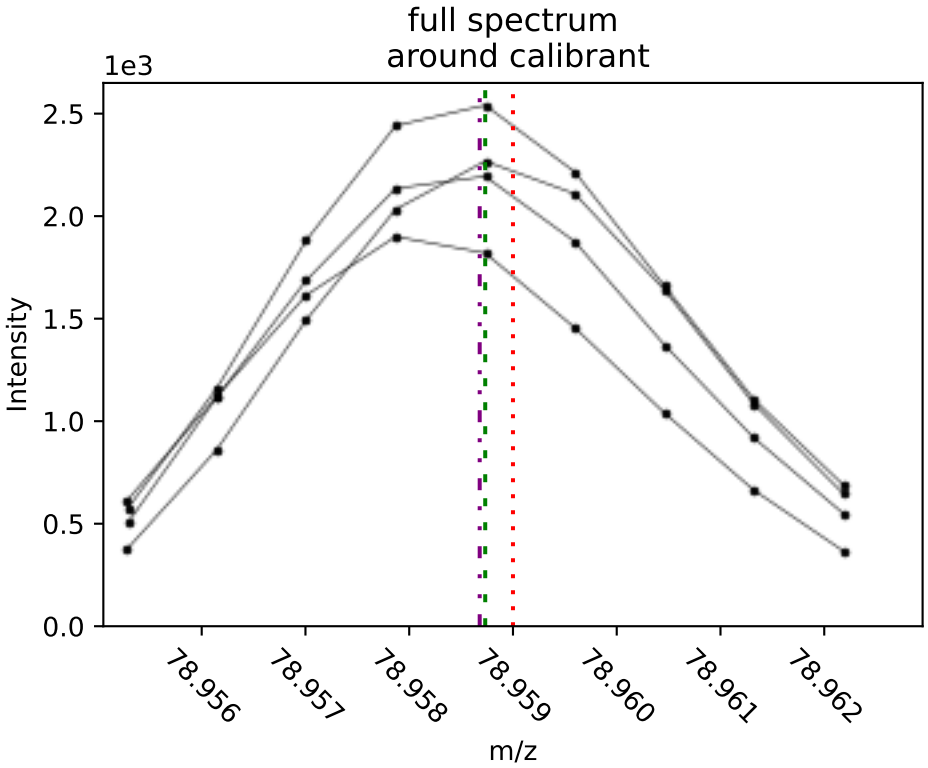
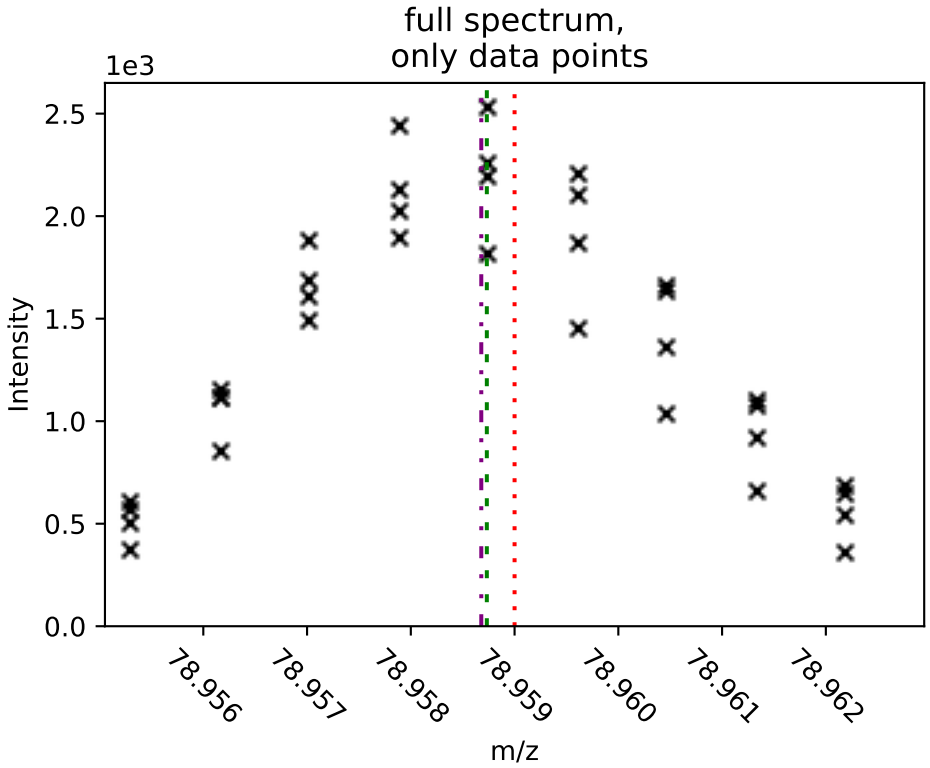
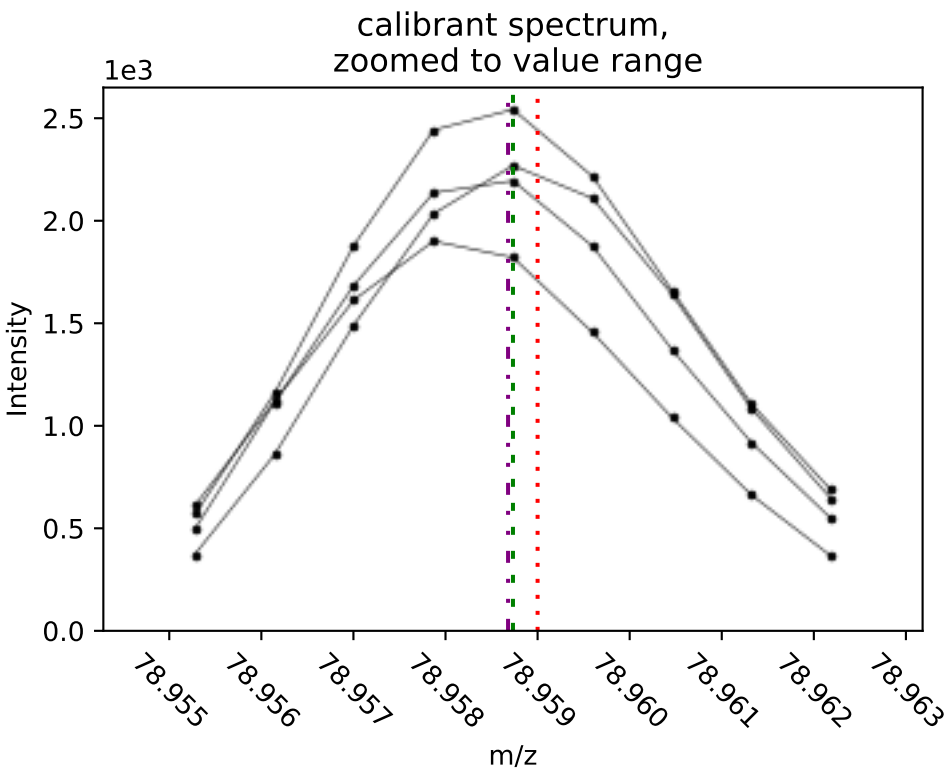
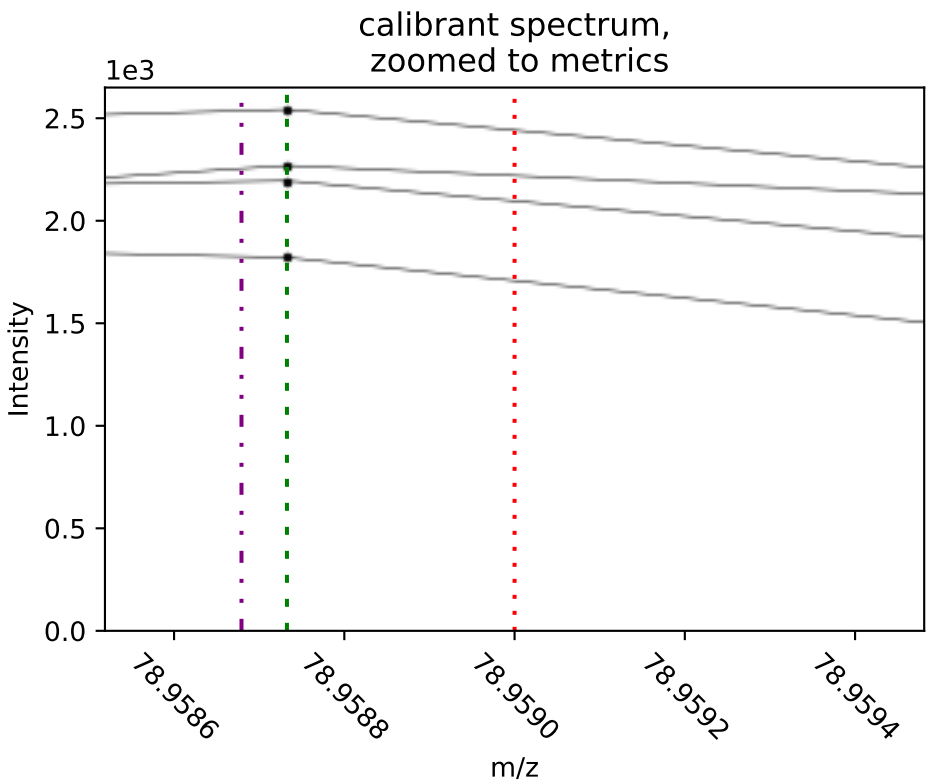
Calibrant spectra for Calibrant A

