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.

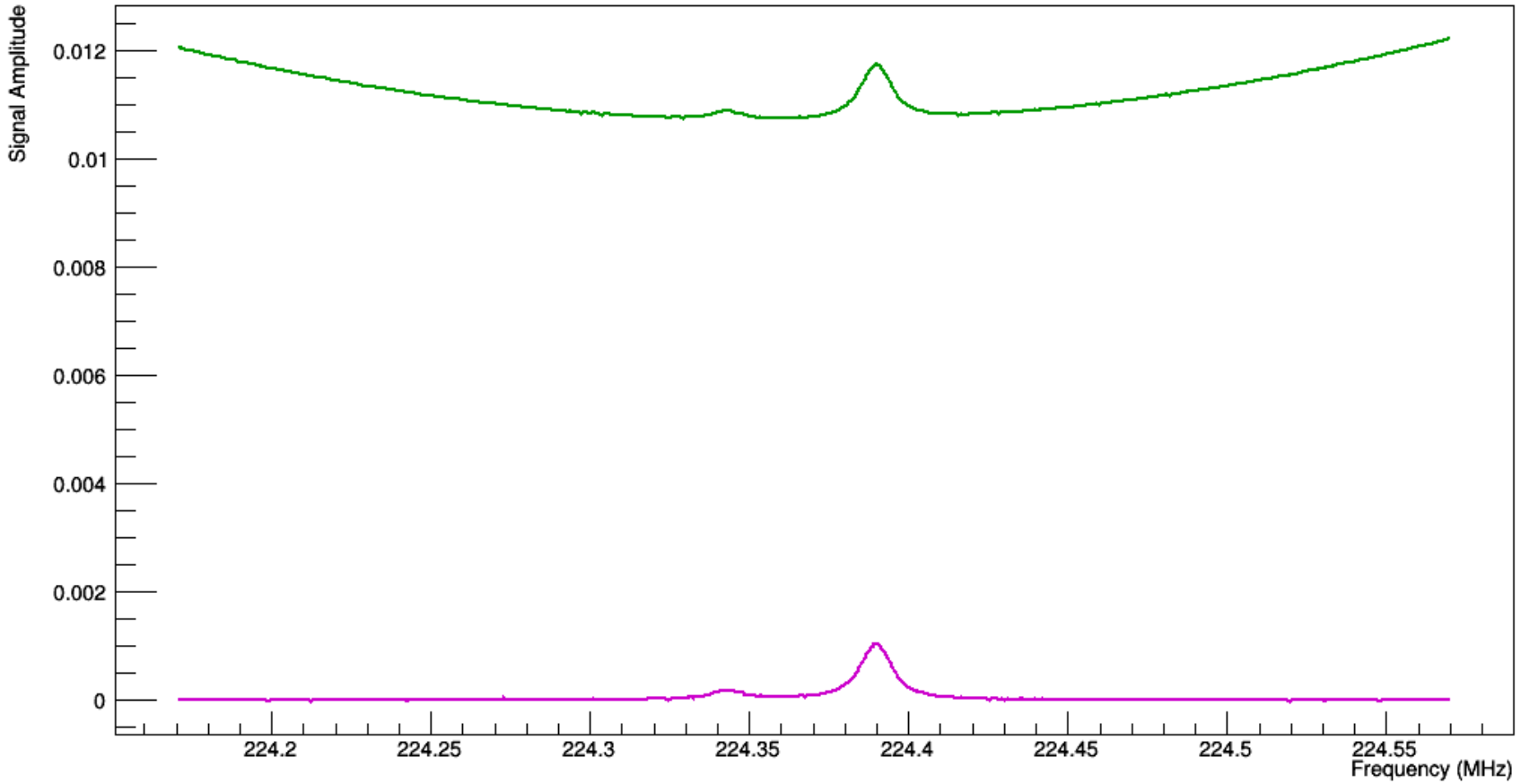
Background was defined by wings of data making up 20% of overall data on each side.

Background determined using OLS polynomial regression.

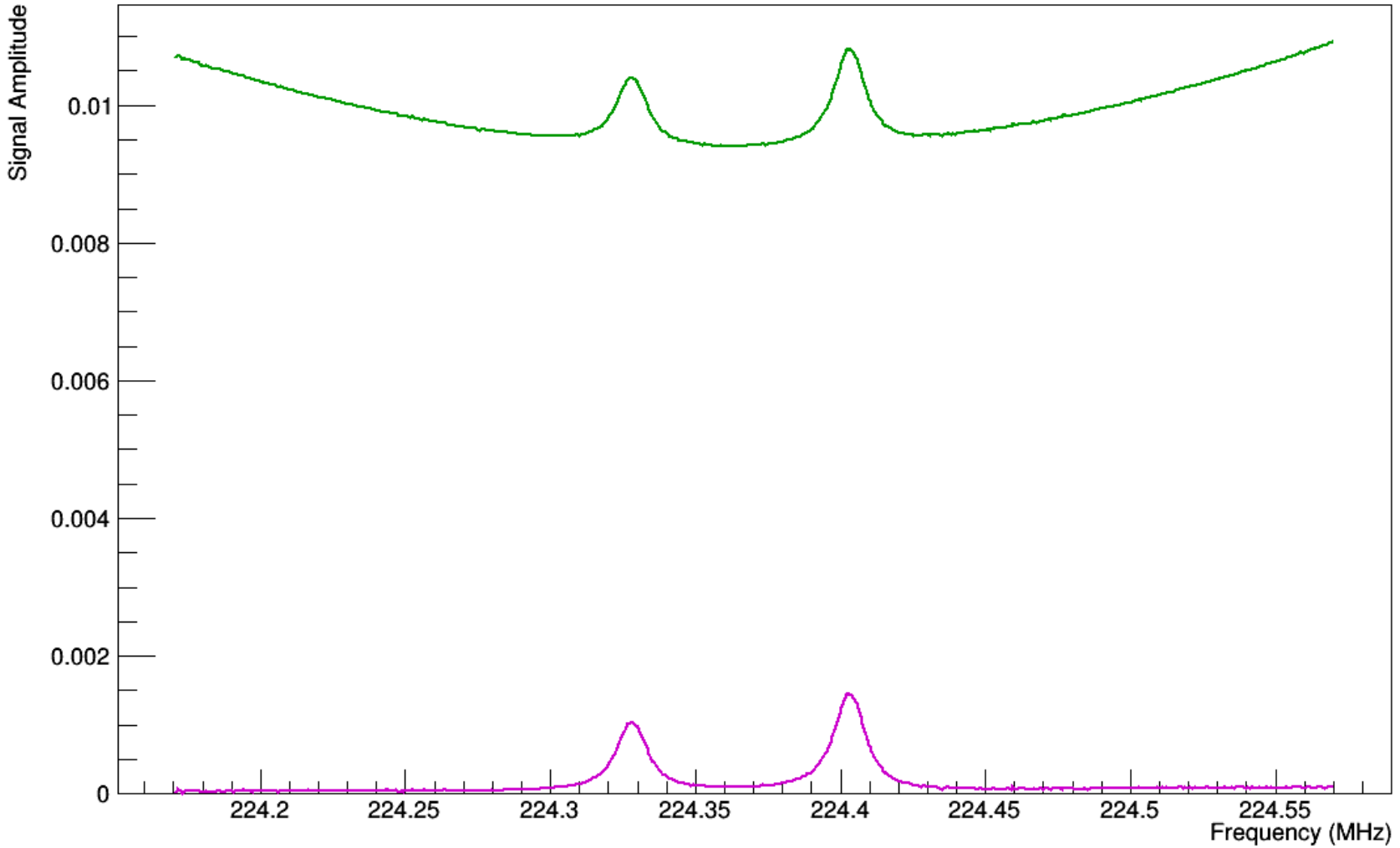
Forth order polynomial used to subtract background of full signal.

Data Set 4

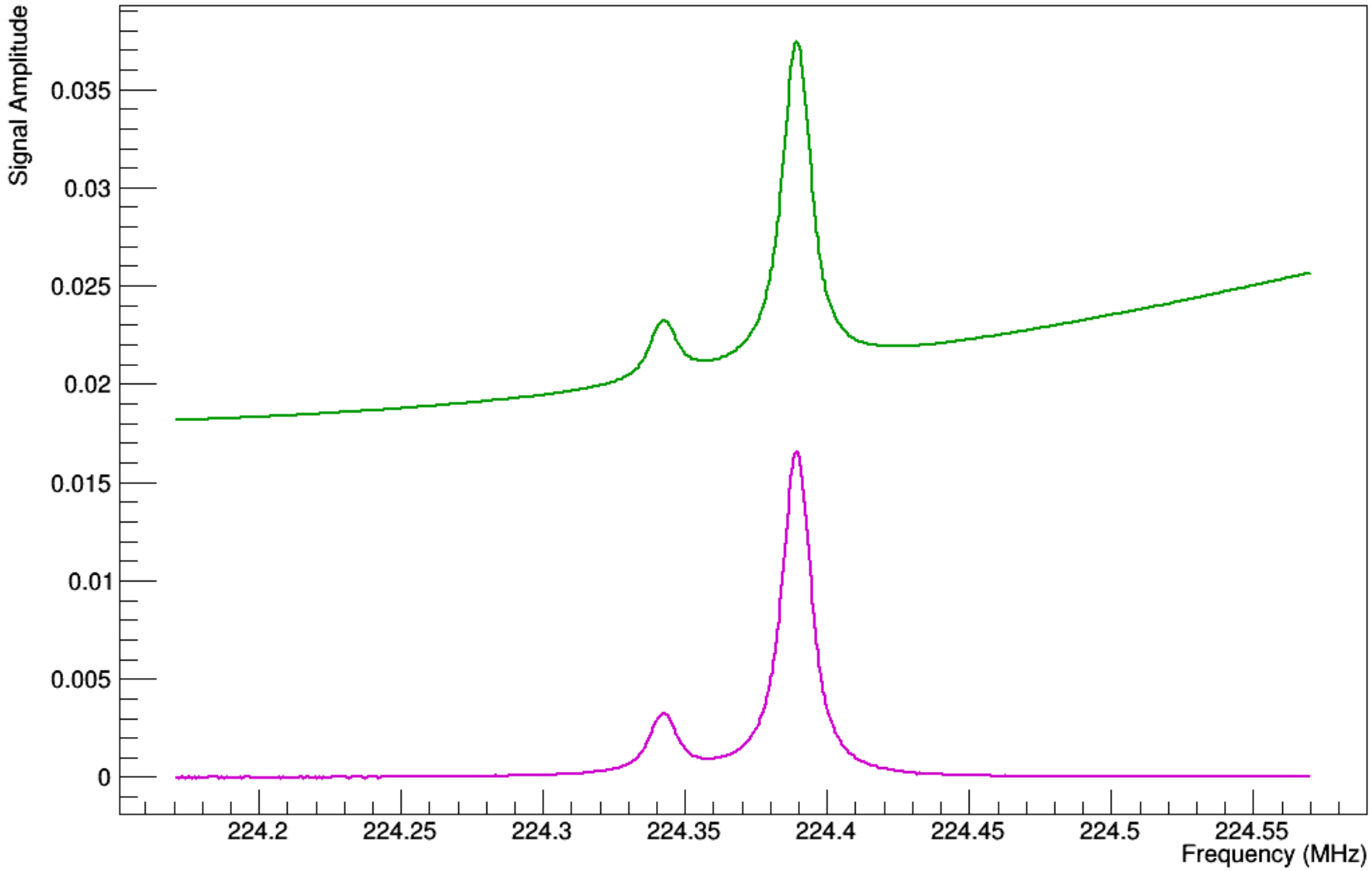
Subtracted Signals: PDP Data 4 Setting 1



