CHEM 115

S2022

How to process and analyze NMR spectra

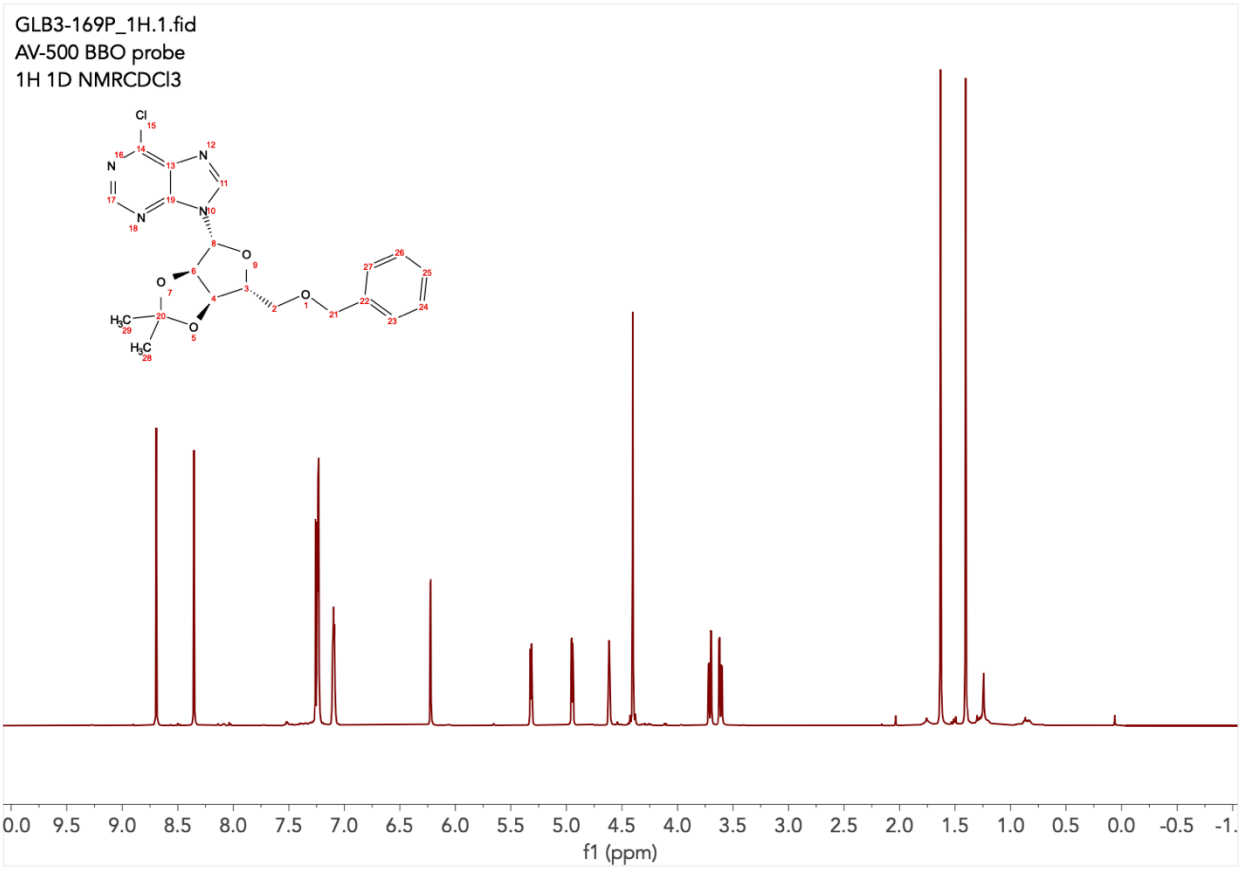
Before going through this tutorial, you may find it useful to load in Logan's MestReNova settings. This way,your spectra will be more readable and cleaner in terms of style. This file and a ReadMe are available on the Drive for 115. This is personal preference, though.

Step 1: Loading Spectra

Open MestReNova and drop in the folder containing your NMR data from the server. Access for this differs based on your operating system. The username and password for the server are **nmrdata** and **cocnmrd11**.

