**What does a good vs. bad peak fit look like?**

Even though DiadFit automates peak fitting, you still need to visually inspect each peak fit to check that it is good, and discard analysis with poor peak fits.

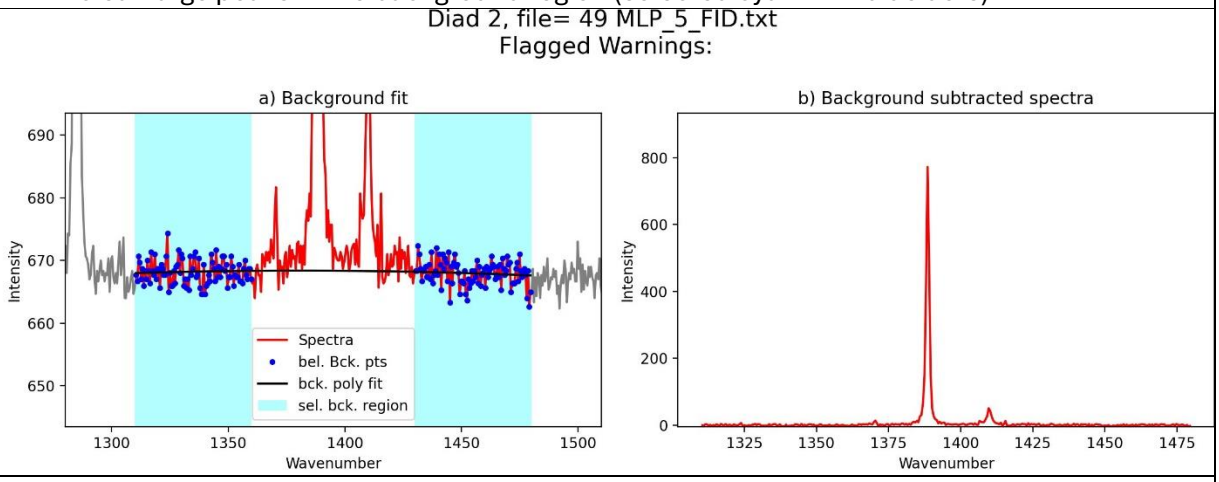
**What makes a good peak fit and what should I check?**

DiadFit makes a 7 panel figure for inspect.

1. inspect the background position.

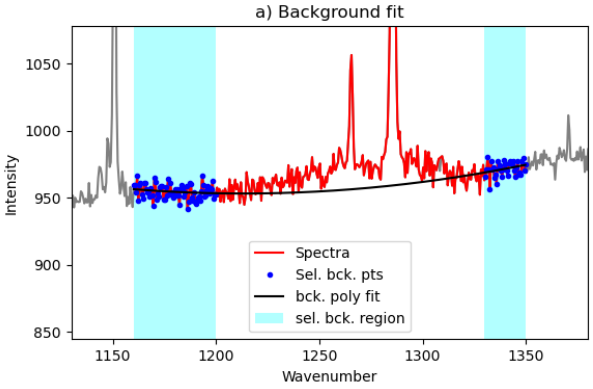
**This is a good background fit**

- The black line best fit line does a good job of passing under the peak, and there are no clear large peaks in the background region (selected cyan with blue dots).