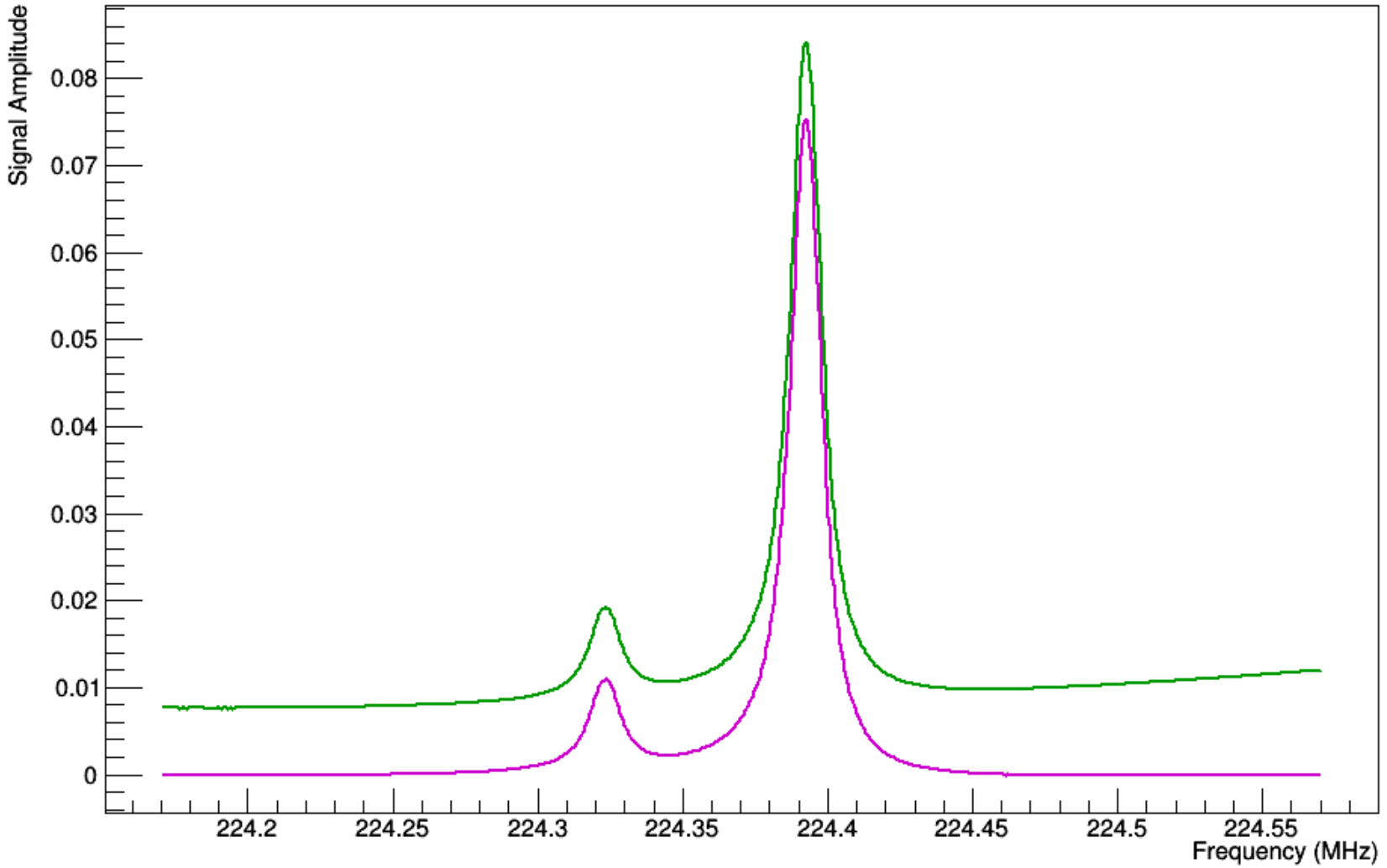
Subtracted Signals: PDP Data 4 Setting 2



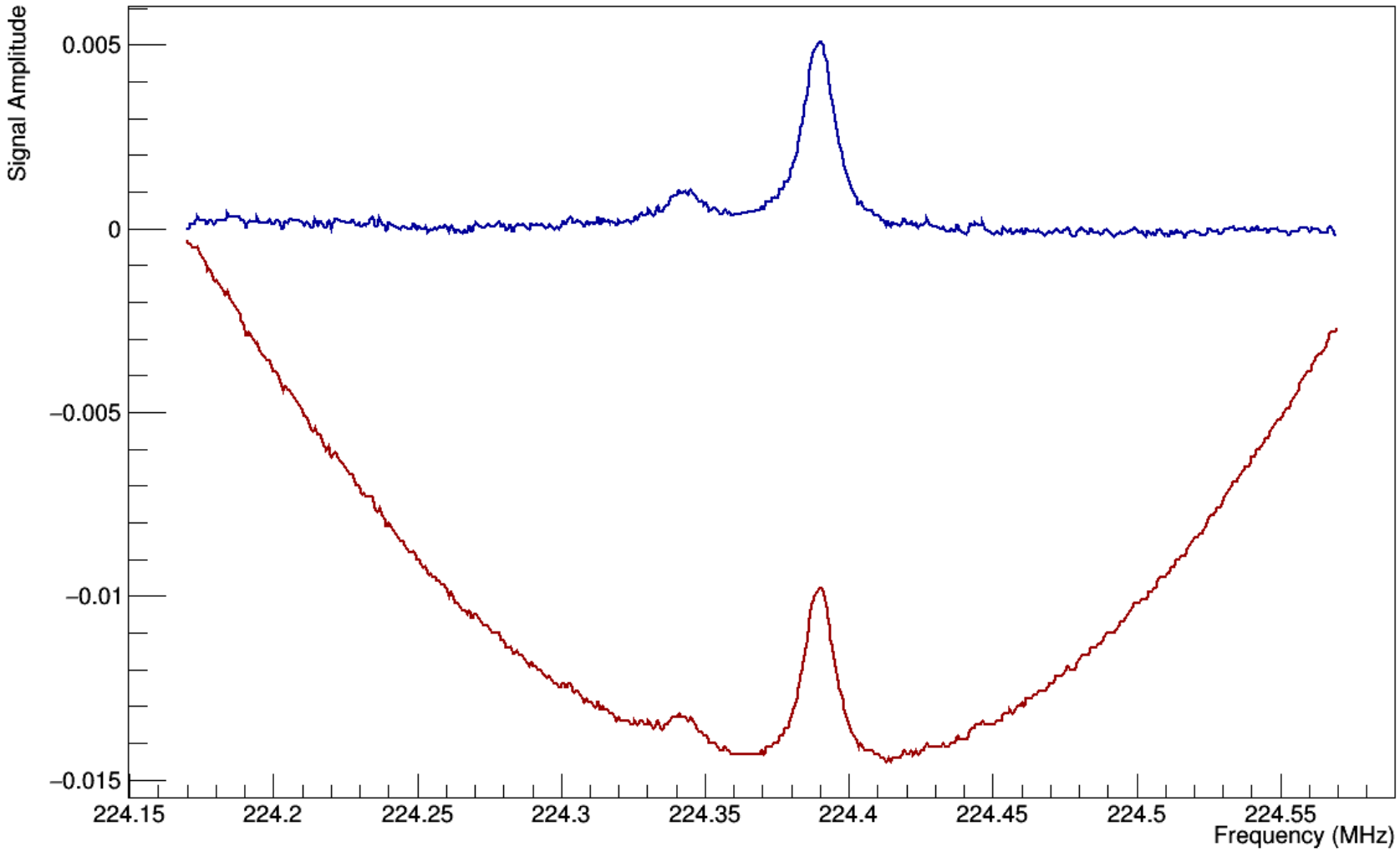
Subtracted Signals: PDP Data 4 Setting 3



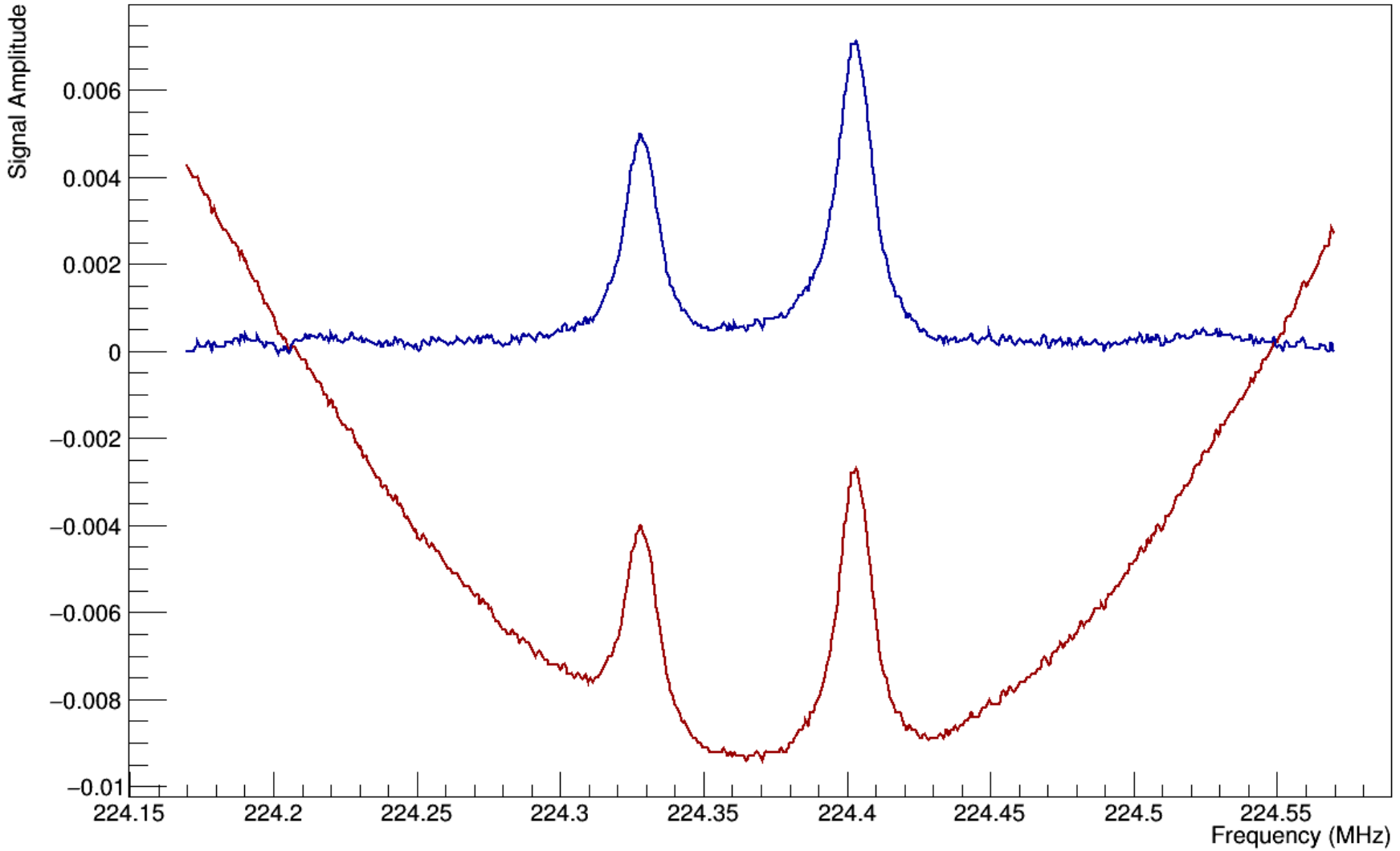
Subtracted Signals: PDP Data 4 Setting 4



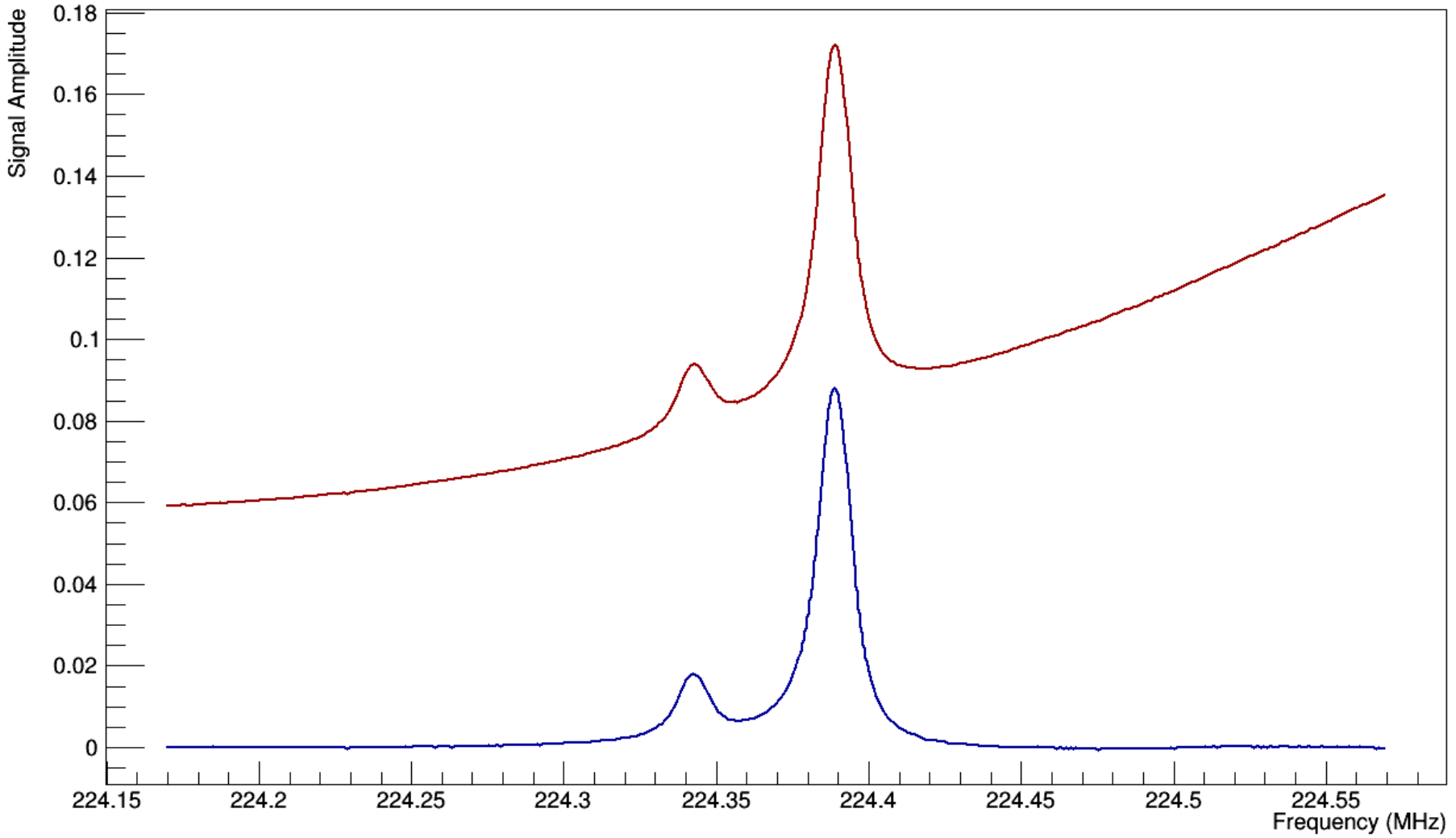
Subtracted Signals: LANL Data 4 Setting 1