Theo. m/z: 78.959000 Most abundant signal: 78.958733 Weighted average: 78.958679



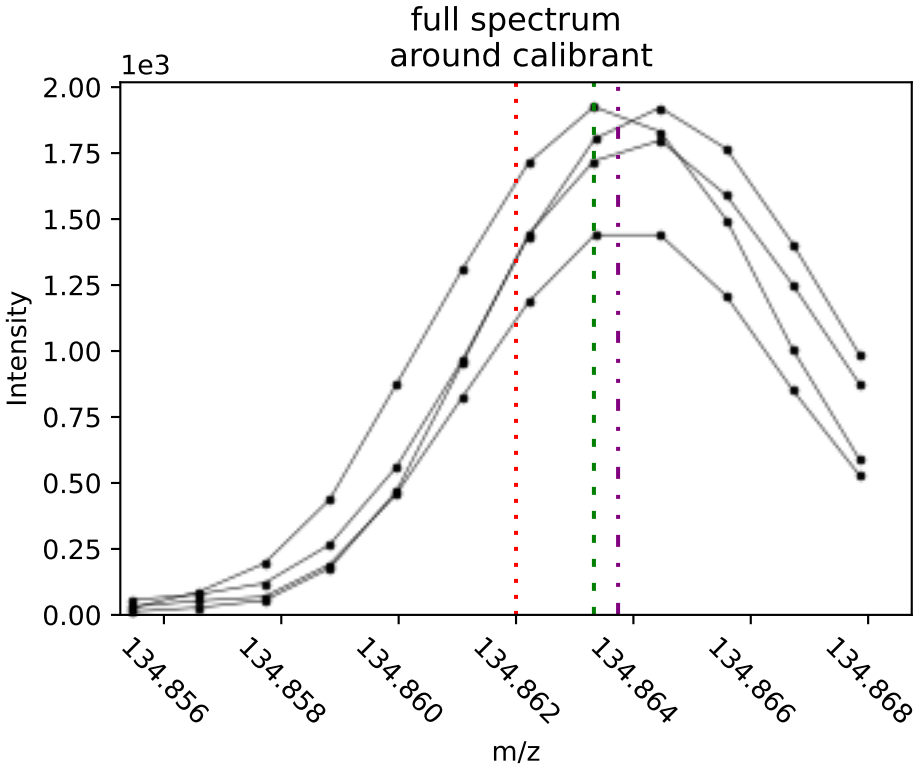


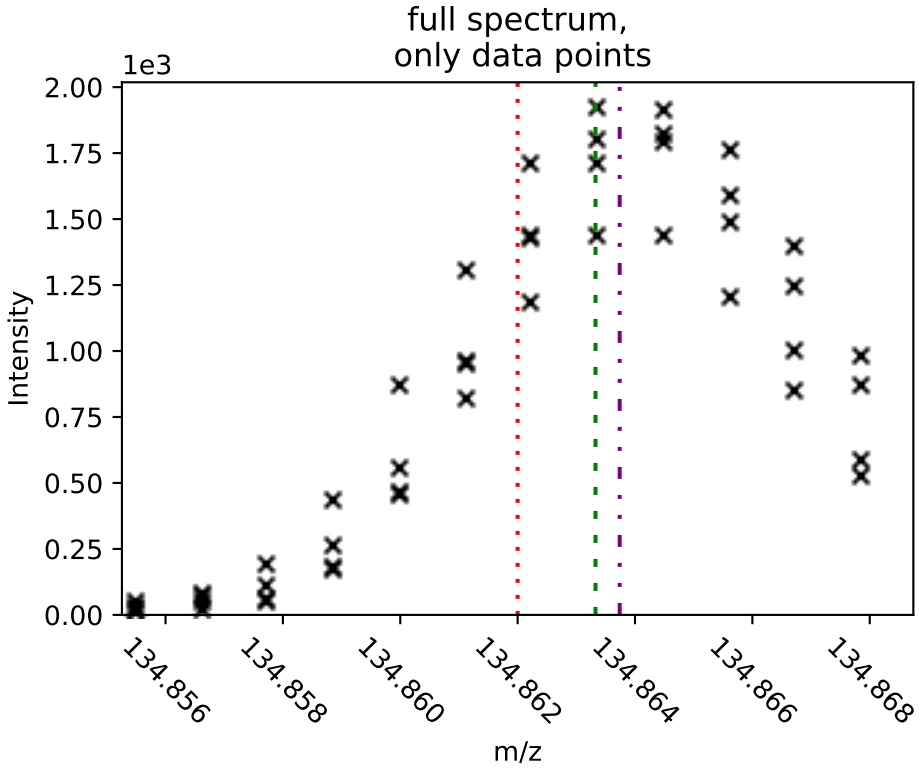


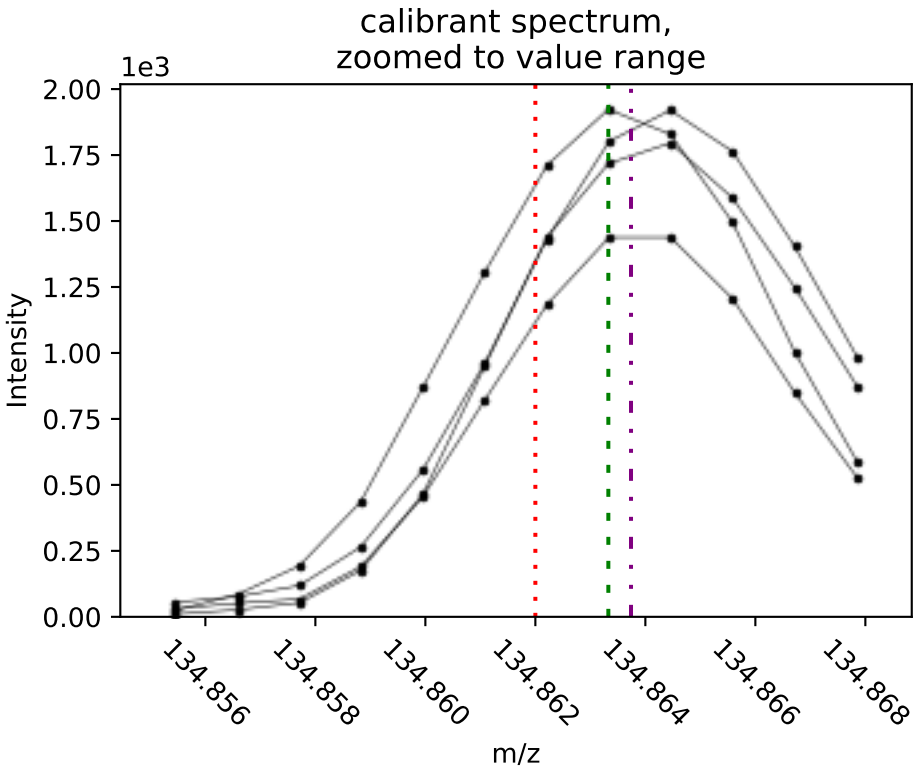


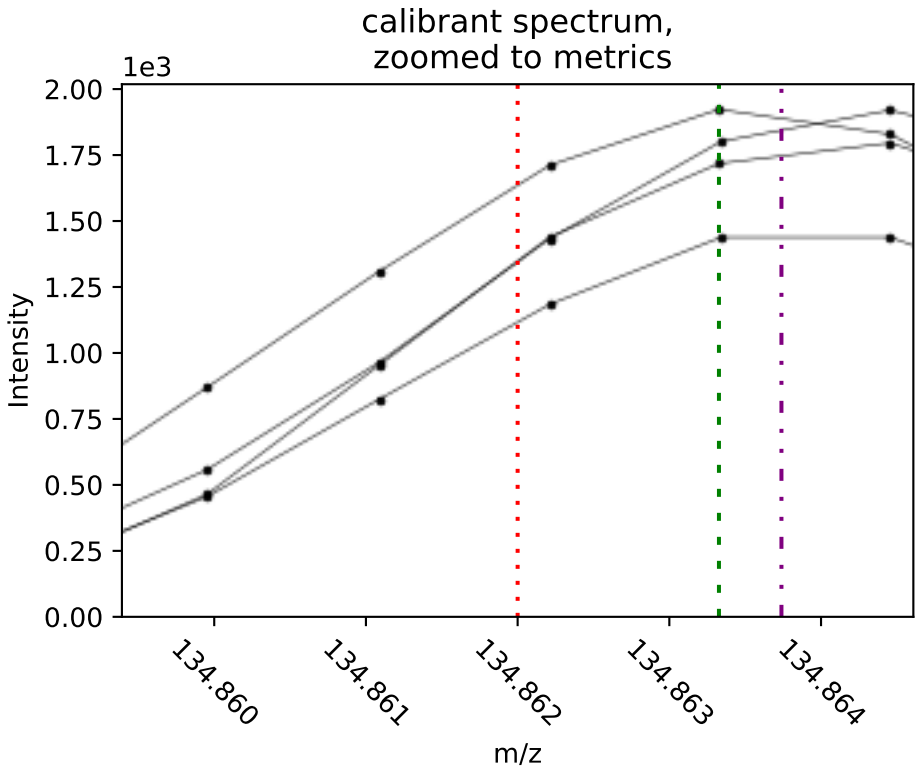
Calibrant spectra for Calibrant B

Theo. m/z: 134.862000 Most abundant signal: 134.863327 Weighted average: 134.863739



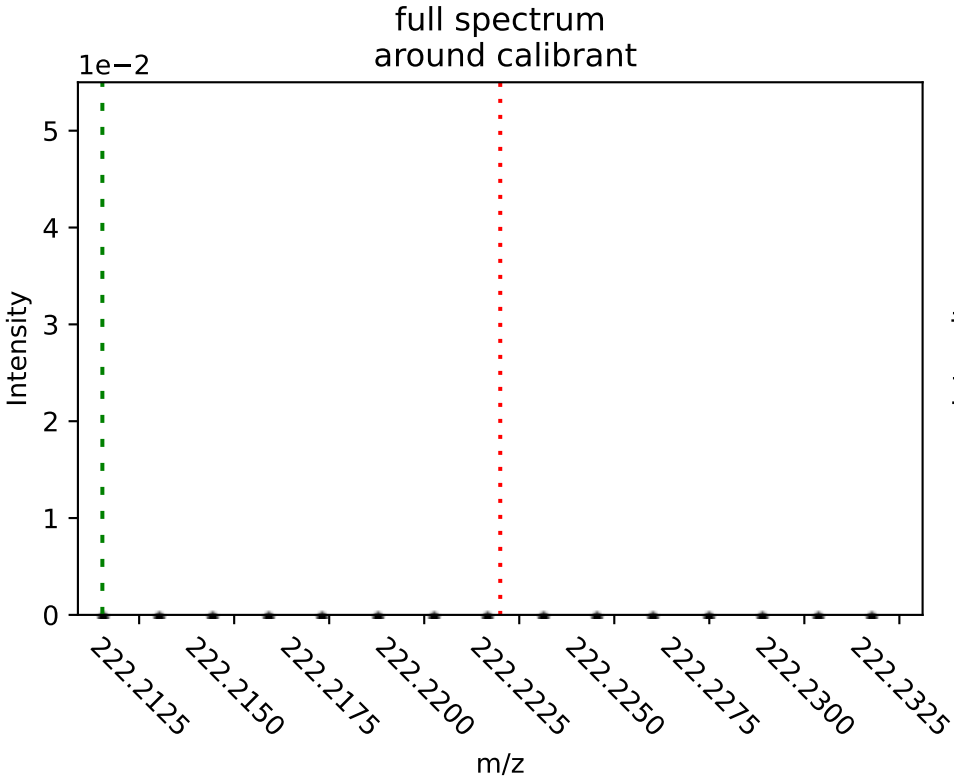


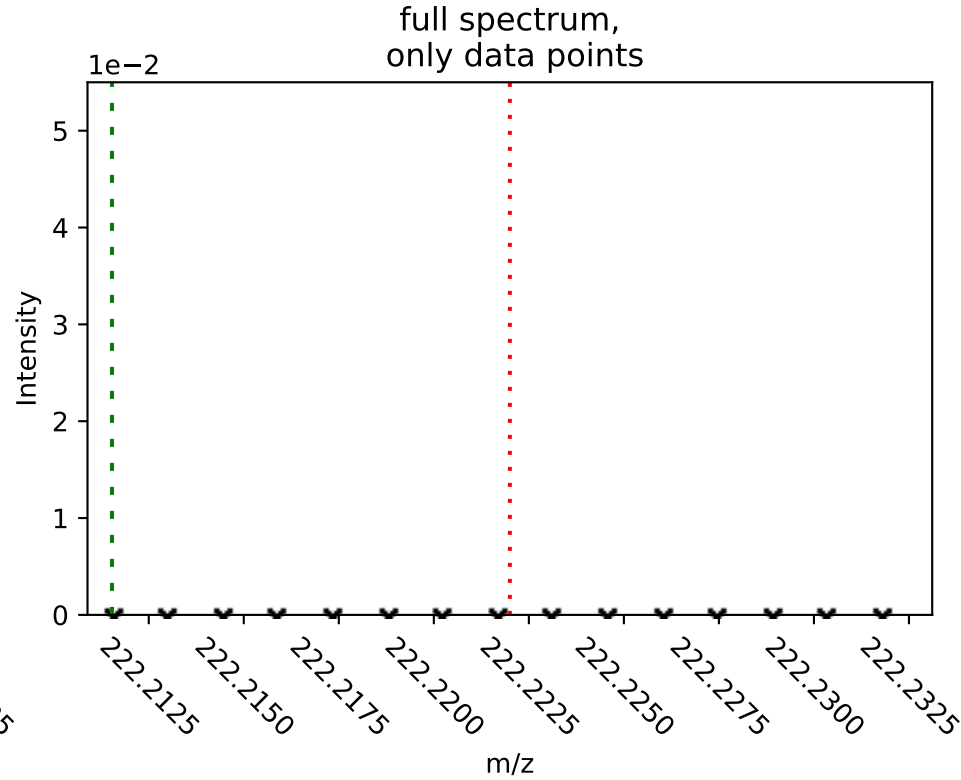


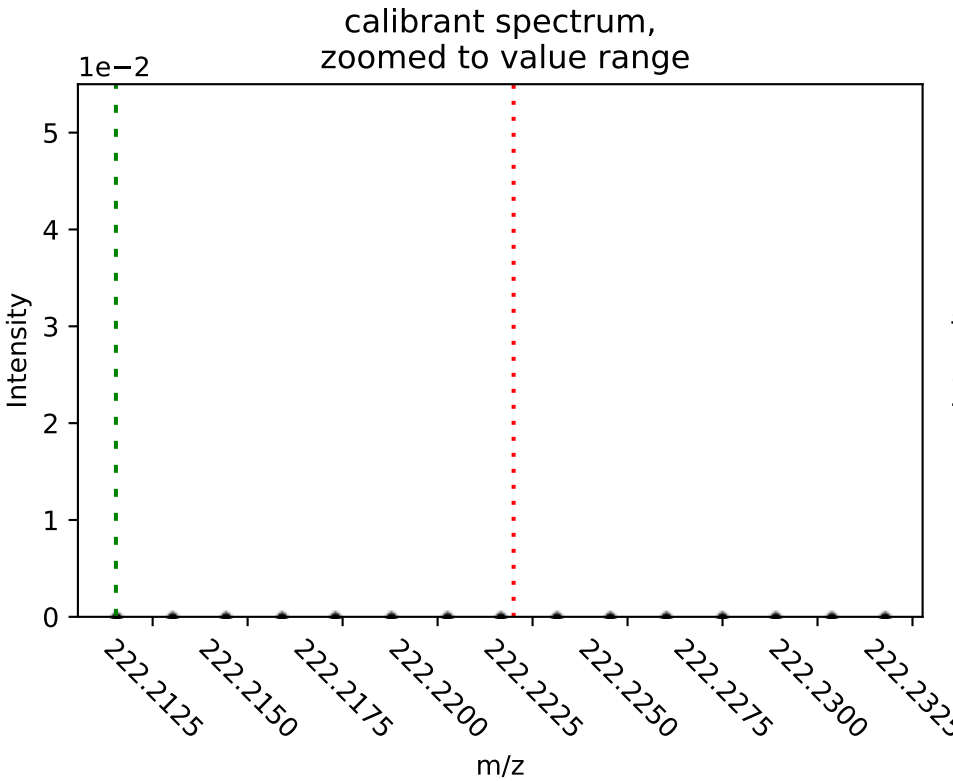


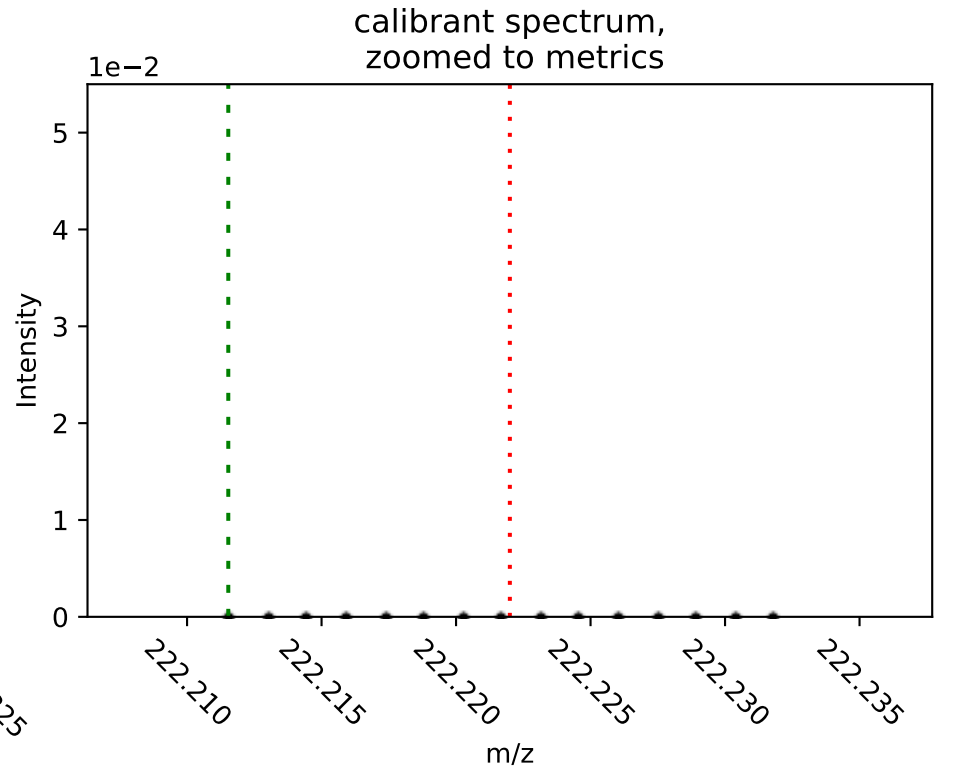