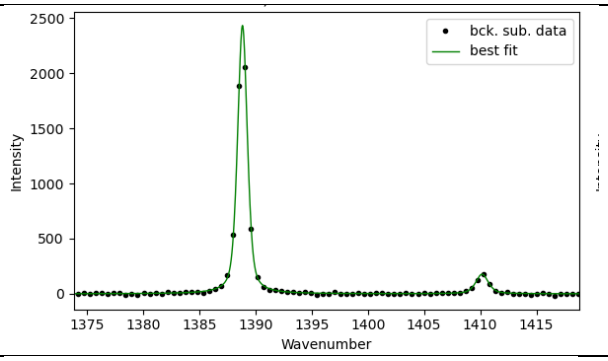
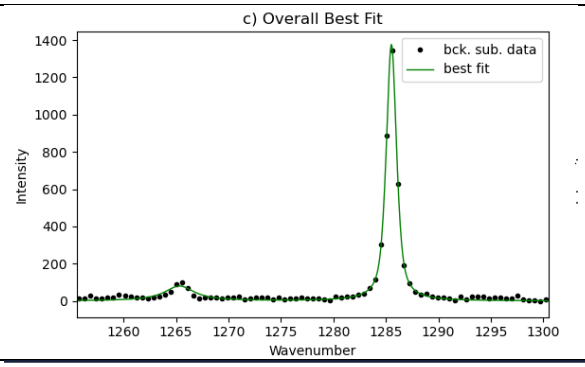
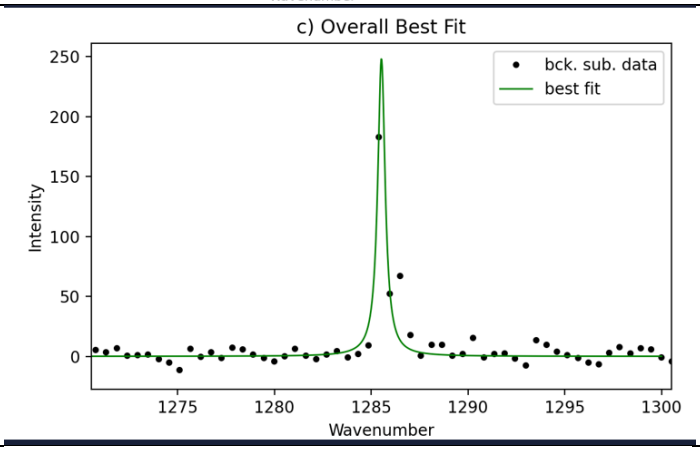
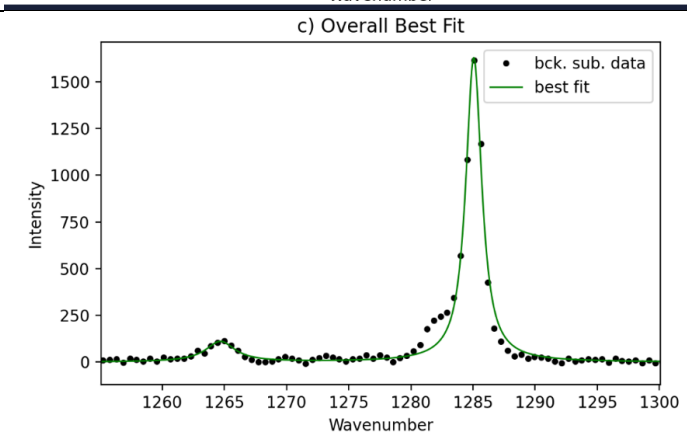


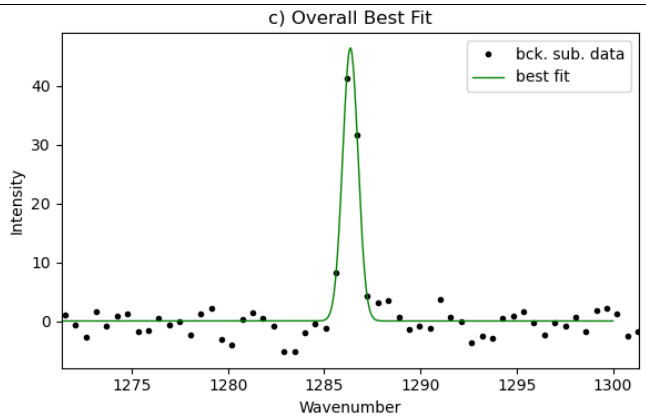

**This is a bad background fit**

- The black line doesn't do a good job of flatting out the background. I would advise moving the background positions in. You might also want to adjust the degree of the poylnomial.