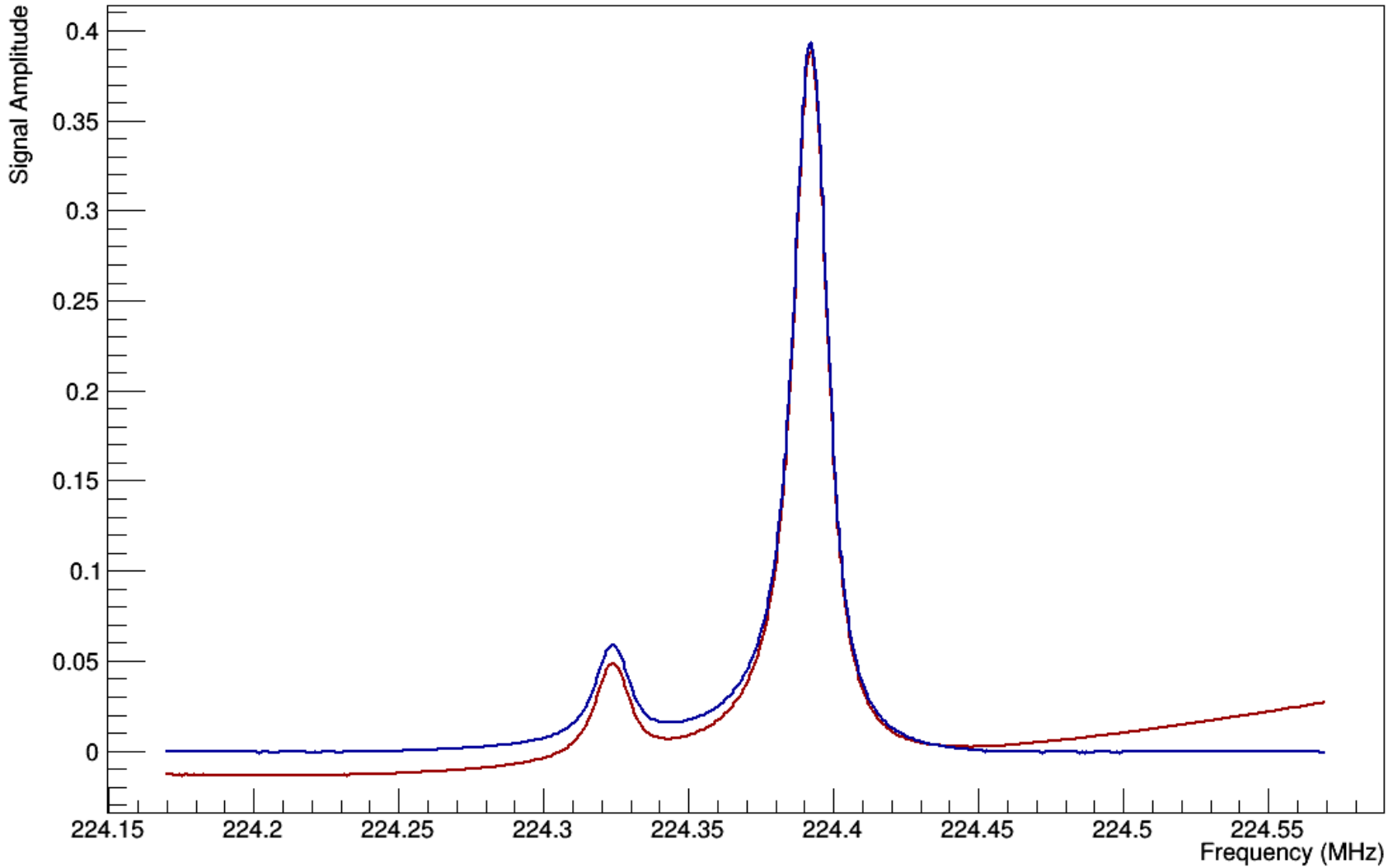
Subtracted Signals: LANL Data 4 Setting 2



