1. Update the variable named "NMRPATH" in the startup.m document according to where you put the NMR folder.

2. Open Matlab, go into the NMR folder.

3. Run 'startup.m', it will ask "Which experiment are you working on?", type the name of the folder you are working on, which is one subfolder in the EXPERIMENTS folder. In the files I sent to you, there is only one subfolder named "crotonic" in the EXPERIMENTS folder, this subfolder is used as an example. You can create new subfolders for other samples in the EXPERIMENTS folder. Please note that in each subfolder there should be a molecule.def, in which is the Hamiltonian data of the sample.

4. The experimental spectra should be put in the results subfolder of the crotonic folder (using crotonic as an example).

5. The codes needed in fitting spectra are in the tomo subfolder of the crotonic folder. The main code is 'fitespec.m'. 'ThermalZ\_fit.m', 'ThermalZ\_fitC2.m', 'ThermalZ\_fitC3.m' and 'ThermalZ\_fitC4.m' use 'fitespec.m' to fit the spectrum of C1, C2, C3 and C4 of crotonic, respectively. Please note the main difference among them, which I labelled in line 6 of 'ThermalZ\_fit.m','ThermalZ\_fitC2.m','ThermalZ\_fitC3.m' and 'ThermalZ\_fitC4.m'. The final executable codes should be like LhZZ23\_save.m or ThermalPPS\_save.m. Please refer to them.

6. The path in createstruc.m should be also updated.

7. The spectrum that is to be fitted should have its middle frequency set to 0. To get such a spectrum, you only need to change the parameter ‘sr’ in Topspin system.