Calibrant spectra for Calibrant C

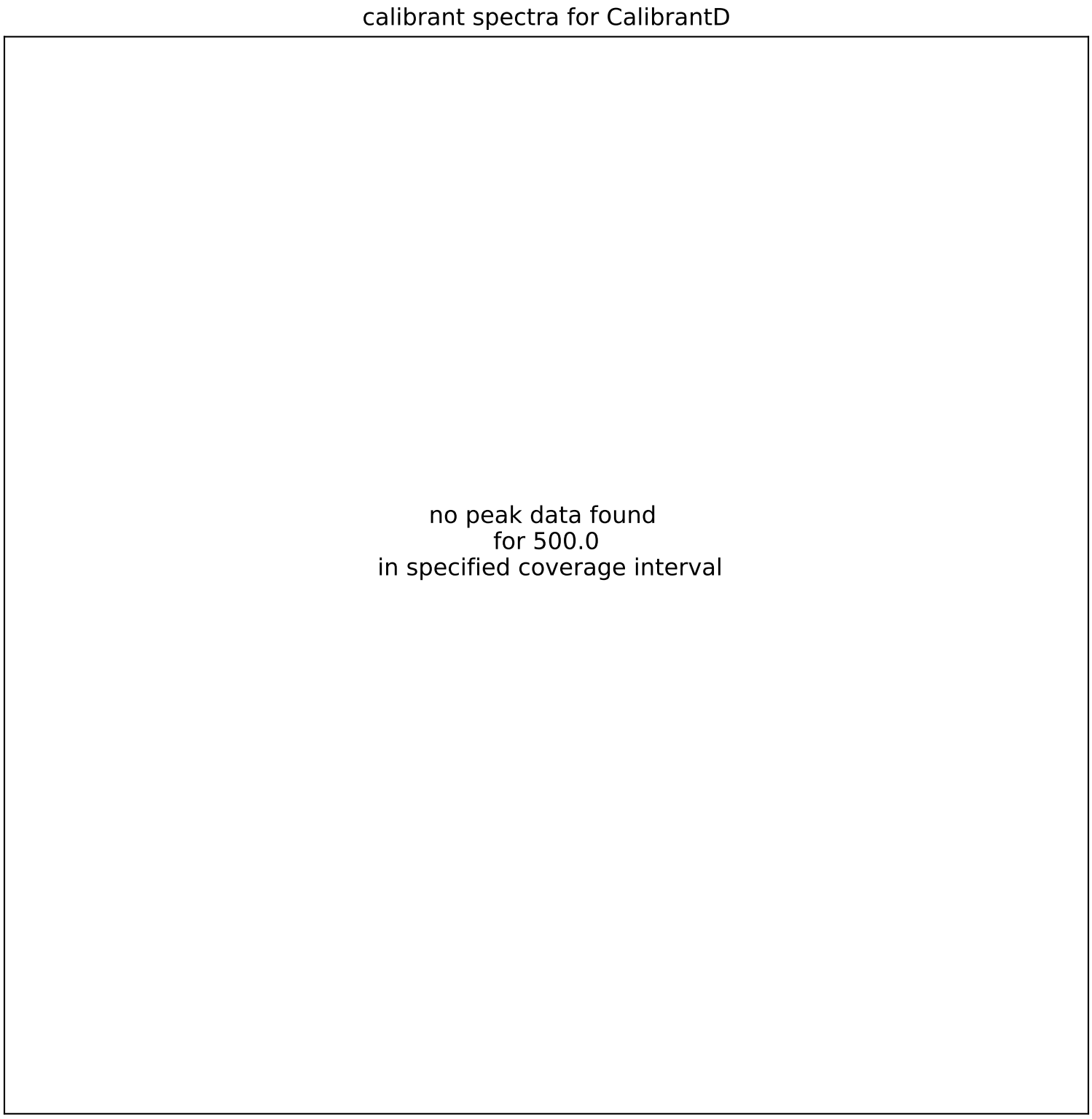
Theo. m/z: 222.222000 | Most abundant signal: 222.211533 | Weighted average: nan

