Chem 220
MNova ^{1}H NMR Processing Guide

1. Open your ^{1}H NMR file in MNova from the NMR-Data$ server. Open the "fid" file to load the data.
2. **Reference**: Normalizes chemical shift using known values ($CDCl_3$ 7.26 ppm or TMS 0.00 ppm)
   Menu Sequence: Analysis < Reference < Reference (hot key "L")
   Once Reference has been activated, select either the $CDCl_3$ or TMS signal and set "New Shift" to the standard value
3. **Autophase**: Adjusts data to ensure all signals are in-phase (positive value)
   Menu Sequence: Processing < Phase Correction < Automatic
4. **Baseline Correction**: flattens the baseline to improve integration accuracy
   Menu Sequence: Processing < Baseline < Full Auto (Bernstein Polynomials)
5. **Define Integrals**: Allows manual designation of integral regions
   Menu Sequence: Analysis < Integration < Manual (hot key "I")
   Once Manual Integration is turned on, click and drag across each signal to define the beginning and end of the integral region.
6. **Normalize Integrals**: Redefines integral ratios to correspond to the number of protons in each signal
   Menu Sequence: Right click on horizontal integral line below spectra < Edit Integral
   a. Set the value for "Normalized" to the expected number of protons for that integral
   b. Click the checkboxes for "Linear Correction" and "Auto" then select "Apply to All"
7. **Peak Picking**: Gives chemical shift for each signal
   Menu Sequence: Analysis < Peak Picking < Manual Threshold (hot key "K")
   Once the Manual Threshold is activated, click and drag across all signals with the vertical threshold at an appropriate height to pick only relevant peaks
8. **Structure and Assignments**: Right click on spectra and select "Copy". Paste into a PowerPoint slide or other appropriate software. Use ChemDraw to generate a labeled structure (a, b, c…etc. for each group of protons) and add corresponding labels to each signal on your spectrum. Clearly label multiplicity for each signal.

Finished Spectrum: