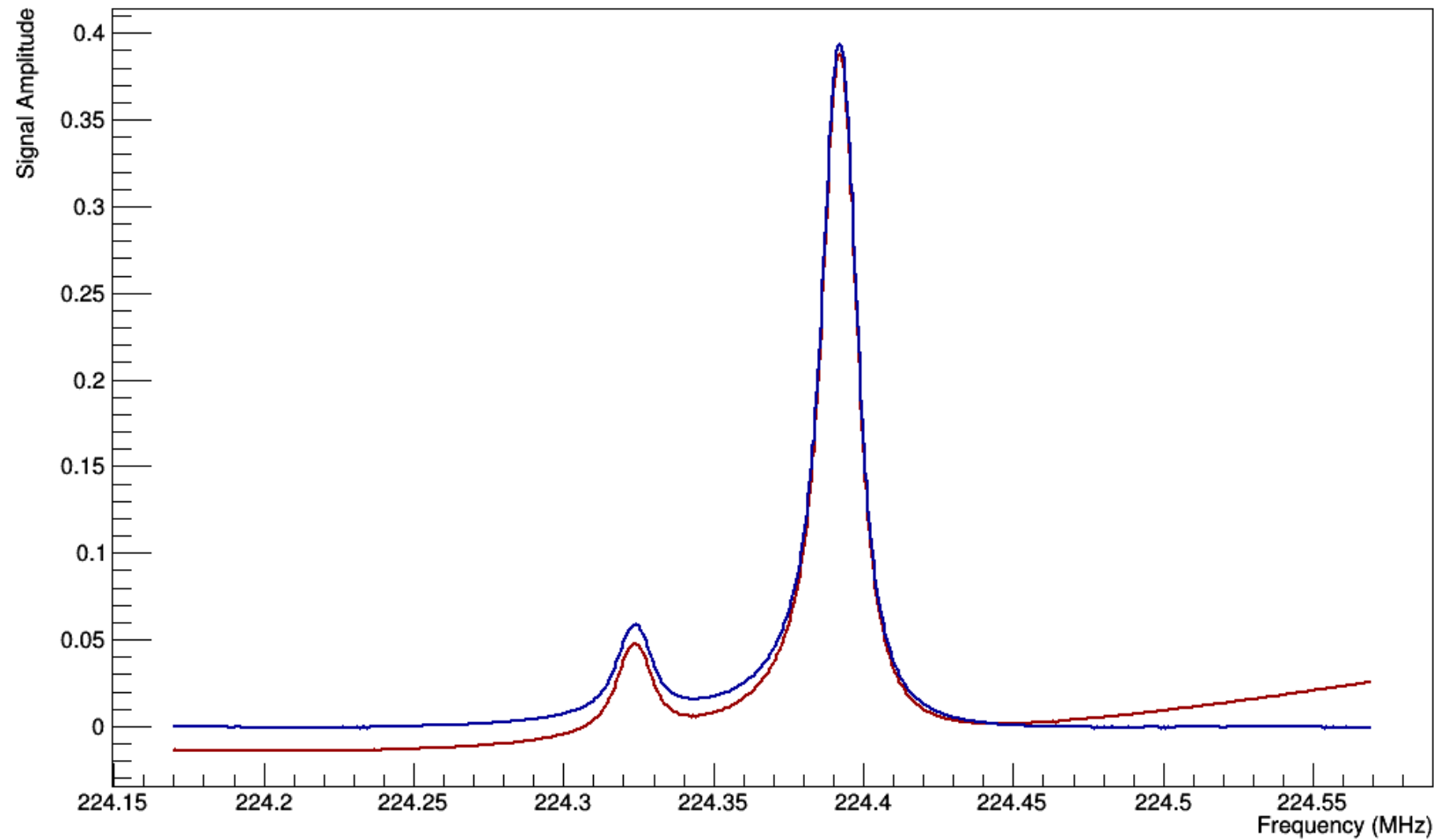
Subtracted Signals: LANL Data 5 Setting 2