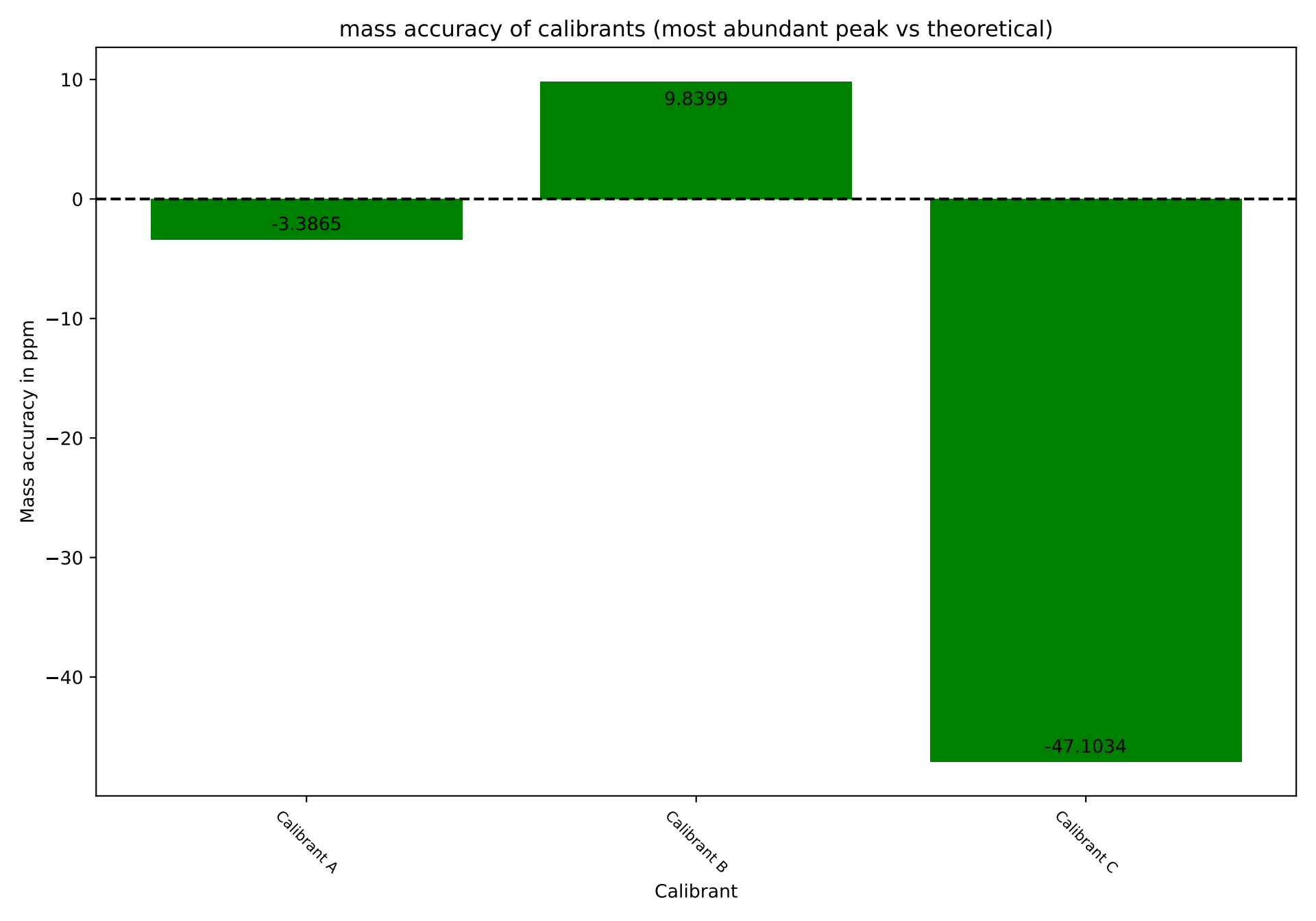


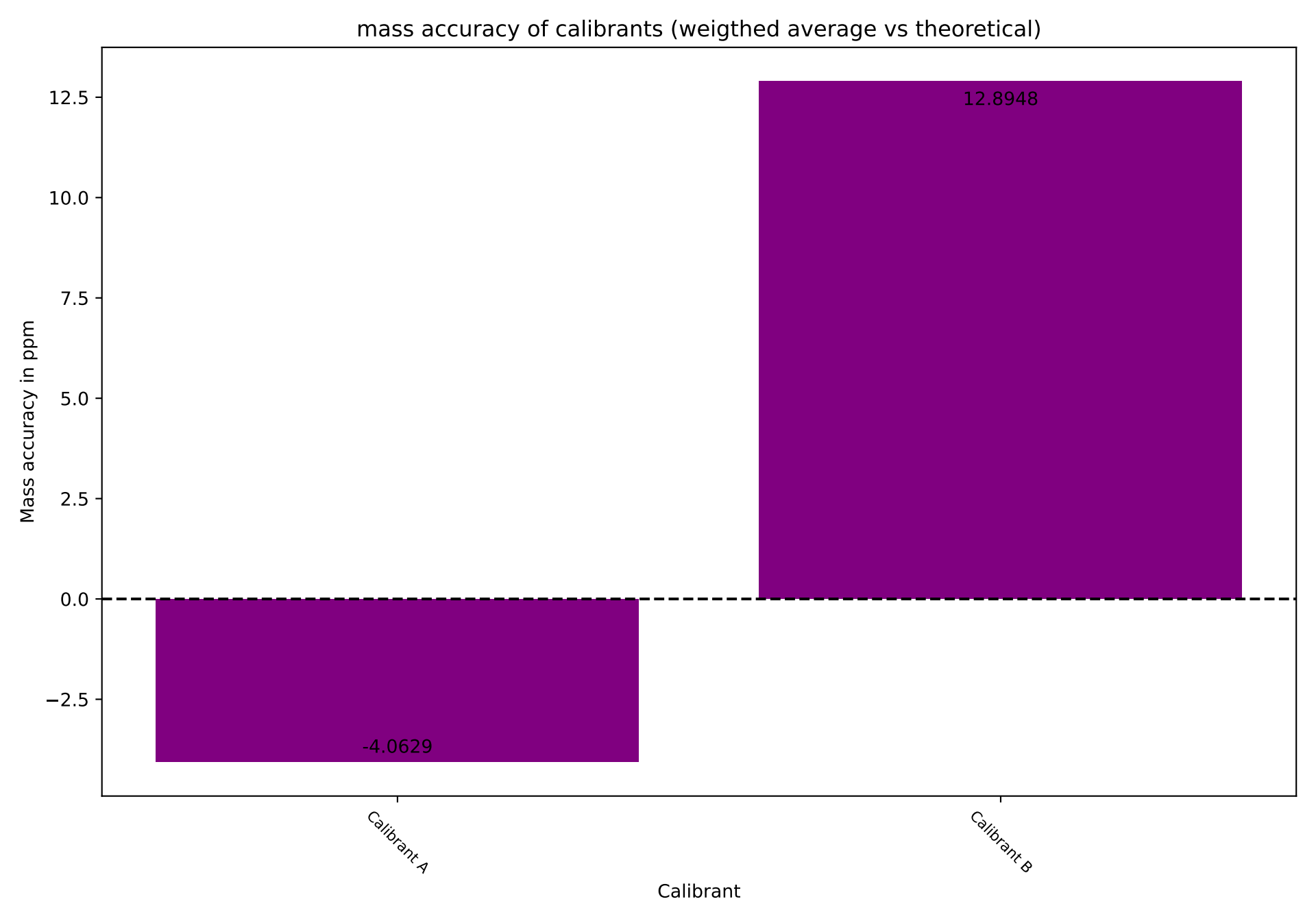


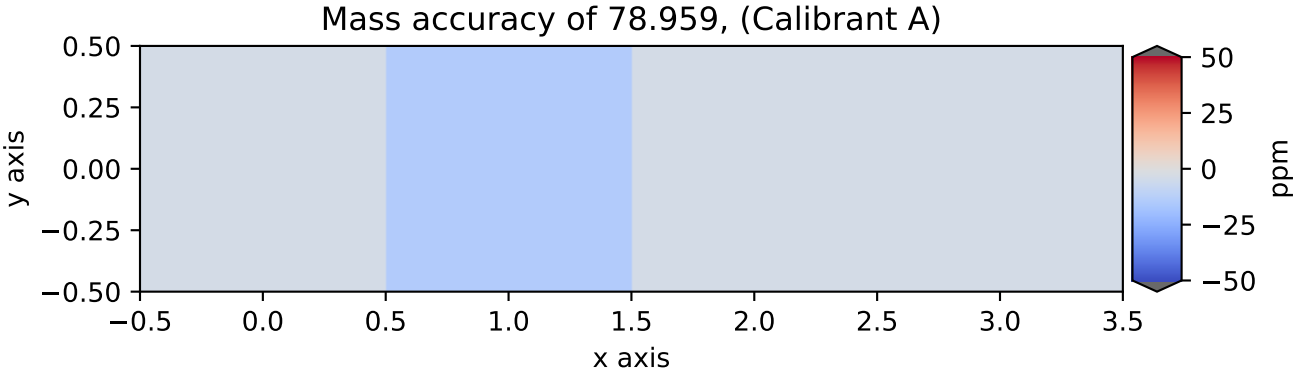


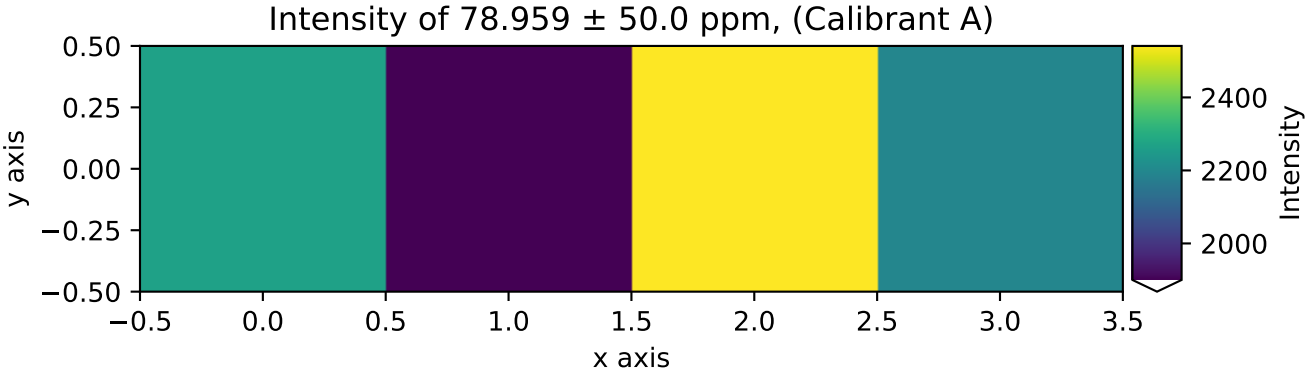


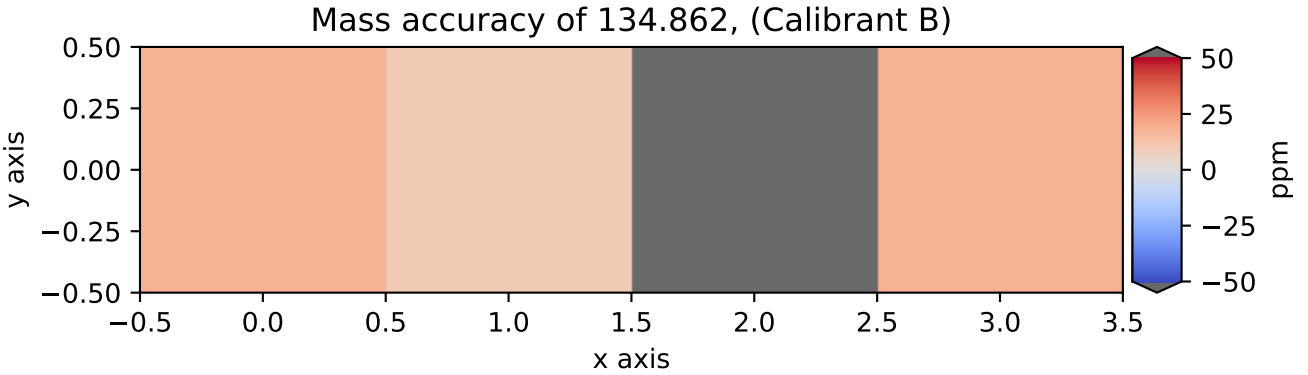

calibrant spectra for CalibrantD
no peak data found