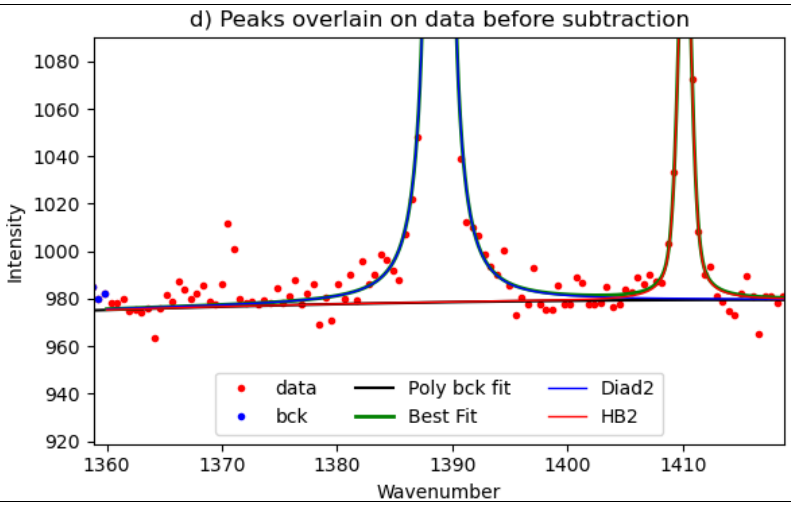
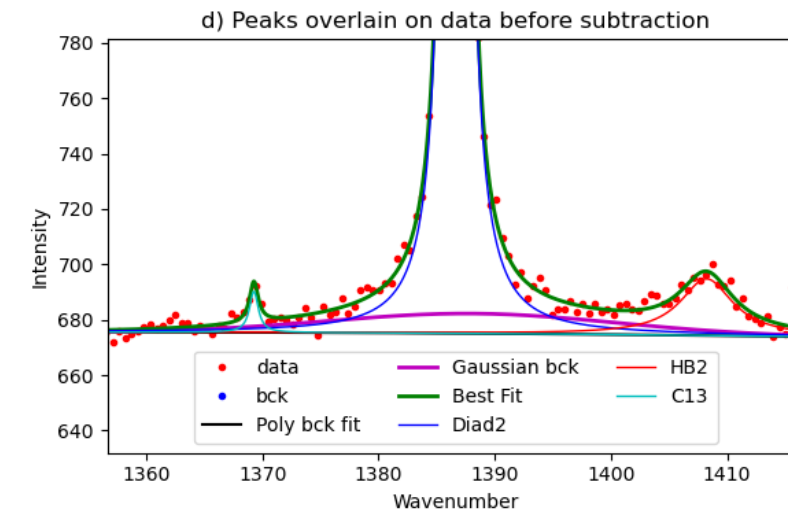


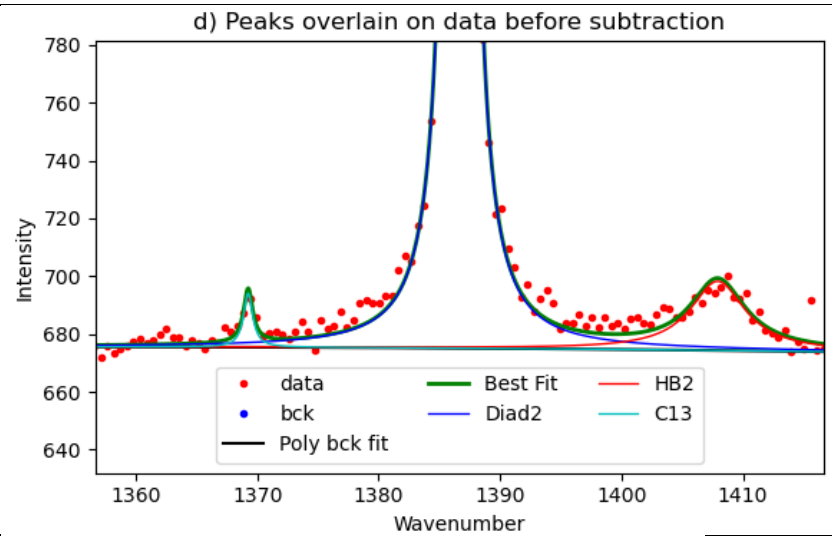
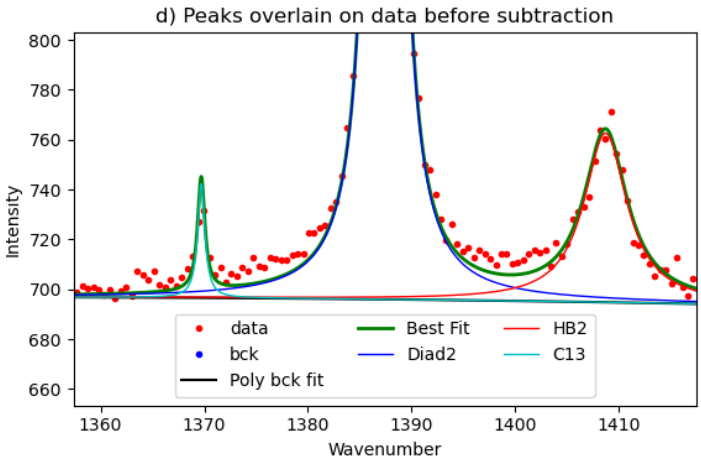

Next, inspect the peak itself in plot c). You ideally will have >3-4 points above background, Check that the green line passes through the points.

| | |
|---|---|
| This is a good fit to the diad and hotband, the green best fit line goes through all the points. |  |
| This is a good peak fit to the diad, but a bad fit to the hot band. Hotbands can be difficult to fit in relatively weak spectra, I would leave this, but just make sure you don't use the hotband position for anything. |  |
| This is a very bad fit to the diad – there are only 2 points above background on the peak, and the one on the right has been totally missed. This isn't going to be possible to fit any better, as the two points on the RHS have similar y and different x. Discard this spectra/try collecting again. |  |
| This is an okay fit to the top of the diad, but that shoulder is concerning, it indicates that there may be liquid + vapour CO2 in the bubble, that is generating peak skewness. See DeVitre et al. (2023) Volcanica for more info. I wouldn't use this diad. |  |

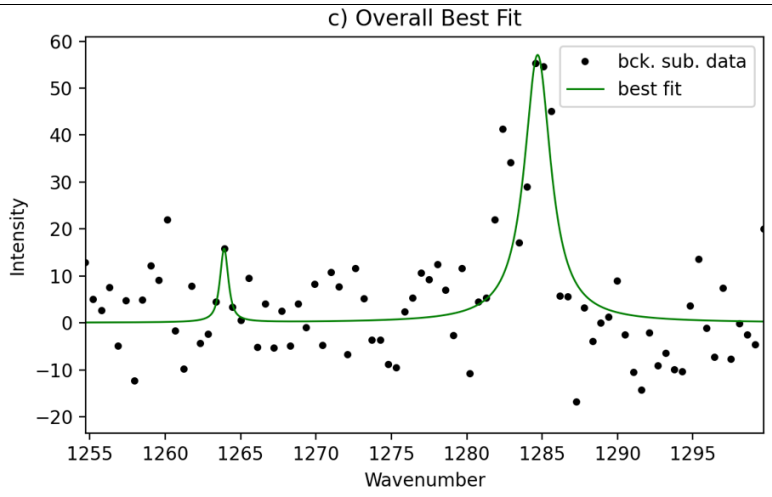
| | |
|---|---|
| This isn't a great fit, there are really only 2-3 points above background. Its possibly okay to use, but Diadfit will give you a big peak fitting error to encompass this uncertainty. |  |

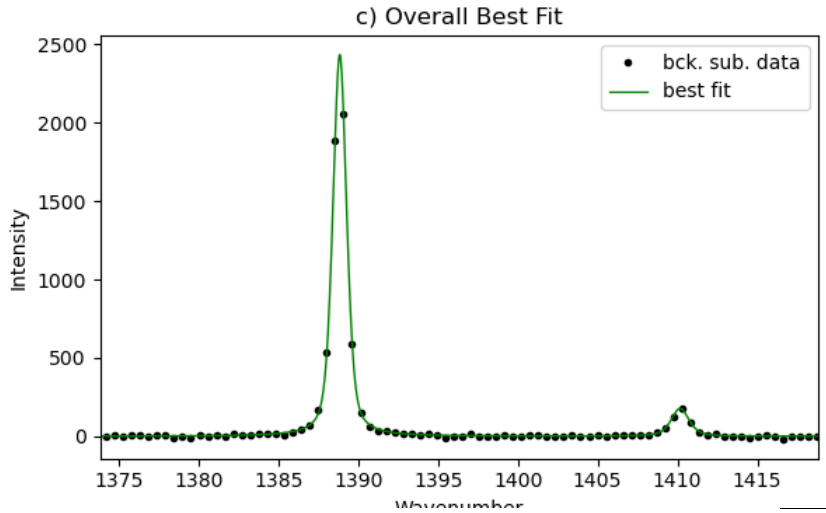
Finally, check panel d. In panel d, you get a zoomed in view of the background, you want to make sure that the points aren't too raised up above the green best fit line between the diad and the hotband.