Subtracted Signals: LANL Data 4 Setting 3

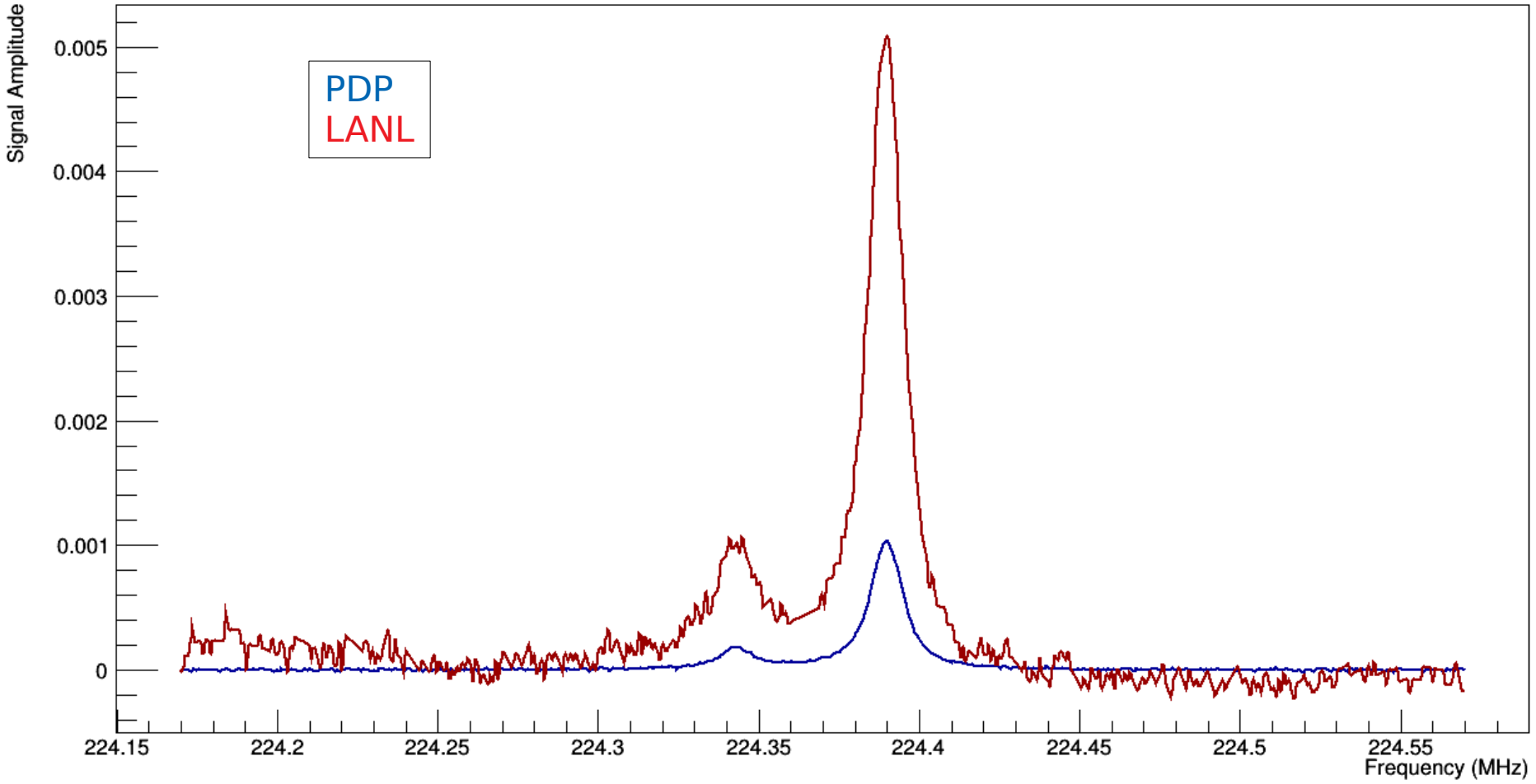


Subtracted Signals: LANL Data 4 Setting 4

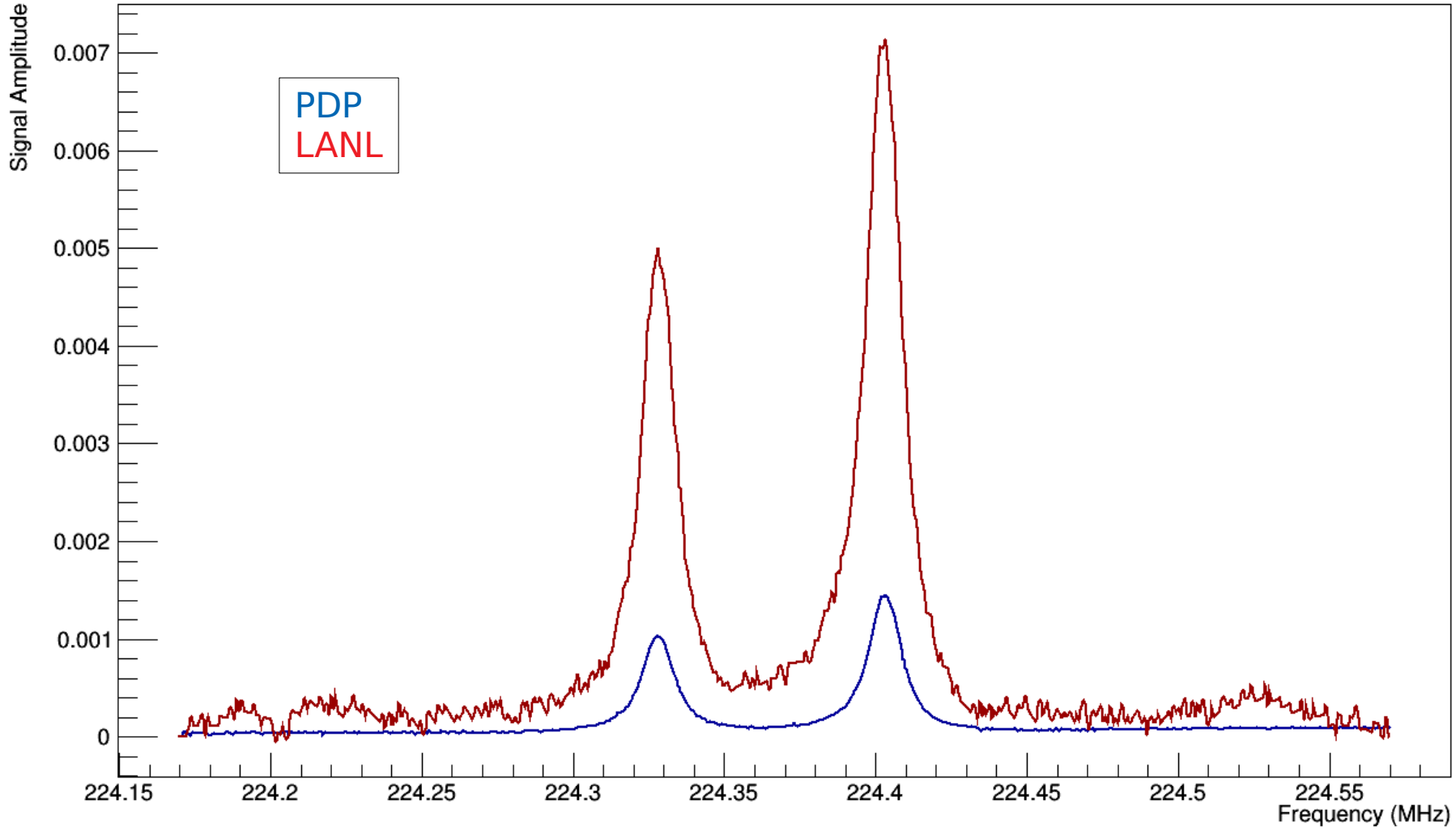


Signal Overlay

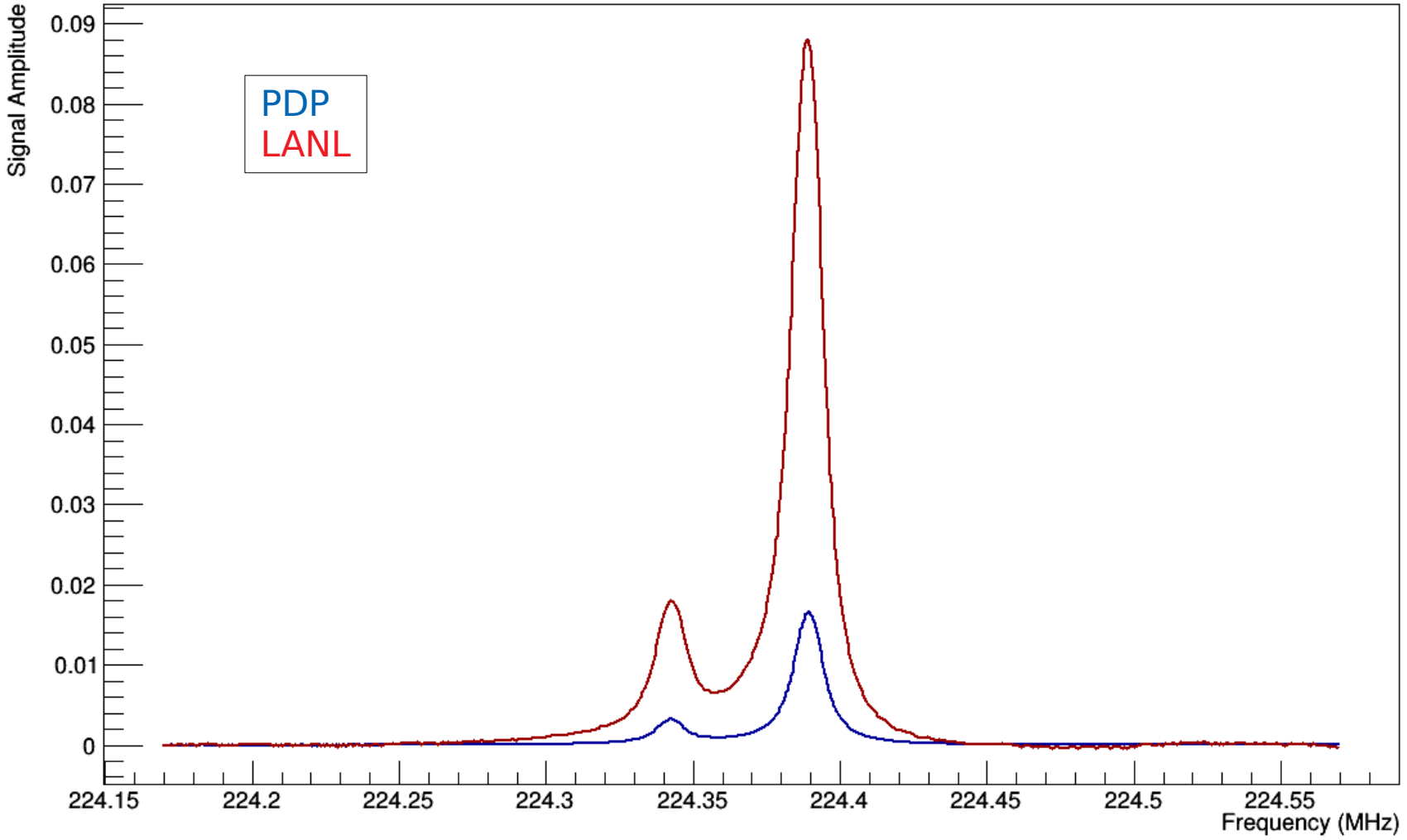
Total Signal: NMR Comparison Setting 1



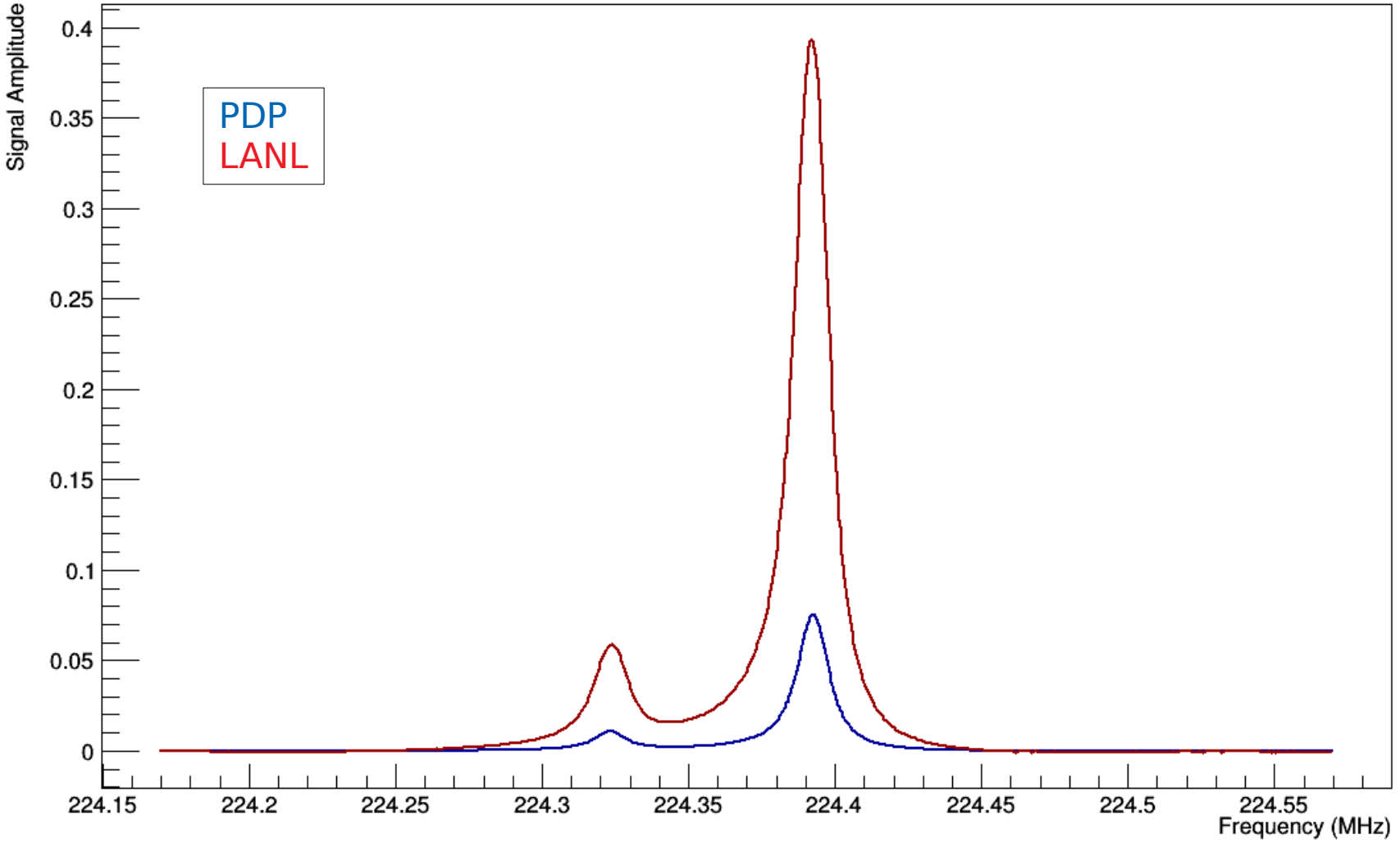
Total Signal: NMR Comparison Setting 2



Total Signal: NMR Comparison Setting 3



Total Signal: NMR Comparison Setting 4



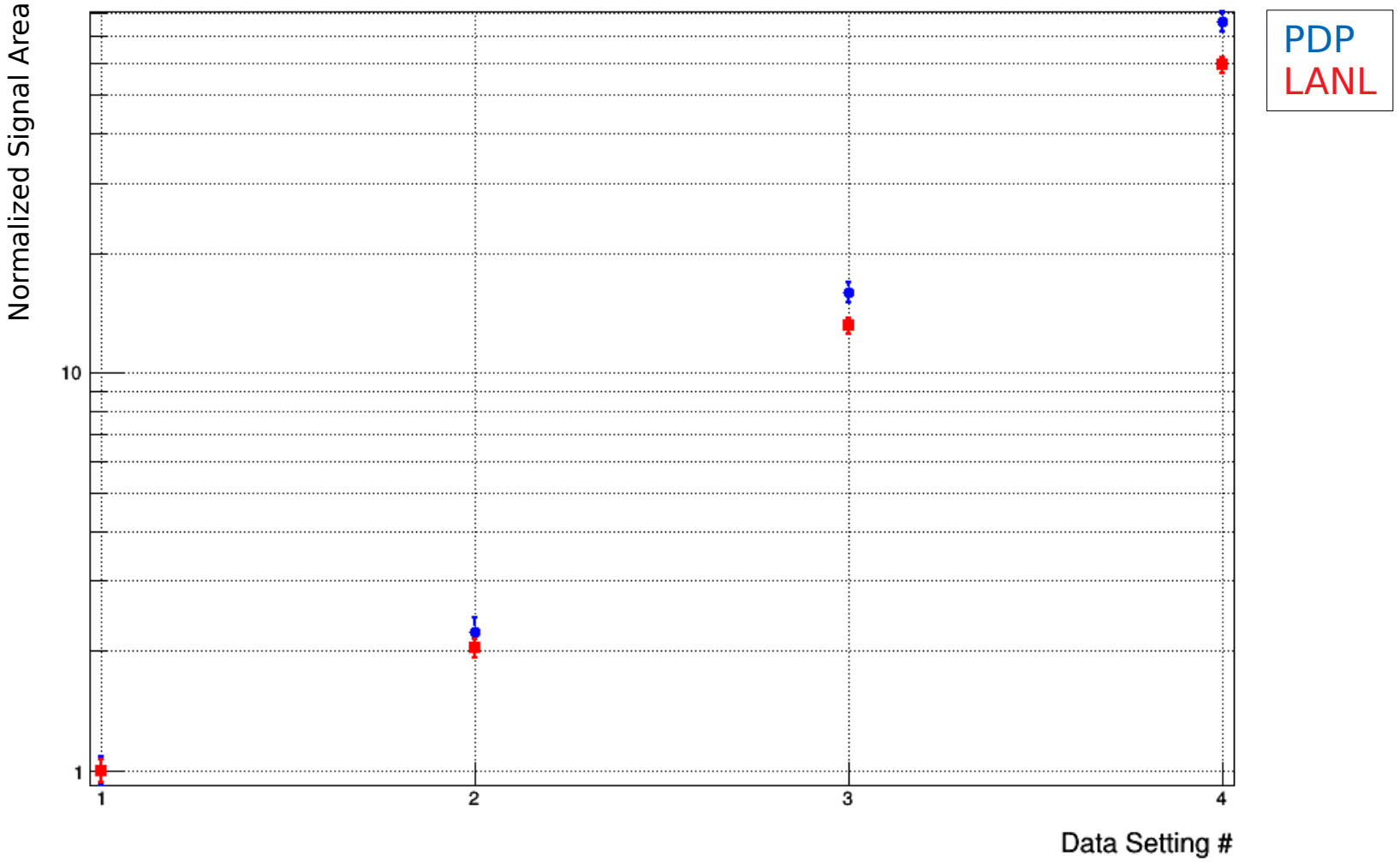
Nomalized Area Comparison

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

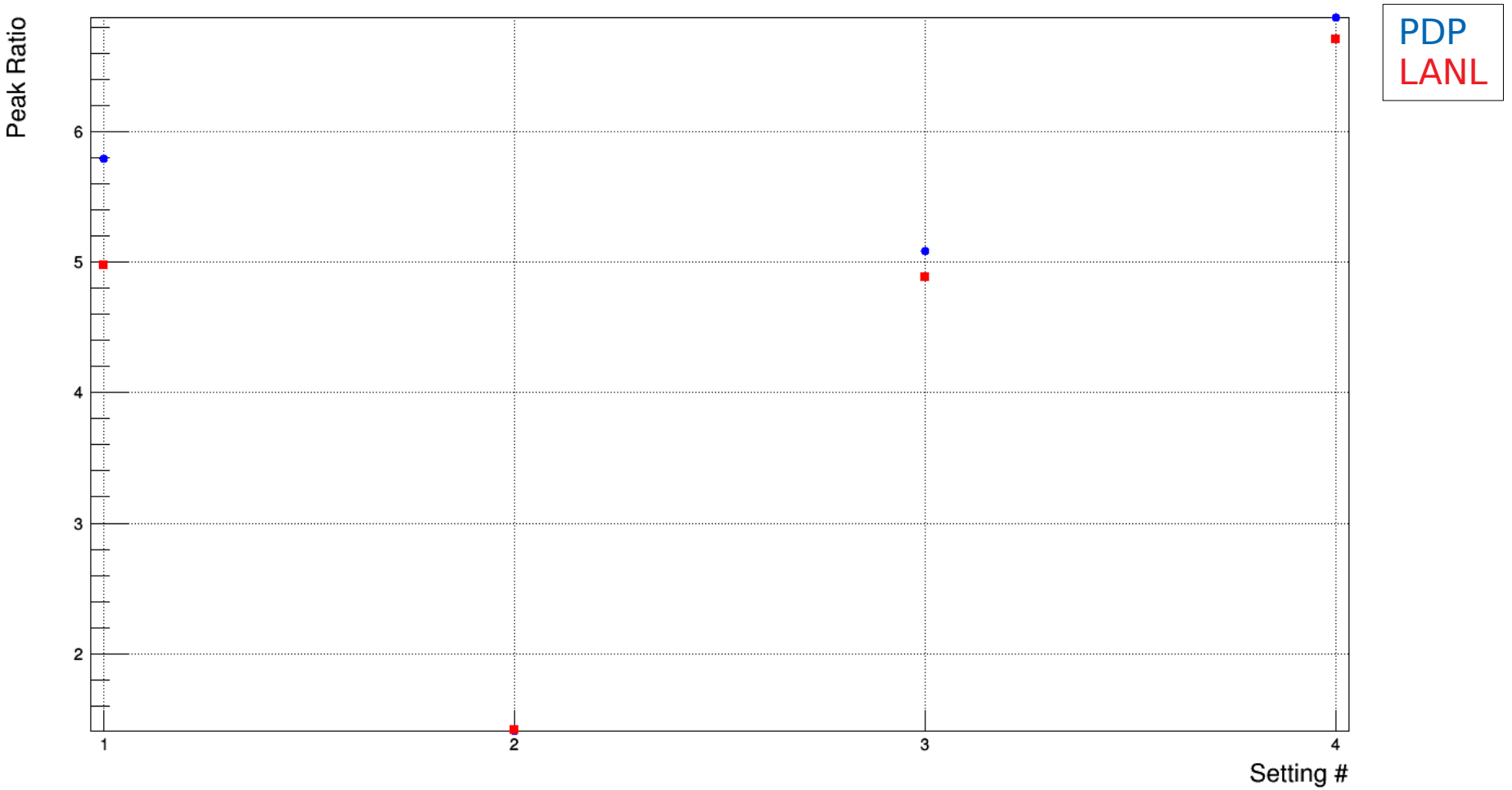


Peak Ratio

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.