for 500.0
in specified coverage interval

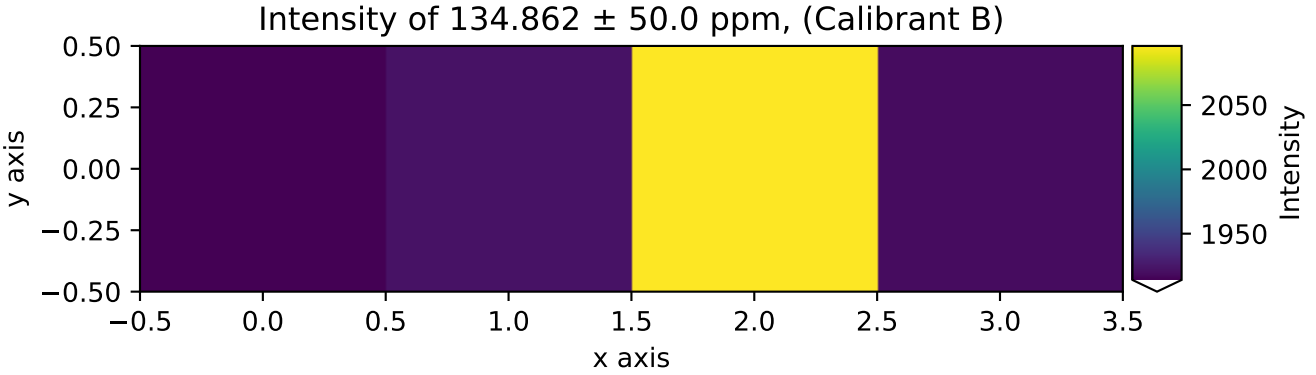

mass accuracy of calibrants (most abundant peak vs theoretical)
Mass accuracy in ppm
10
0
−10
−20
−30
−40
9.8399
-3.3865
-47.1034
Calibrant A
Calibrant B
Calibrant C
Calibrant