Subtracted Signals: LANL Data 5 Setting 3

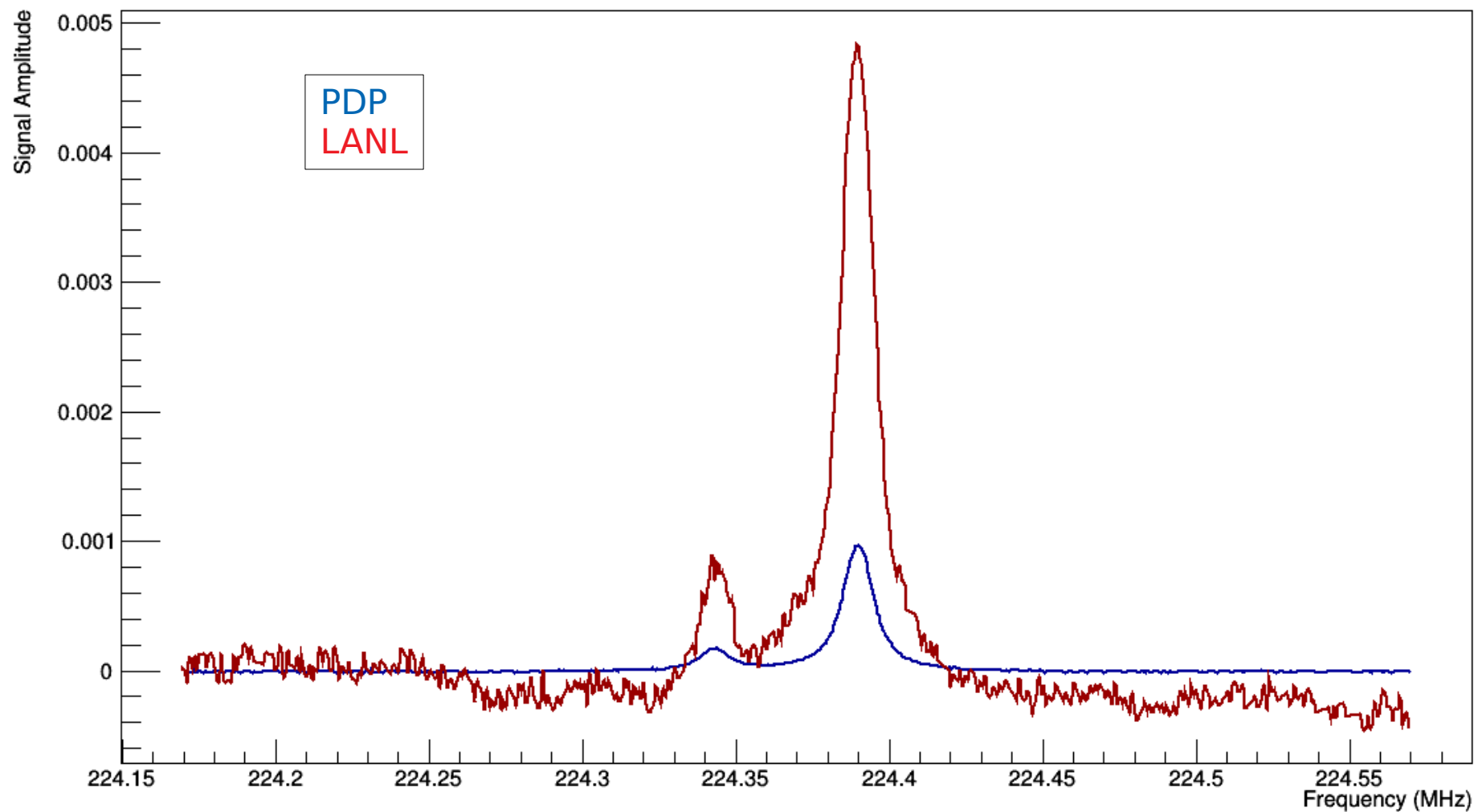


Subtracted Signals: LANL Data 5 Setting 4