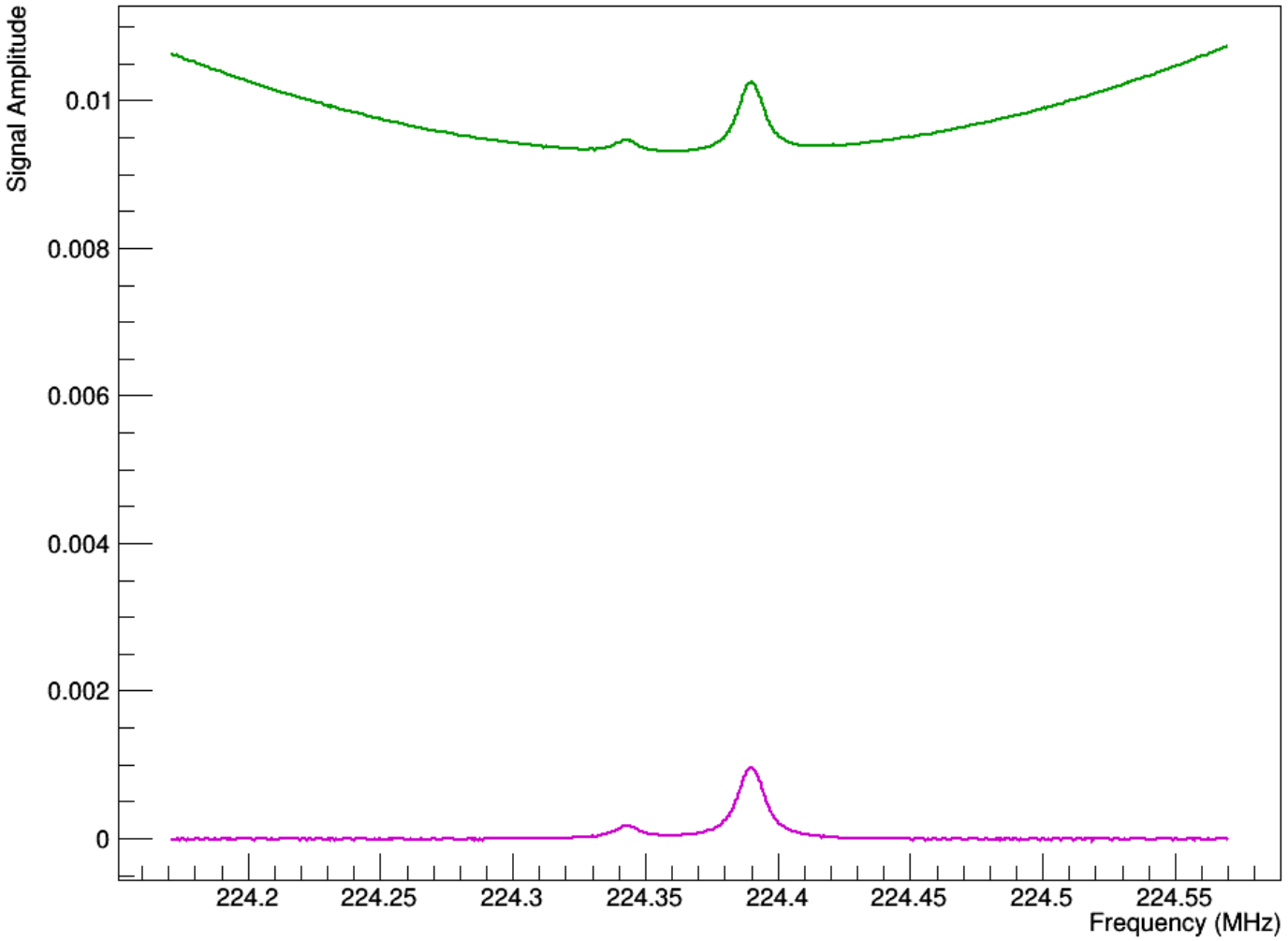
This was plotted versus signal setting.

Normalized Signal: NMR Peak Comparison

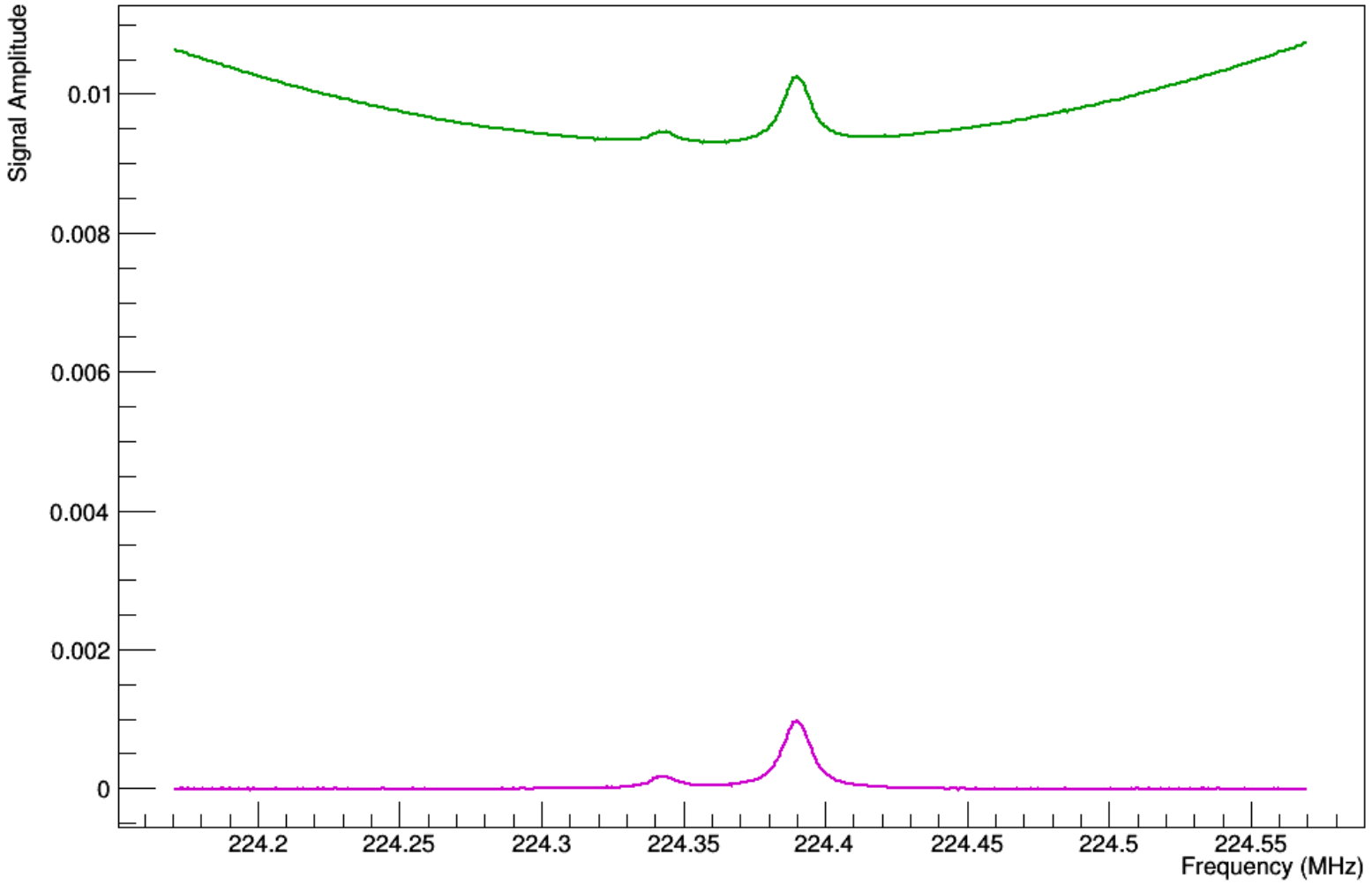


Data Set 5

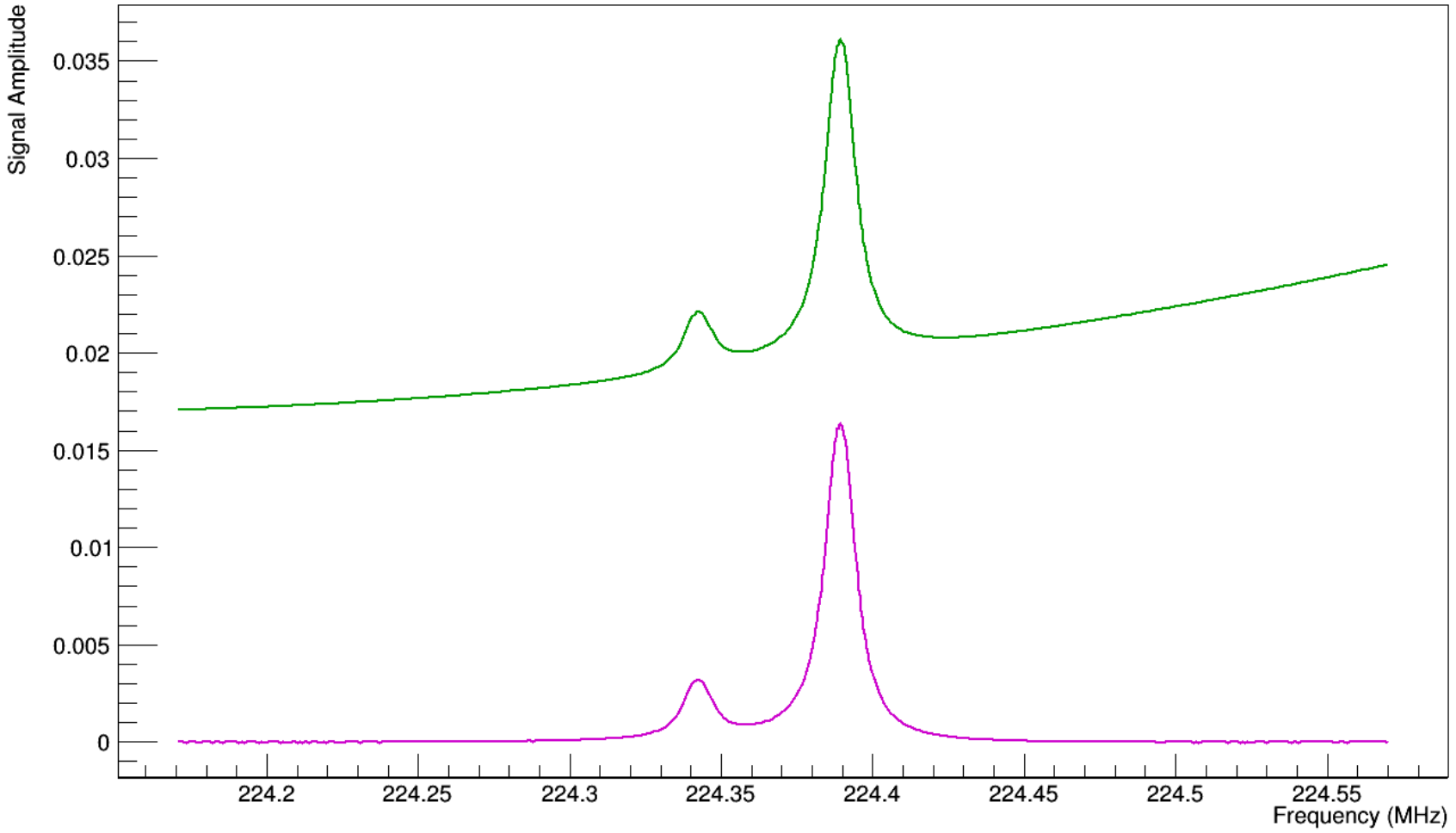
Subtracted Signals: PDP Data 5 Setting 1



Subtracted Signals: PDP Data 5 Setting 2



Subtracted Signals: PDP Data 5 Setting 3



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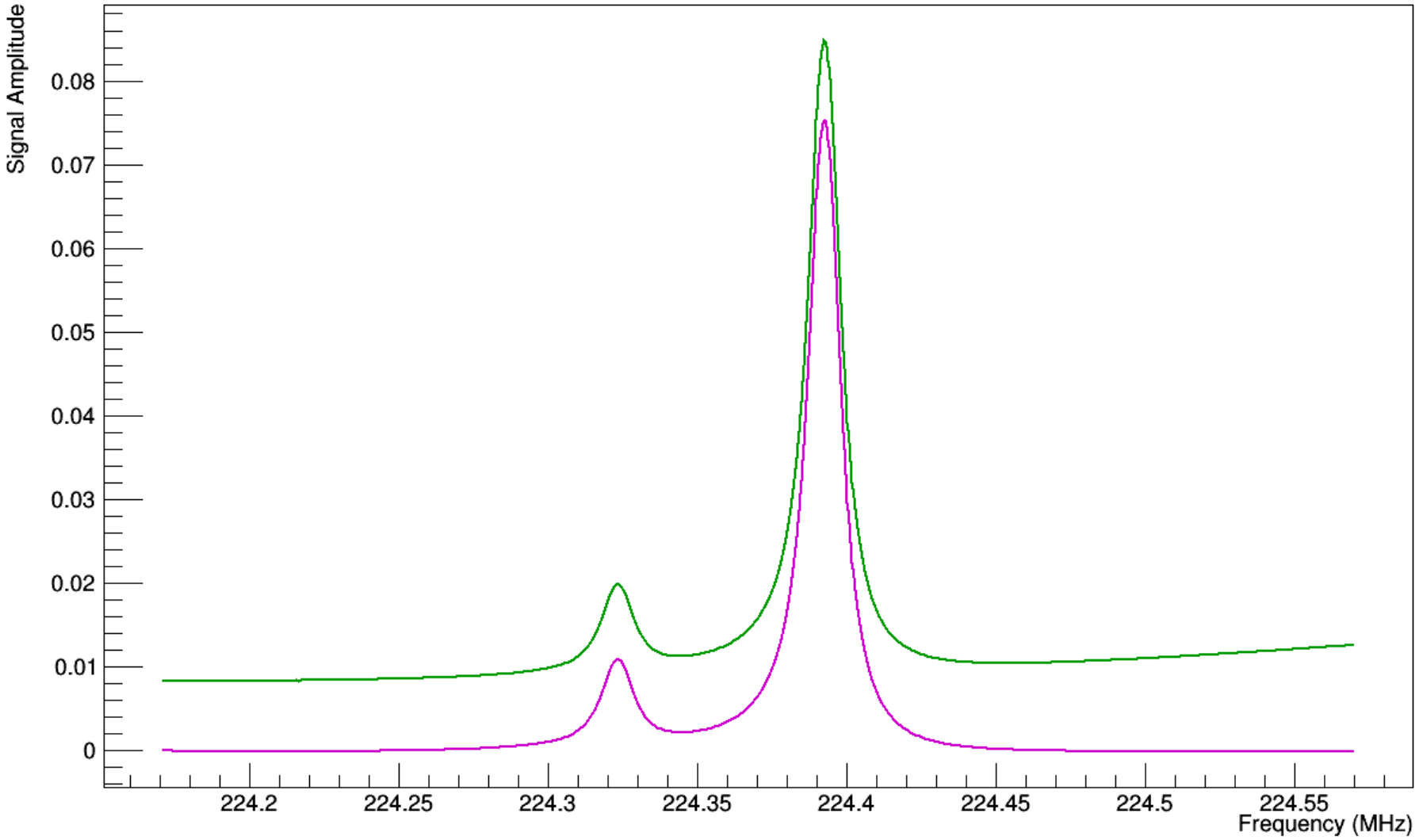
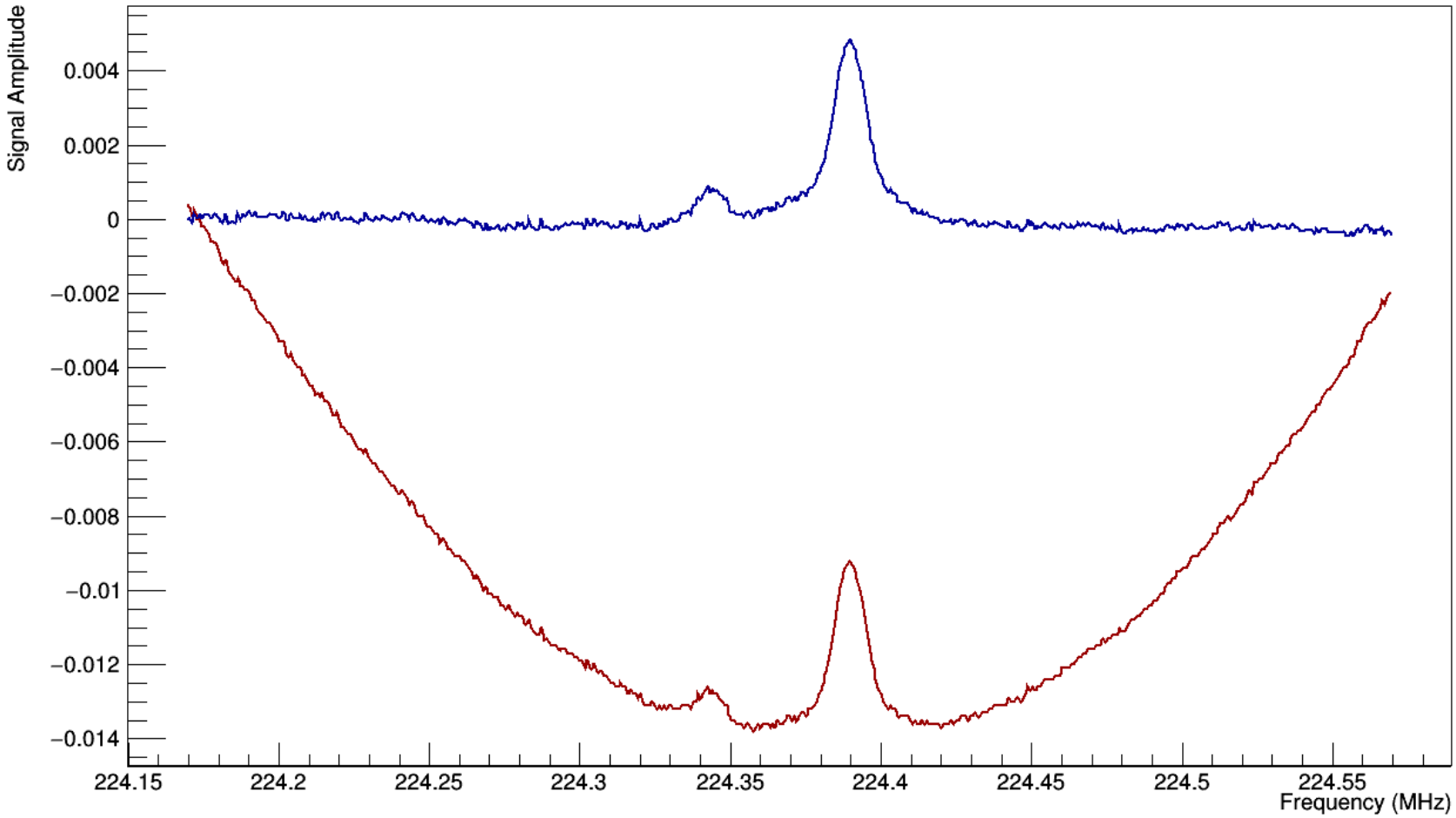
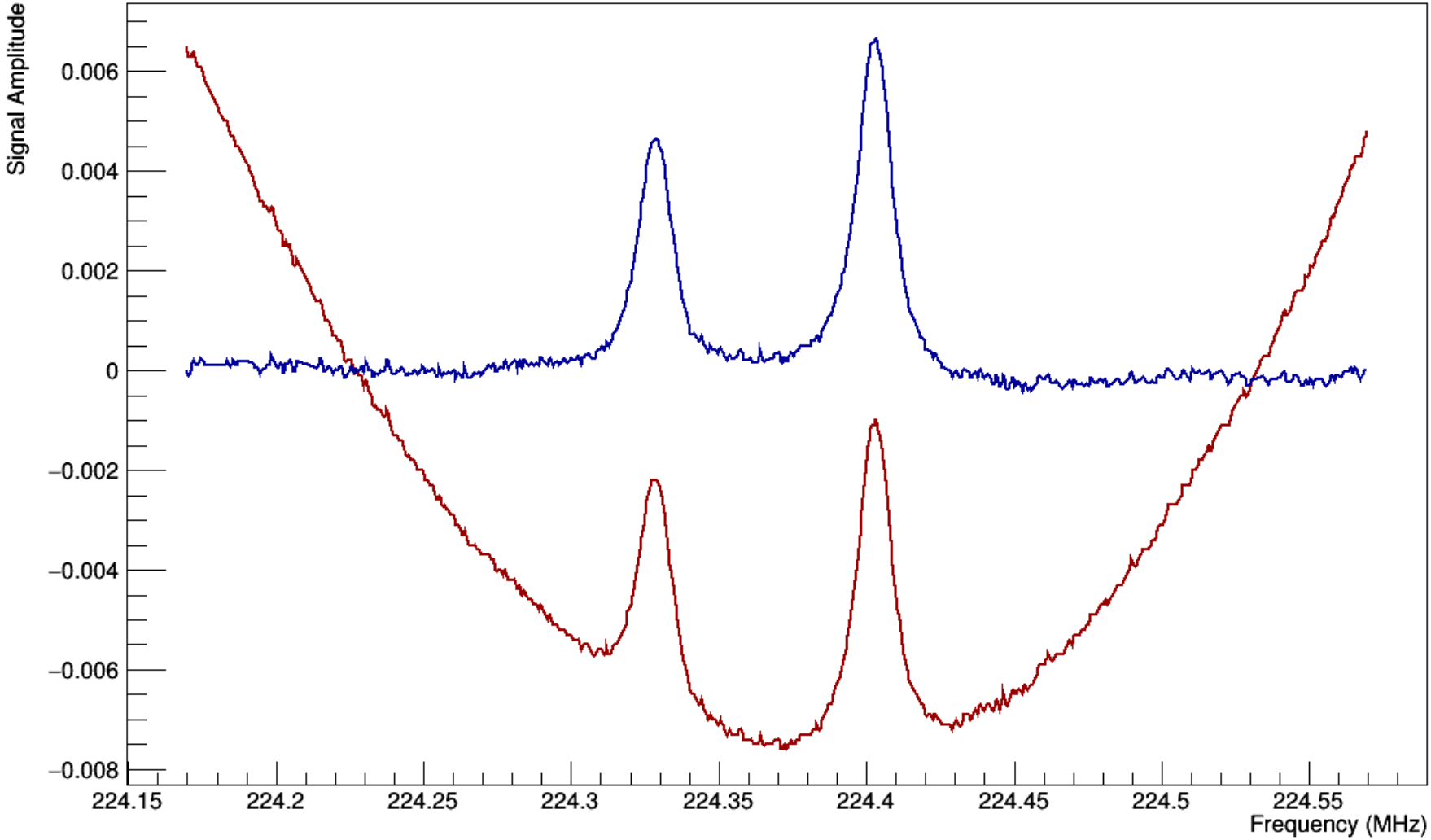


Subtracted Signals: LANL Data 5 Setting 1



Subtracted Signals: LANL Data 5 Setting 2



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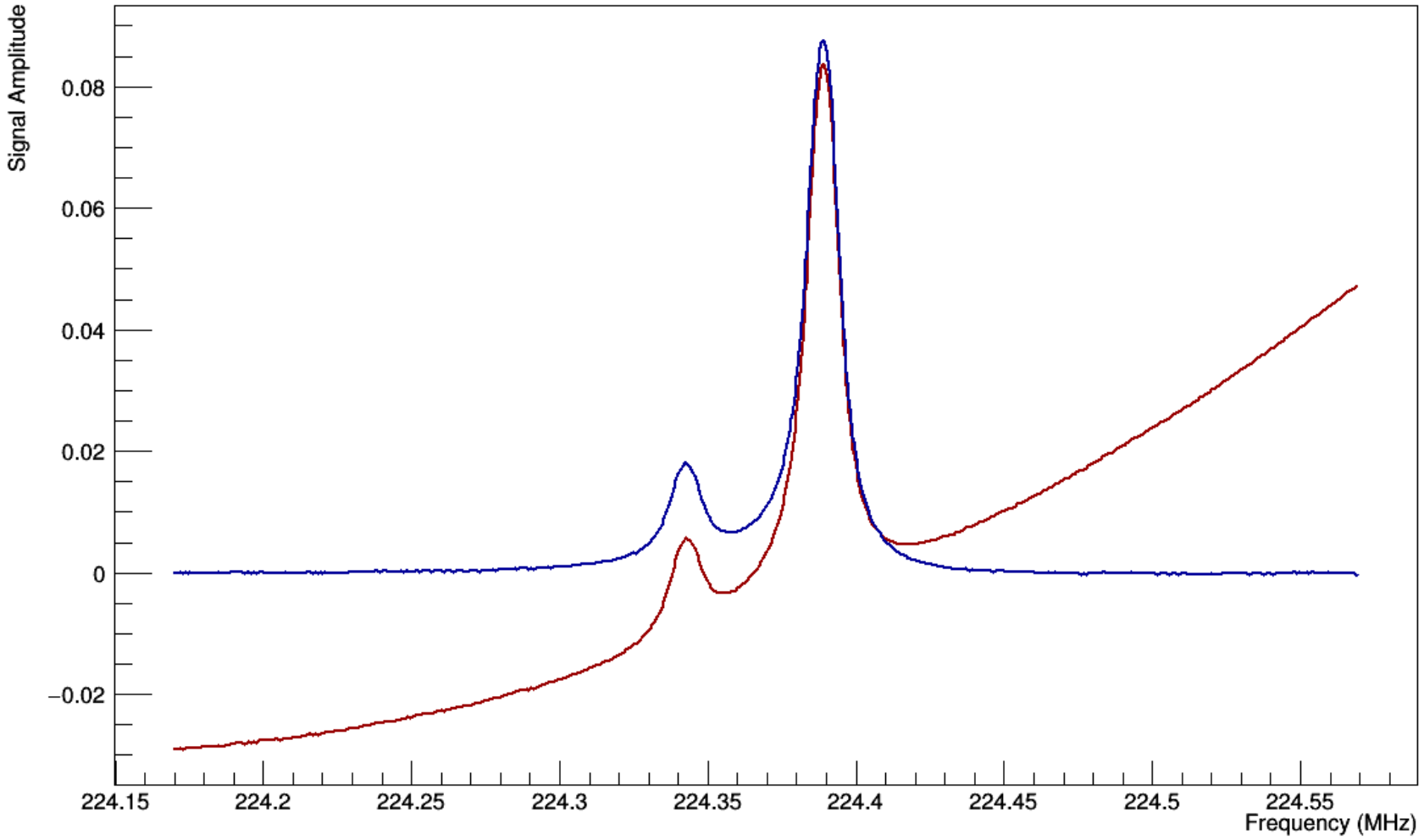

