Things that you will likely want to change for your data:f

for filename in glob.glob(os.path.join(path, '\*.txt')): as is this will deconvolute any file in the current folder with .txt adjust this to one file (by just putting in the full name of the file you want to deconvolute; for example ‘testspectrum.txt’) or several files using normal unix wild card symbols etc.

mancentcol: this is the center of the peak colorings, adjust this to the center of your peak of interest

manrangecol: this is how much ppm the rainbow ranges over

peaks\_to\_fit: adjust to about twice the number of peaks that you can readily see by eye or lower

freqsig: this needs to be changed to the basic frequency of the magnet/nuclei that the spectrum comes from

left: put in desired left limit of analysis in ppm

right: put in desired right limit of analysis in ppm

maxph: you may want to give a little more freedom to the phasing of the fits but I would say no more than π/10 (m.pi/10) and only change this if you understand why you are changing it.

mc0123: False or True ; set to True if you want to run montecarlo refining, however in my experience this rarely changes the outcome and sometimes makes it run a lot longer.

minFWHM: set this to be no more than half of the line broadening that you apply to the spectrum when processing the spectrum.

maxsplit: IF using split (to turn on peak splitting change savemetime=[False] to savemetime=[True]) this number limits the maximum number of peaks that will be fit. Peak splitting in general will not overfit the data, but it will increase the time it takes to fit by a lot. For a data set I analyze them all without or with speak splitting enabled so that the deconvolutions are comparable.