***Igor for Peak Fitting Methyl IR Data***

**Loading the Data:**

* Command loadIRMatrix()
* Select all of the files that are to be uploaded in the dialog box. The file paths are printed to the command window. Check here to ensure that everything is loaded in the correct order.
* As written, this method is specific to the methyl region. It finds the data point at 2557.19 cm-1 and then loads from there the next 1216 data points (to 3143.45 cm-1). If the region of interest or the data point spacing changes, this will need to be adjusts in the code
* Note: If you run this method multiple times, the data will be appended to “irMatrix”
* Good Practice: In the folder, select all the files being loaded. Shift+right click the first file and copy as path. Paste into a notebook.
  + The same information will exist in the command window, but often having the files in a separate notebook is helpful.

**Plotting the Data**

* Command plot2Das1D()
* This just allows a quick check that everything looks like it loaded correctly.
* This command will plot and 2D wave as traces. It also sets the axes for IR data.

**Setting the background correction**

* We’ll check the background on one trace first. The trace subset is that last wave loaded and can be used to check the background.
* Start by displaying the trace with Display subset
* The command for an asymmetric least squares fit is ALS(w\_data, lambda, asymmetry)
  + W\_data is a 1D wave
  + Lambda is a number between 10^2 and 10^9
  + Asymmetry is a number between 0.001 and 0.1
* Start ALS(subset, 5\*10^7, 0.001)
* To visually check the fit

SetScale/I x 2557.19, 3143.45,"", w\_base

AppendtoGraph w\_base

* + Try different values until the fit looks good
  + To check the first wave if needed

Duplicate/R=[][0] irMatrix firstWave

Redimension/N=-1 firstWave

AppendtoGraph firstWave

* + Attribution details at end
* To run the fit on all traces matrixALS(irMatrix, *lambda*, *asymmetry*)
  + This creates a matrix of baseline fits called baselines, but this can take a while to run.
  + You can plot these if you want to check how it went

**Subtracting the baseline**

* Command subtractBaselines(irMatrix, baselines)
* Creates new matrix called correctedIR

plot2Das1D(correctedIR)

**Running an Initial Peak Fit**

* Make a new wave to test the fit with:

Make/N=1217 peakFitWave = subset- w\_base

SetScale/I x 2557.19,3143.45,"", peakFitWave

* Under Analysis > Packages > Multipeak Fit, start new with peakFitWave
* Autofind peaks and run
* Use these coefficients with the batch fit
  + I’ve found opening an excel file at this point to keep track of peak parameters separately really helps.
* Under Analysis > Packages > Batch Curve fit, stat new with correctedIR and equation fitManyGaussian
* Tab through the fit to ensure that everything looks good

**Plotting parameters cheat sheet**

•Display wave0,wave3,wave6,wave9,wave12,wave15

•ModifyGraph margin(left)=70,width=226.772,height=226.772

•Label left "delta";DelayUpdate

•Label bottom "Trace Number";DelayUpdate

•ModifyGraph mirror=2,fSize=14

•ModifyGraph mode=3,marker=19

•TextBox/C/N=text0/F=0/A=MC "\\Z14Amplitude"

•TextBox/C/N=text0/F=0/A=MC "\\Z14Position"

•TextBox/C/N=text0/F=0/A=MC "\\Z14FWHM/2.35482"

•Legend/C/N=text1/J/F=0/A=MC "\\Z14\\s(wave1) 2822\r\\s(wave4) 2856\r\\s(wave7) 2929\r\\s(wave10) 2927\r\\s(wave13) 2960\r\\s(wave16) 3003"

•Legend/C/N=text1/J/B=1

*// Originally developed by tony withers:*  
*//*  
*// by*[*tony.withers@uwo.ca*](mailto:tony.withers@uwo.ca)*, using method of Eilers, PHC and Boelens, HFM*  
*// (2005) Baseline correction with asymmetric least squares smoothing.*  
  
*// Creates (and overwrites) w\_base, a baseline estimate for w\_data. The*  
*// asymmetry parameter (Eilers and Boelens' p) generally takes values*  
*// between 0.001 and 0.1. Try varying lambda in orders of magnitude*  
*// between 10^2 and 10^9. Not efficient for large N, try it for w\_data*  
*// with fewer than 1000 points.*  
*//*  
*//*  
*// I just changed the code to avoid the slow matrix multiplication.*  
*// The H-matrix is now constructed "manually". This saves time and memory*  
*// allows larger datasets.*  
*// (*[*kmichel@wzw.tum.de*](mailto:kmichel@wzw.tum.de)*)*