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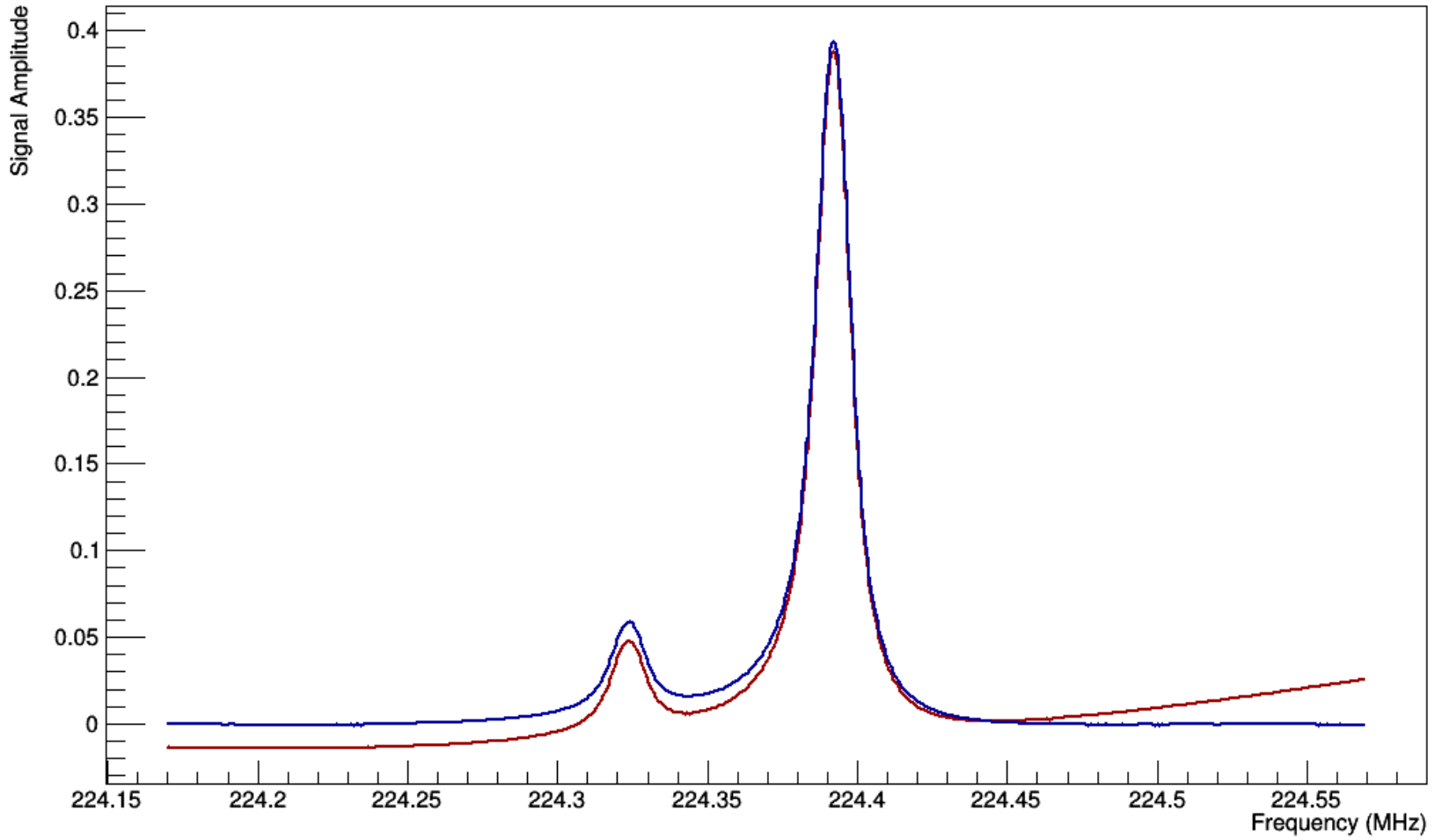

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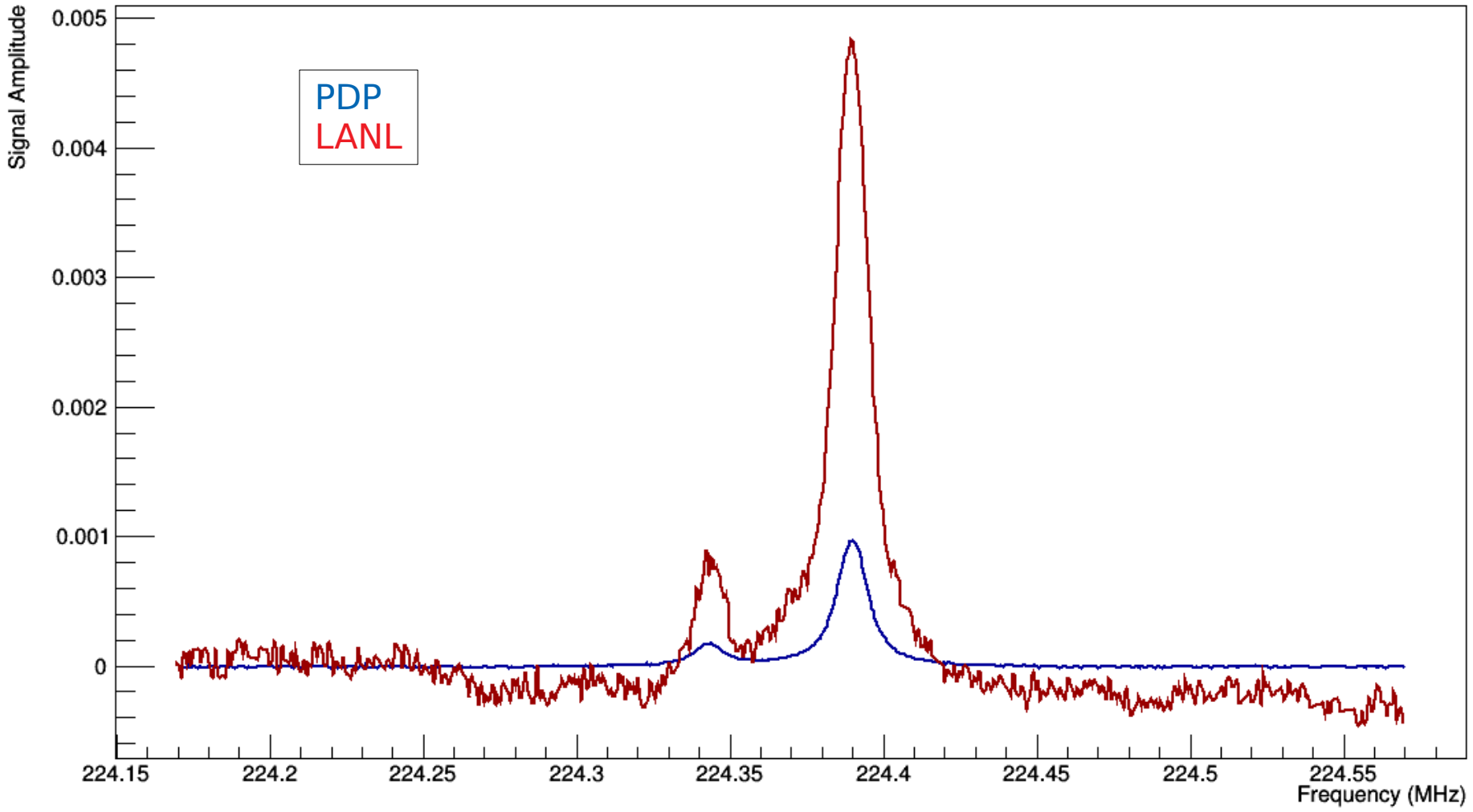
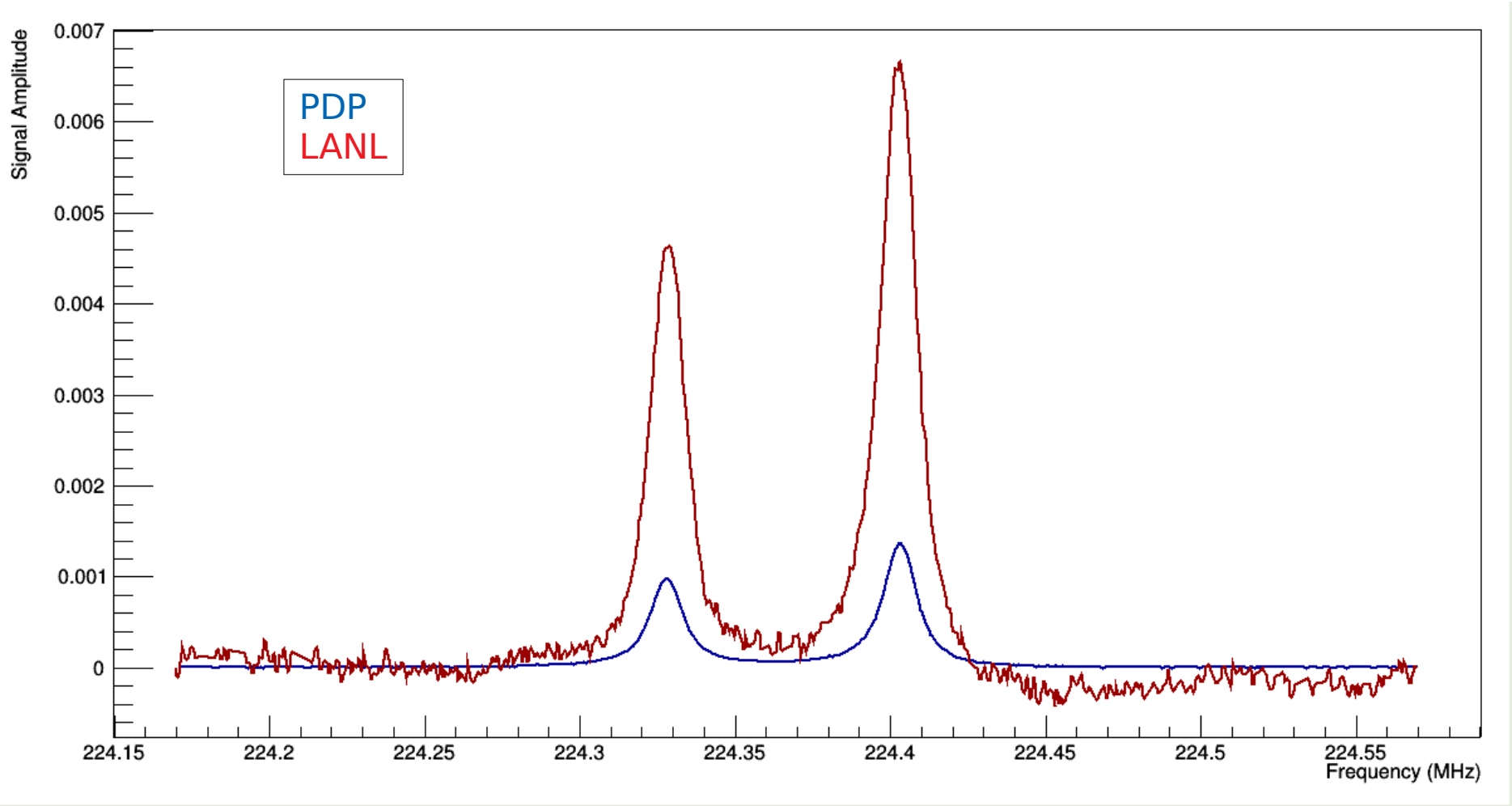