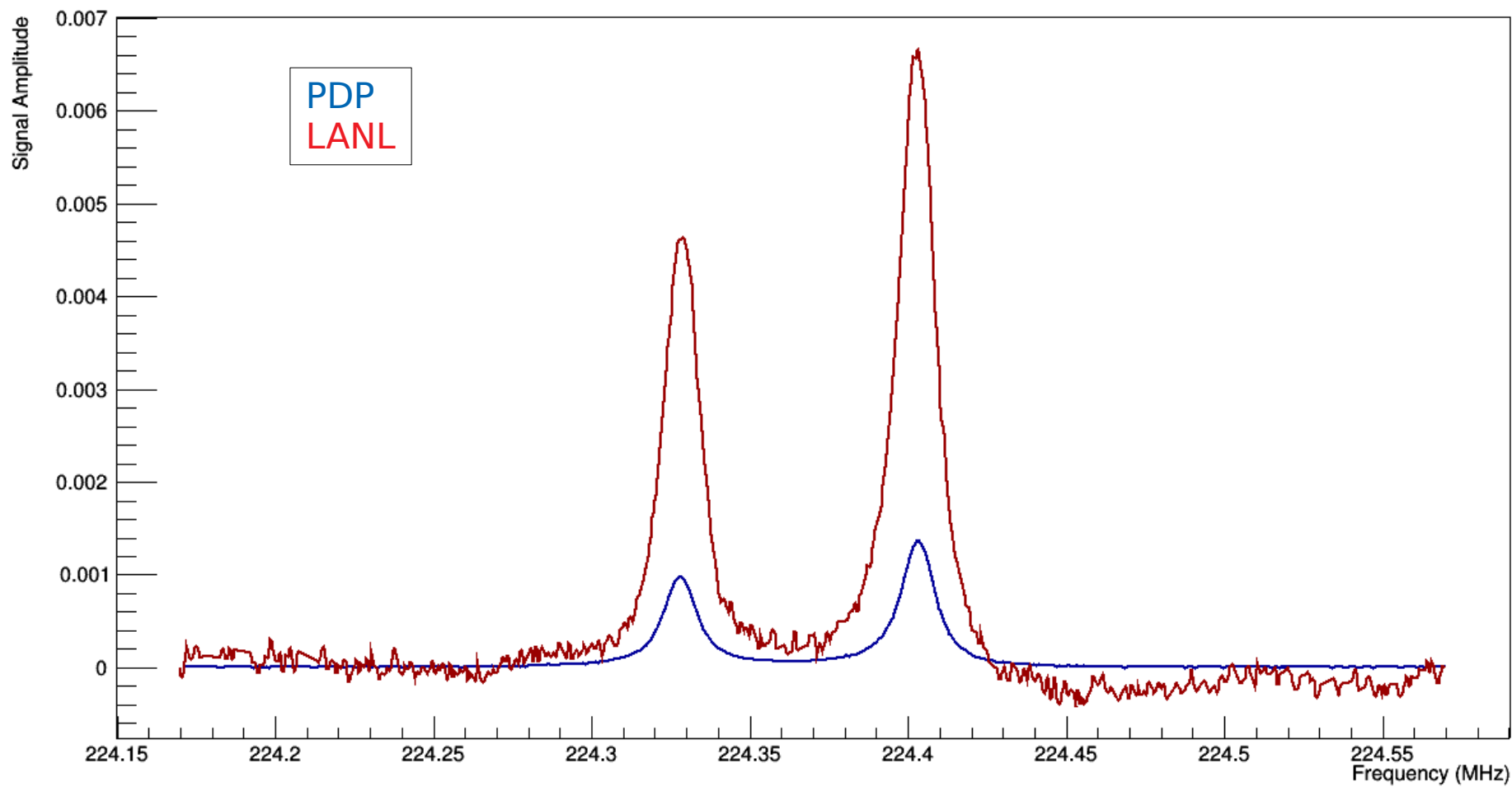


Signal Overlay

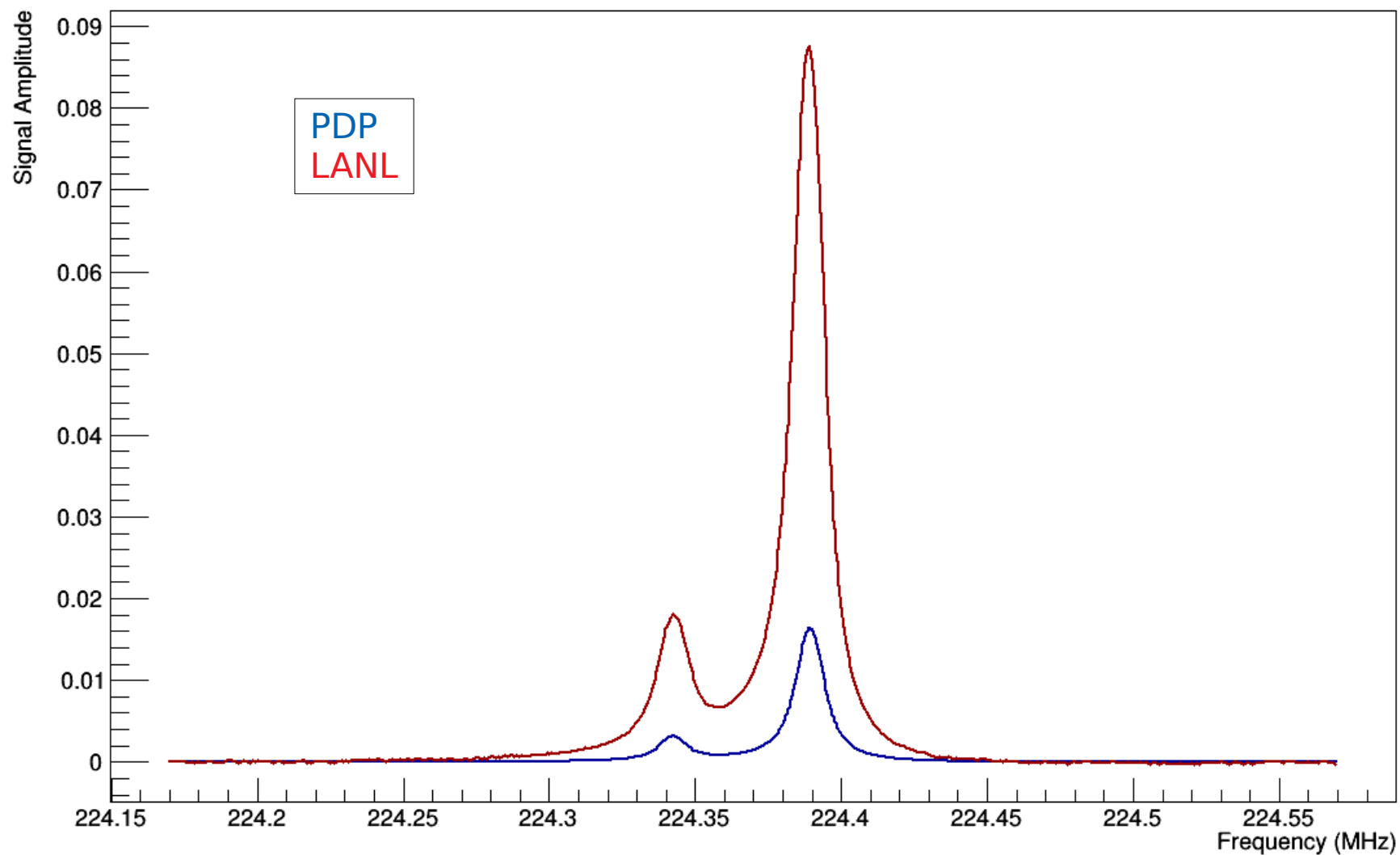