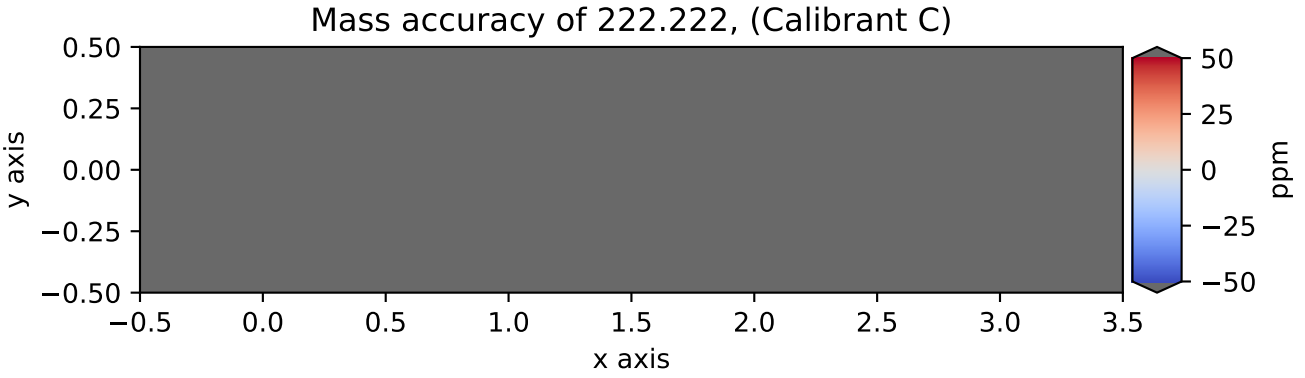

mass accuracy of calibrants (weigthed average vs theoretical)
12.8948
-4.0629
12.5
10.0
7.5
5.0
2.5
0.0
−2.5
Mass accuracy in ppm
Calibrant A
Calibrant B
Calibrant

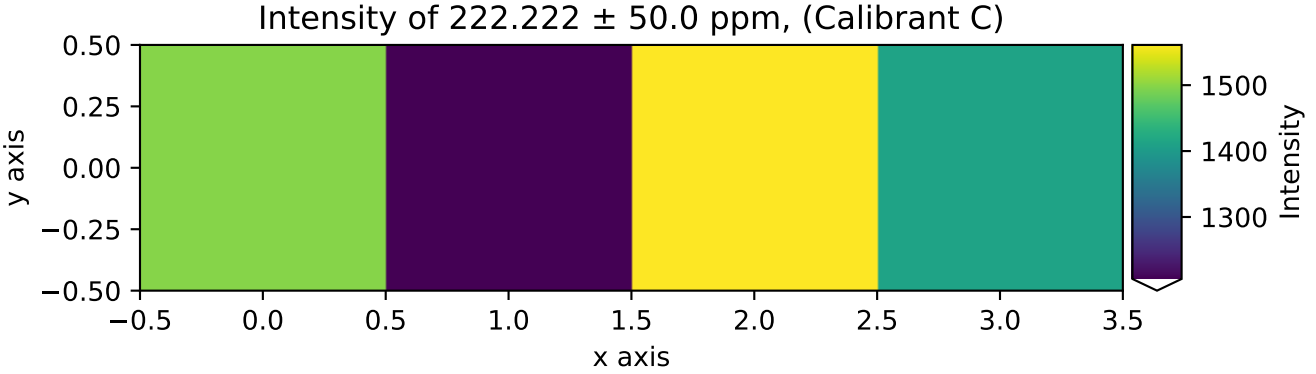

Mass accuracy of 78.959, (Calibrant A)
0.50
0.25
0.00
−0.25
−0.50
y axis
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x axis
50
25
0
−25
−50
ppm

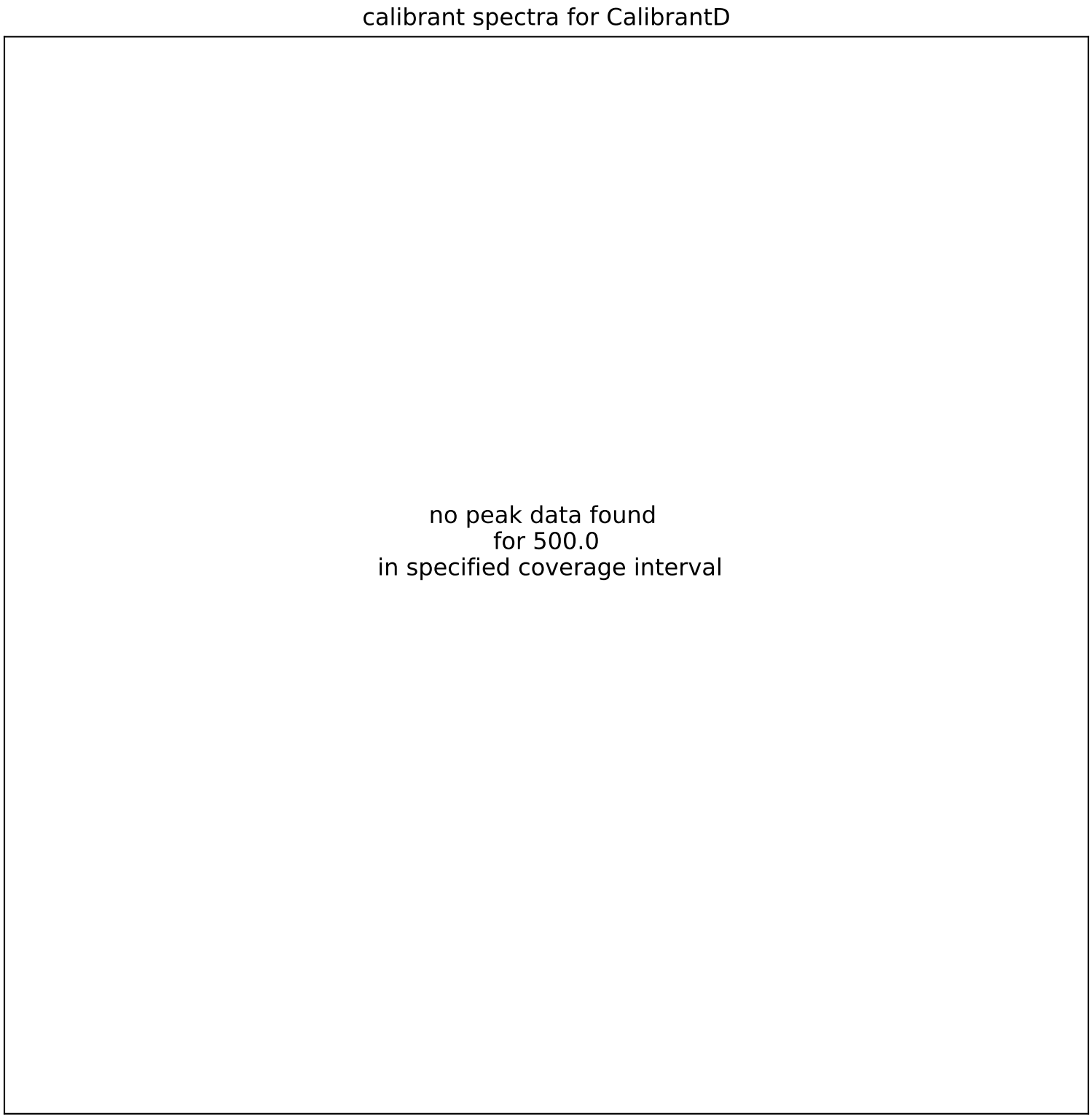

Intensity of 78.959 ± 50.0 ppm, (Calibrant A)
0.50
0.25
0.00
−0.25
−0.50
y axis
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x axis
2400
2200
2000
Intensity