Total Signal: NMR Comparison Setting 2



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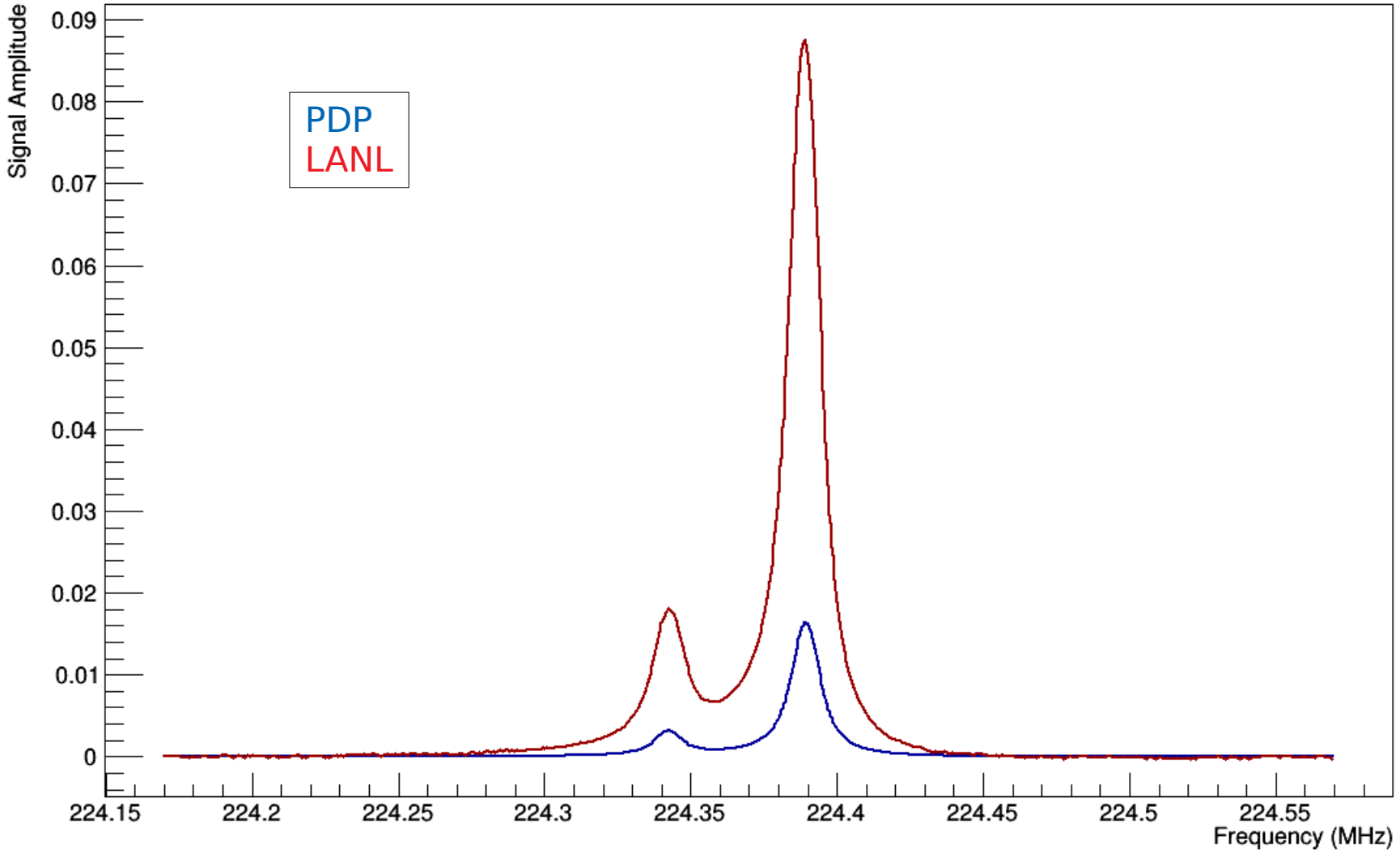

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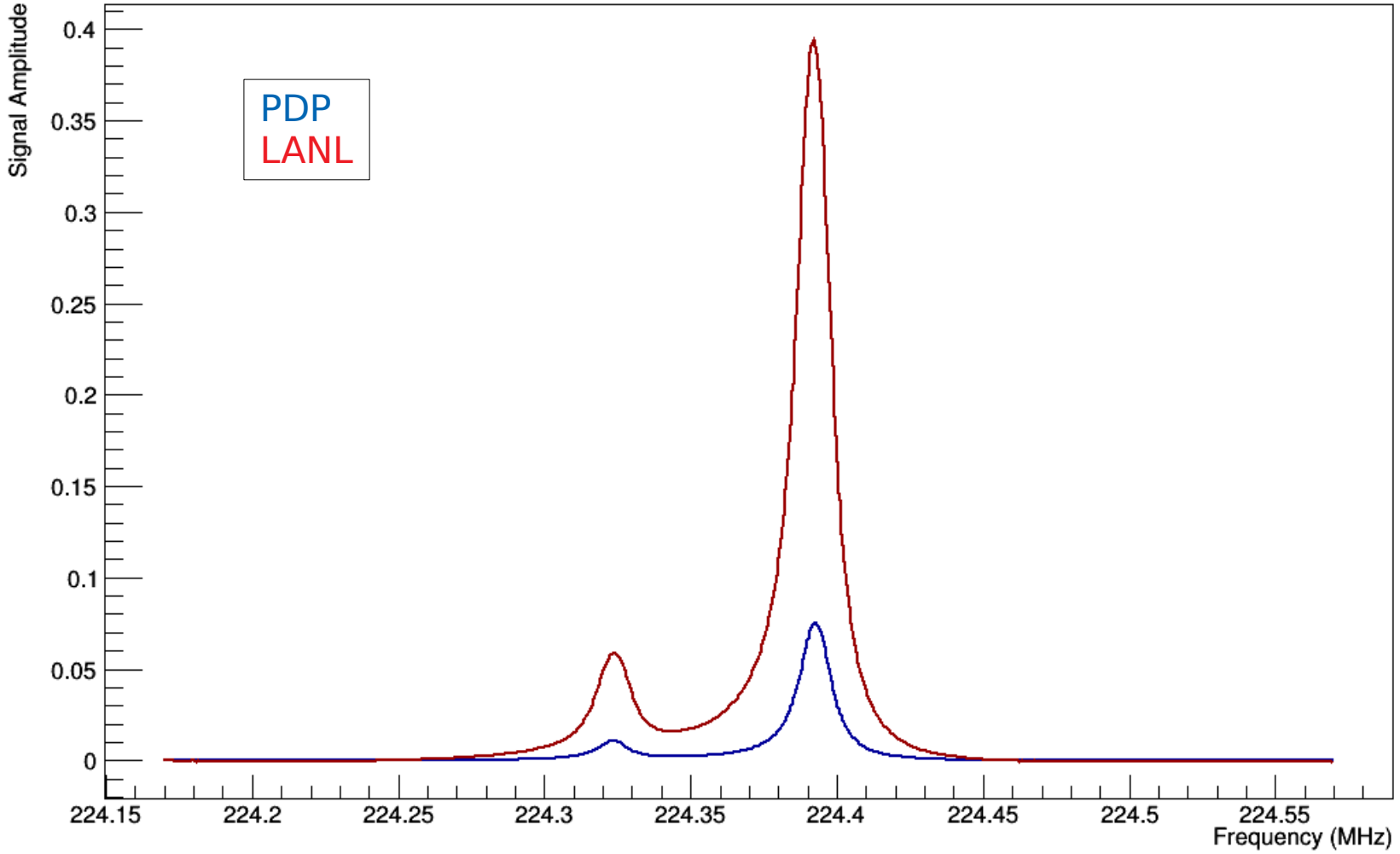

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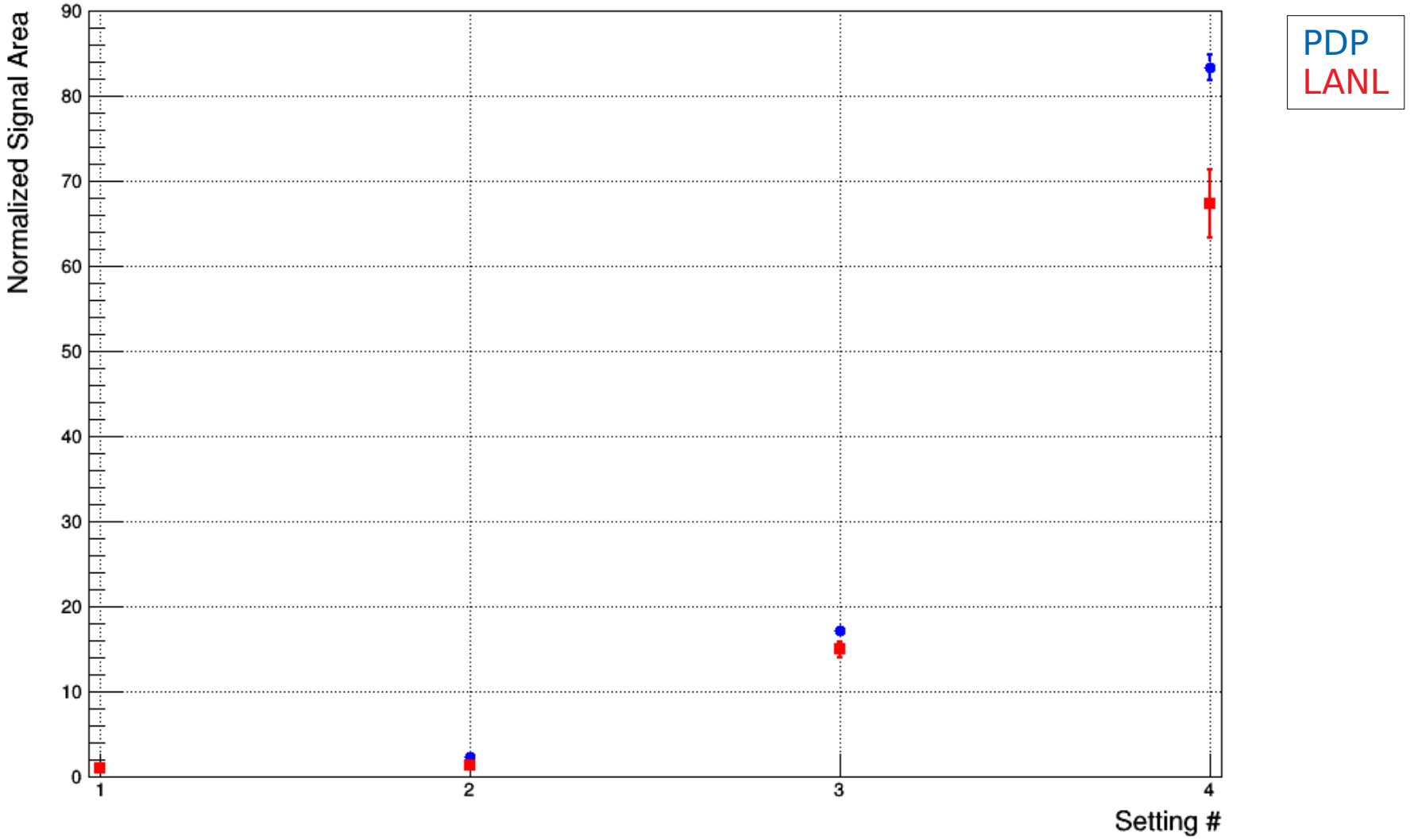

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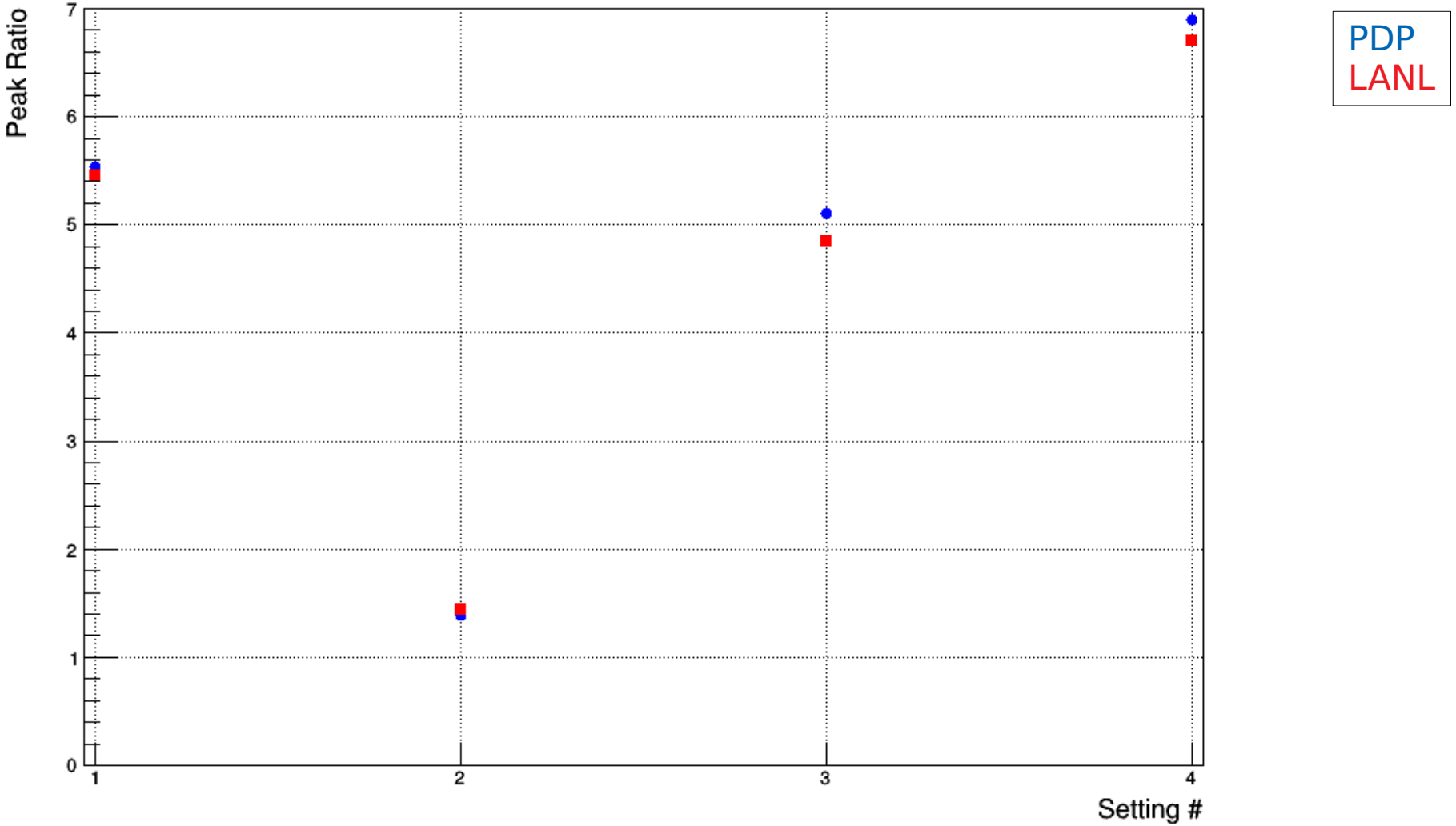
Normalized Signal: NMR Peak Comparison