Total Signal: NMR Comparison Setting 1



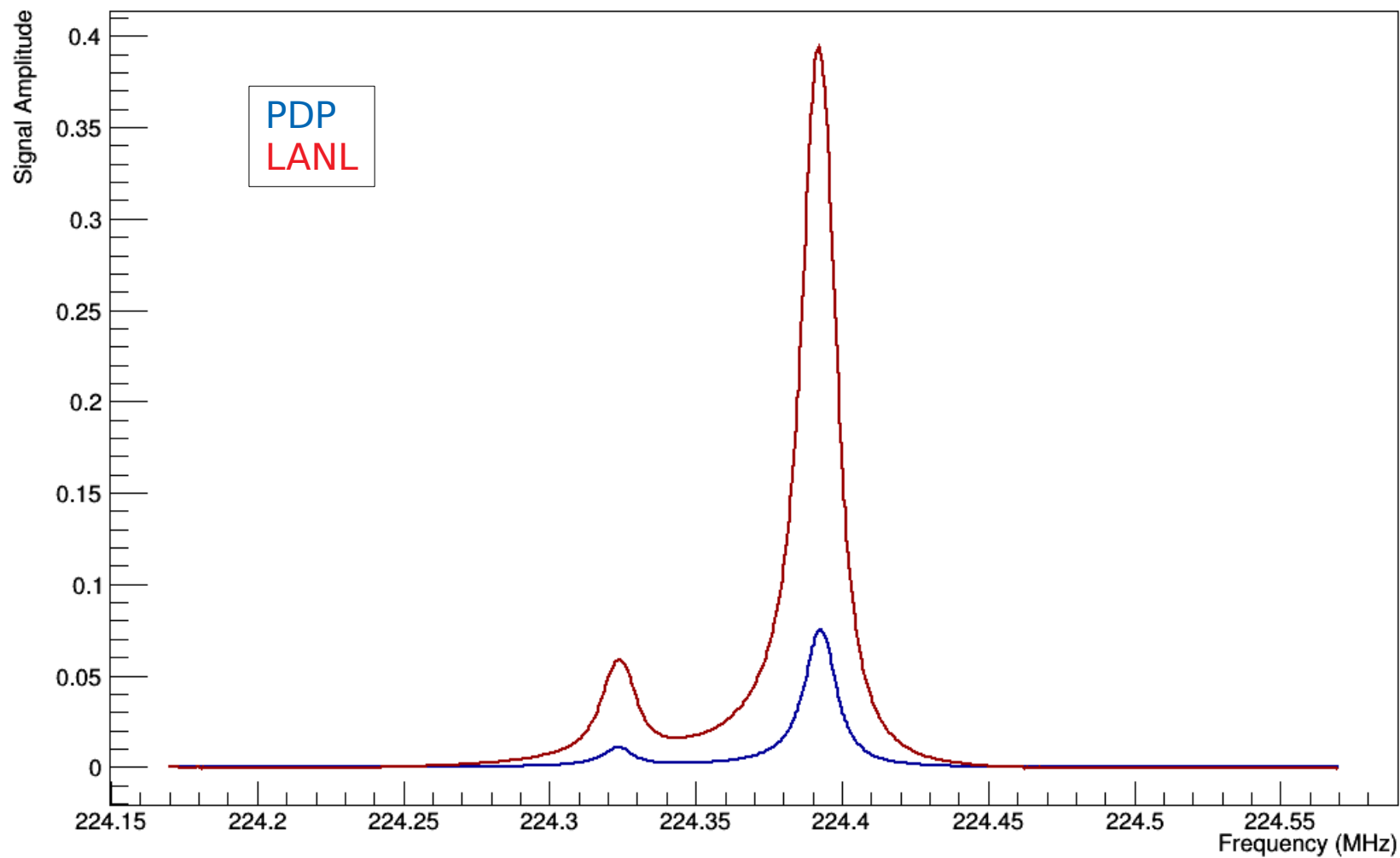
Total Signal: NMR Comparison Setting 2