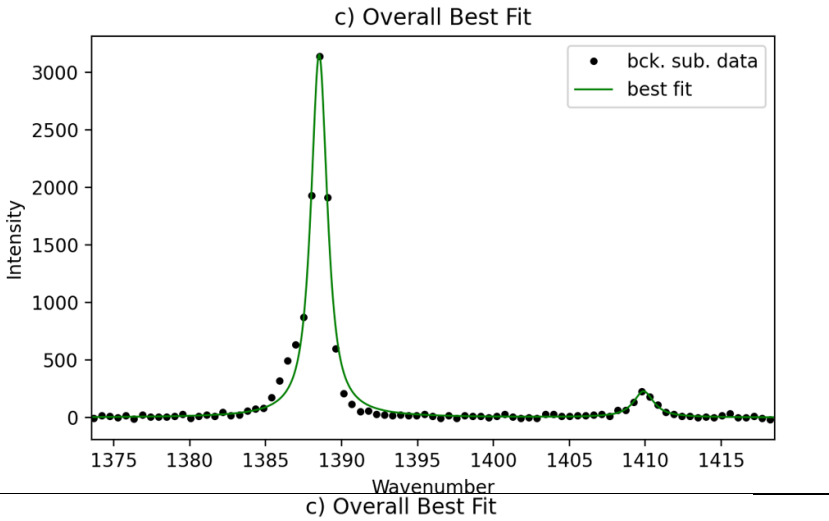
| | |
|---|---|
| This is a good fit, there is some background noise around 1370, this is where C13 is but its too weak to fit in this spectra, but the fit looks good around 1400. |  |
| This is a good fit – you can see the addition of the purple gaussian has meant that the green best fit line is passing through the data nicely at 1400 cm-1. |  |

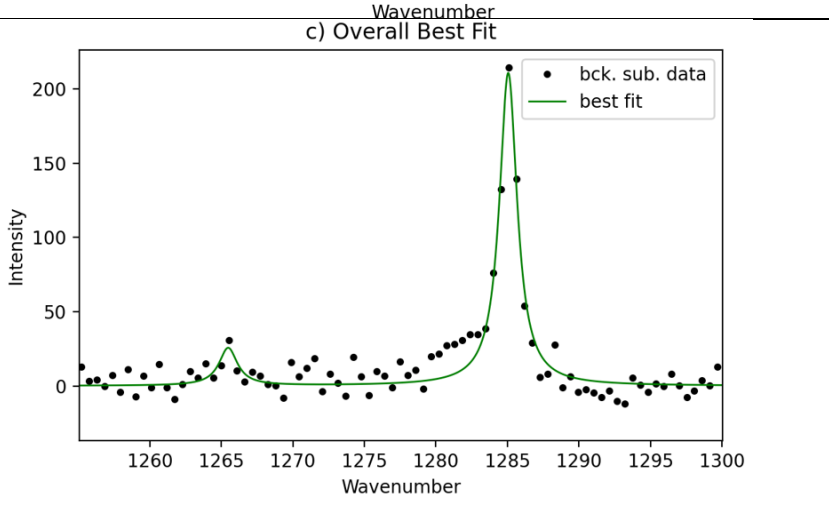
| | |
|---|---|
| This is the same fit as above, but without the Gaussian. Its not terrible, the red dots are still skimming the green line, but anything stronger than this, you really need the Gaussian. |  |
| This is where you really need to start adding a Gaussian to get the background under control. |  |

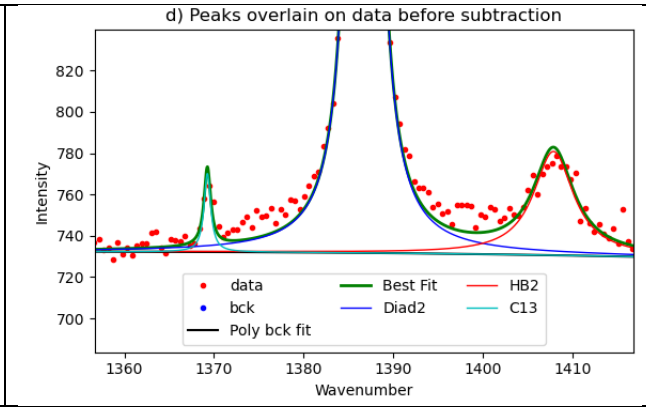
Here are some to try yourself! Is it a good/bad fit? What would you do to resolve?

| | |
|---|---|
| |  |


c) Overall Best Fit
bck. sub. data
best fit
Intensity
2500
2000
1500
1000
500
0
1375
1380
1385
1390
1395
1400
1405
1410
1415


c) Overall Best Fit
bck. sub. data
best fit
Intensity
3000
2500
2000
1500
1000
500
0
1375
1380
1385
1390
1395
1400
1405
1410
1415
Wavenumber


c) Overall Best Fit
bck. sub. data
best fit
Intensity
200
150
100
50
0
1260
1265
1270
1275
1280
1285
1290
1295
1300
Wavenumber


d) Peaks overlain on data before subtraction
Intensity
Wavenumber
820
800
780
760
740
720
700
1360
1370
1380
1390
1400
1410
data
bck
Poly bck fit
Best Fit
Diad2
HB2
C13