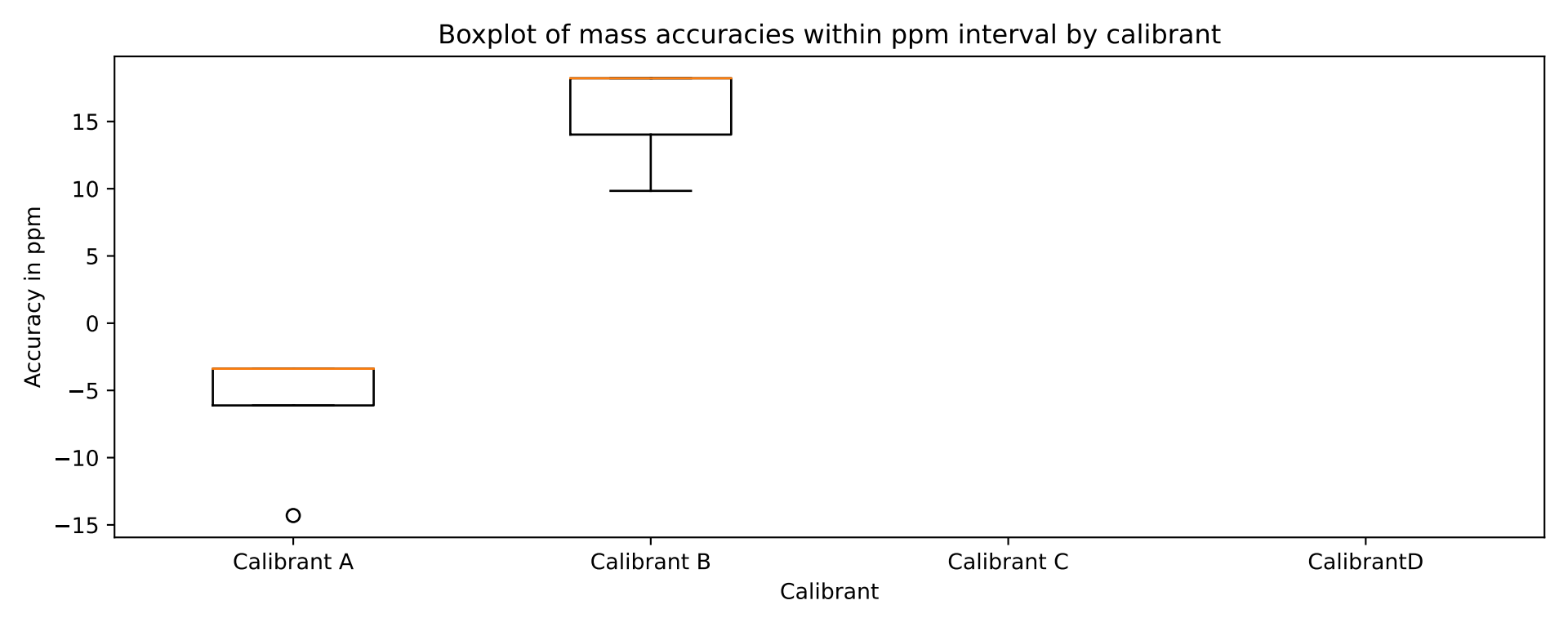

Mass accuracy of 134.862, (Calibrant B)
0.50
0.25
0.00
−0.25
−0.50
y axis
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x axis
50
25
0
−25
−50
ppm

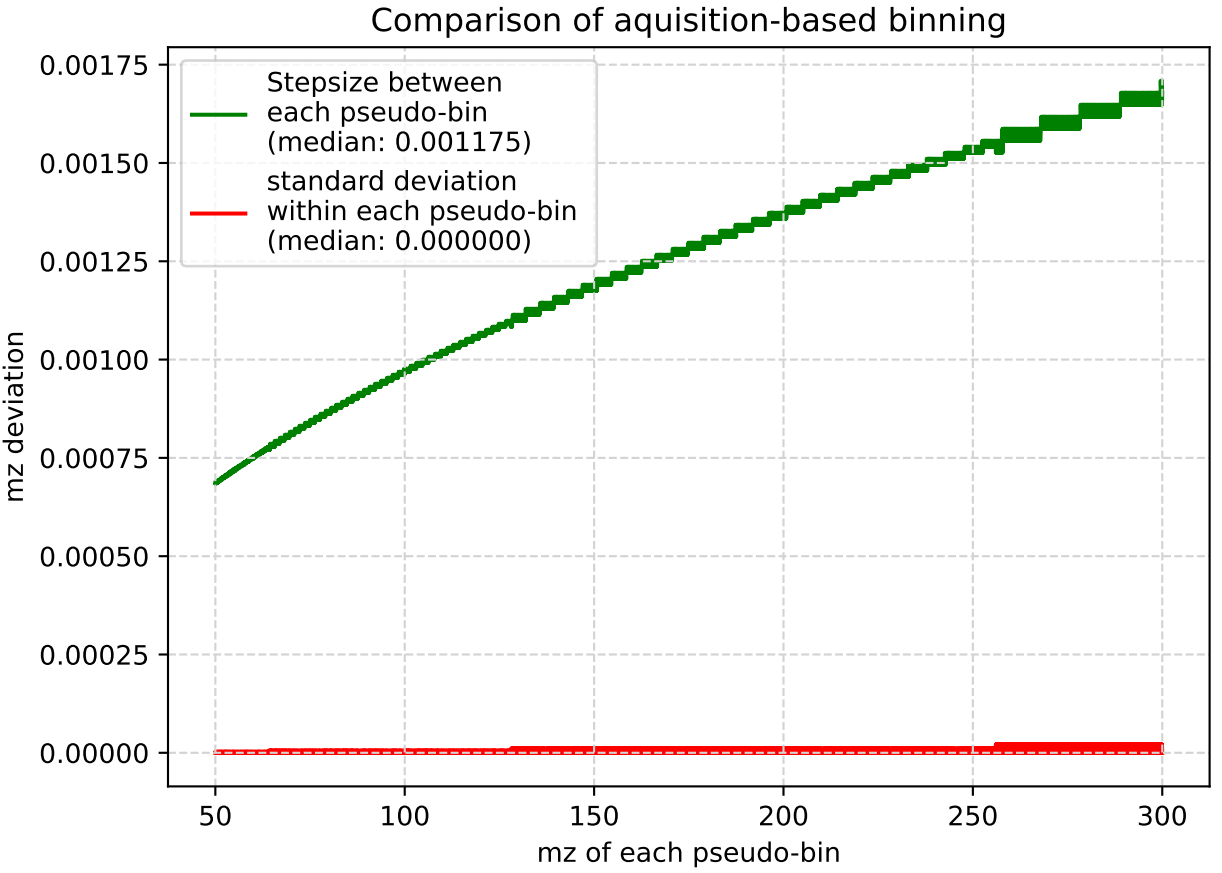

Intensity of 134.862 ± 50.0 ppm, (Calibrant B)
0.50
0.25
0.00
−0.25
−0.50
y axis
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x axis
2050
2000
1950
Intensity


Mass accuracy of 222.222, (Calibrant C)
0.50
0.25
0.00
−0.25
−0.50
y axis
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x axis
50
25
0
−25
−50
ppm


Intensity of 222.222 ± 50.0 ppm, (Calibrant C)
0.50
0.25
0.00
−0.25
−0.50
y axis
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
x axis
1500
1400
1300
Intensity


calibrant spectra for CalibrantD
no peak data found
for 500.0
in specified coverage interval


Boxplot of mass accuracies within ppm interval by calibrant
Accuracy in ppm
15
10
5
0
−5
−10
−15
Calibrant A
Calibrant B
Calibrant C
CalibrantD
Calibrant


Comparison of aquisition-based binning
Stepsize between each pseudo-bin (median: 0.001175)
standard deviation within each pseudo-bin (median: 0.000000)
mz deviation
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
50
100
150
200
250
300
mz of each pseudo-bin

mz	name	comment	found	value_wavg	distance_wavg	value_map	distance_map	coverage	interval
78.959	Calibrant A	in all pixel	True	78.958679	-4.0629	78.958733	-3.3865	1.0	0.00394795
134.862	Calibrant B	in pixel 2	True	134.863739	12.8948	134.863327	9.8399	0.75	0.006743099999999999
222.222	Calibrant C	no signal	True	nan	nan	222.211533	-47.1034	0.0	0.0111111
500.0	CalibrantD	out of mz range	False	nan	nan	nan	nan	0.0	0.025