Total Signal: NMR Comparison Setting 3



Total Signal: NMR Comparison Setting 4



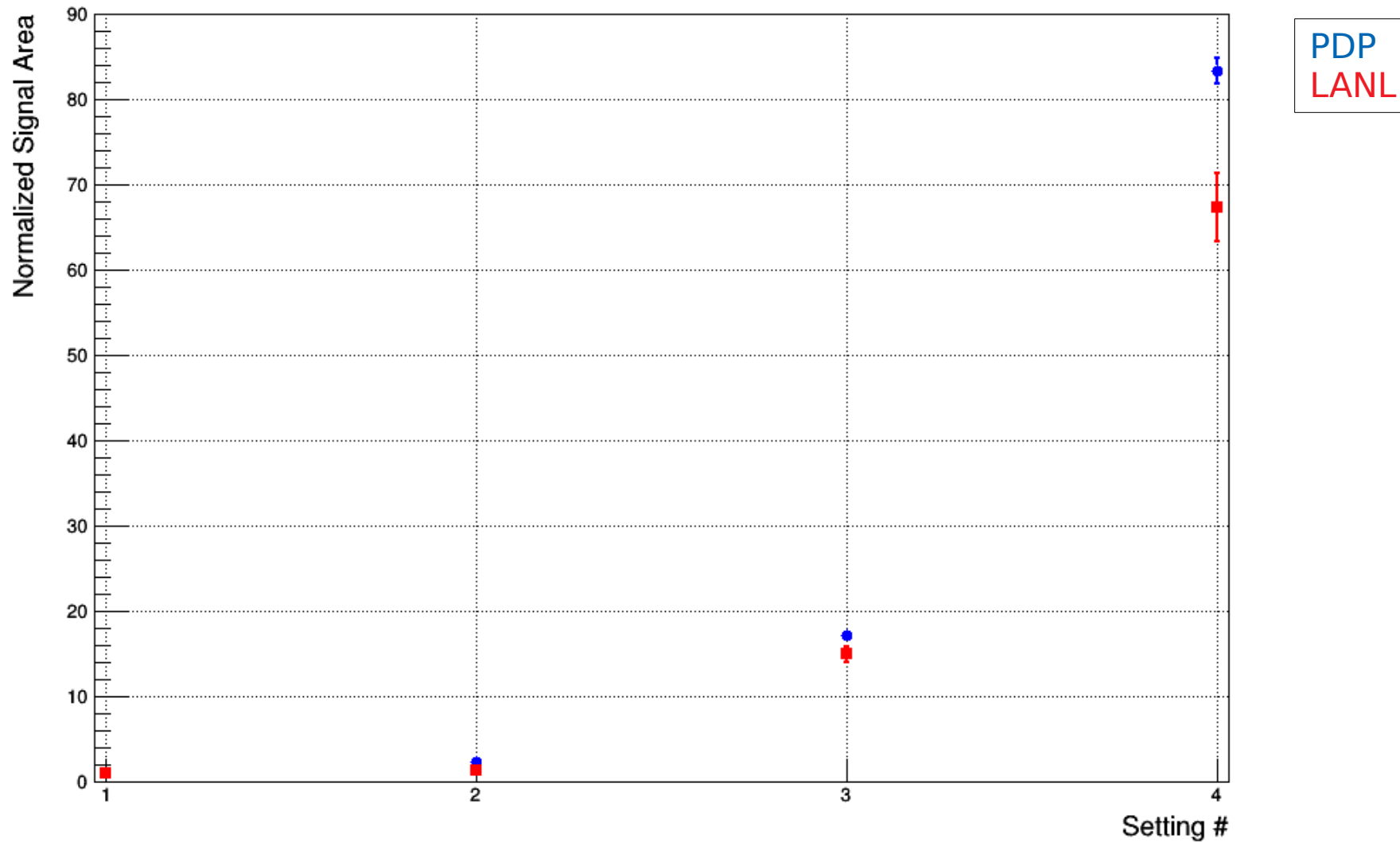
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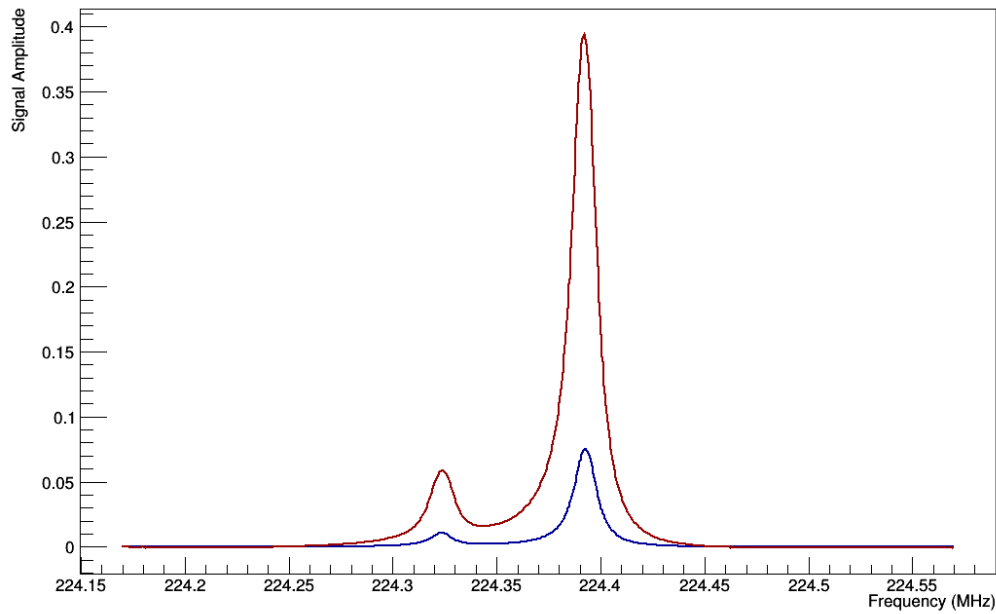
Normalized Signal: NMR Comparison



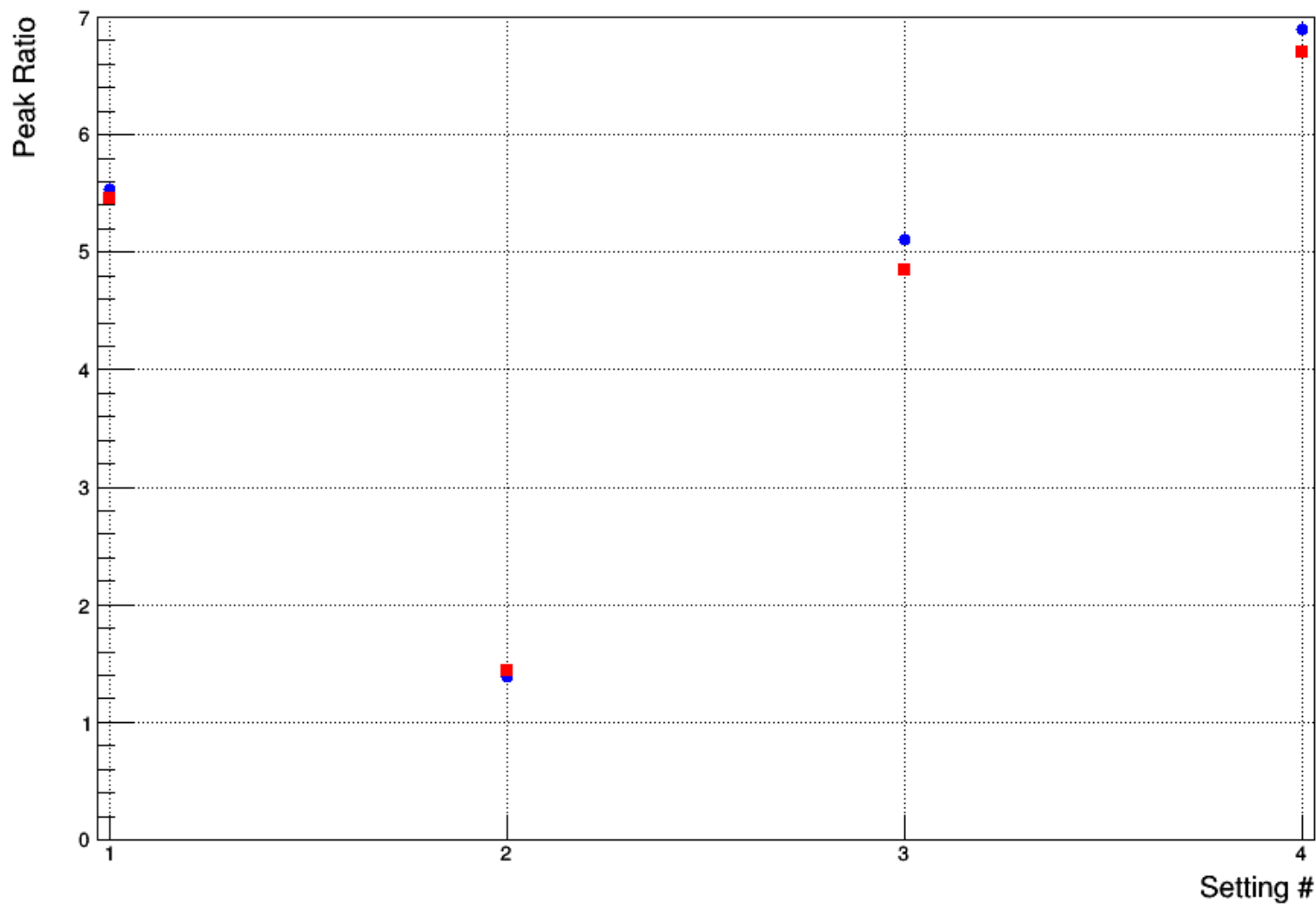
Peak Ratio

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This was plotted versus signal setting.



Normalized Signal: NMR Peak Comparison



PDP
LANL

Conclusion

Systematic differences can be seen post-background subtraction in some cases.

Both comparisons show a difference between the two systems to some degree.

There are differences in the actual gain of each systems versus gain setting but these show but canceled out when normalizing by the area of the first setting.

There seems to be a legitimate difference between the two systems response to a given signal.