Step 2: Initial Processing

Go to the **Processing** tab in MestReNova. Click **Auto Baseline Correction** and **Auto Phase Correction**. This will assuage any errors in the shape of the baseline and the phasing of the peaks. Use ChemDraw to build the structure of the target compound, then copy and paste this structure onto the spectrum within MestReNova. Press **Z** on your keyboard to access the **zoom** tool (there are 3: horizontal, vertical, and box zoom; pressing Z will cycle through these) and zoom in on your peaks to eliminate unnecessary white space; 1.00 ppm around the most downfield and upfield peaks is sufficient. Your spectrum will look like the following:



CHEM 115

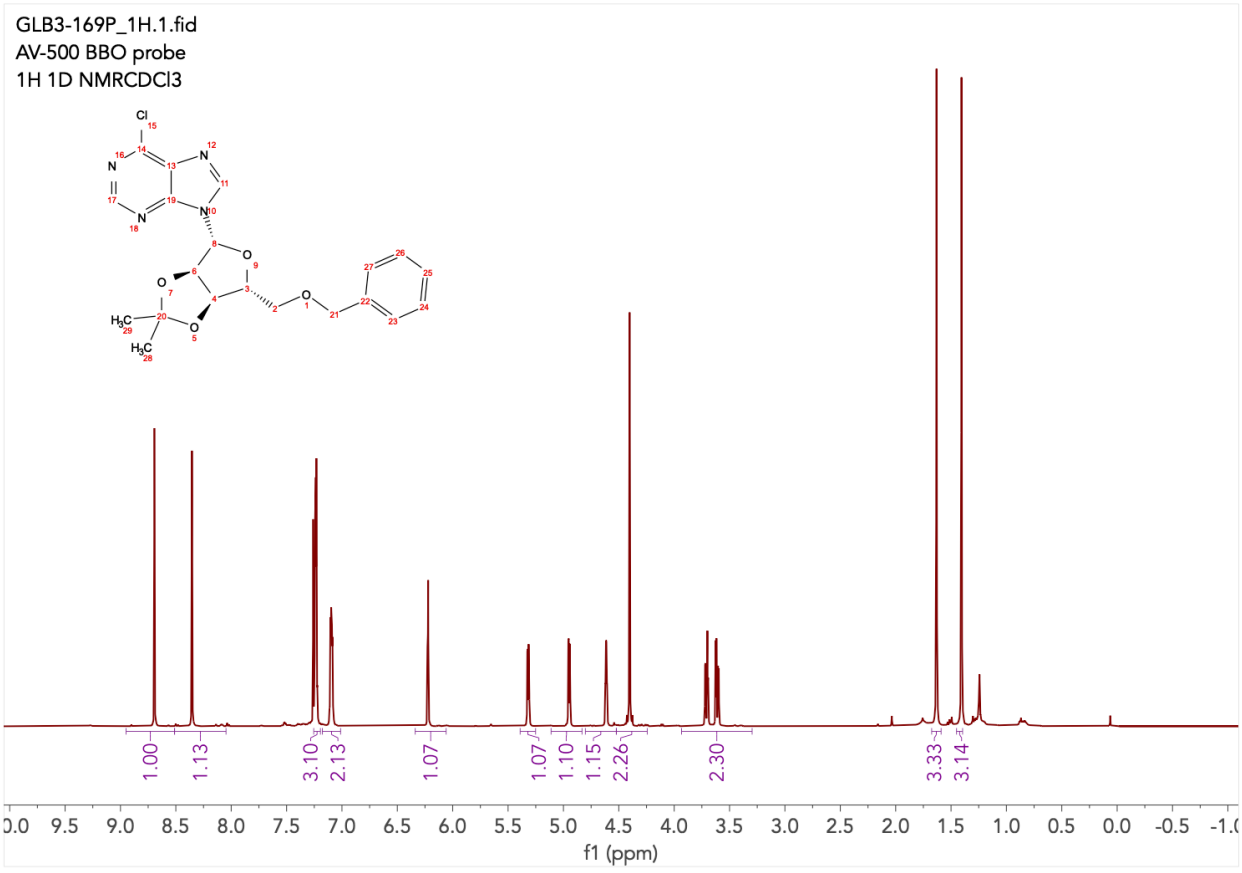
S2022

Step 3: Integration

Press **L** on your keyboard to access the peak-snapping **reference tool** and identify the NMR solvent peak. A table of these (and common shifts for other solvents in common NMR solvents) can be found on the Drive for 115. Select the solvent peak and set its chemical shift to the known ppm value using the **L reference tool**. For example, the proton in $CHCl_3$ often appears around 7.19 ppm though should appear at 7.26 ppm.

Identify a peak on your spectrum of known integration. This may be a methyl peak, a methylene, a vinyl proton, or any proton you are reasonably certain of. Press **I** on your keyboard to access the **integration tool** and **integrate** this peak *including the baseline around the peak*. MestReNova will set this peak to 1.00 protons automatically and will reference the rest of your peak integration to this **normalization**; this can be changed later. For example, if you know the peak you've chosen should be 2.00 protons, you can right-click on the integration number below the peak and change its normalization from 1.00 to 2.00.

Zooming in may help here. Selecting the zoom tool with **Z** then pressing **F** for "full" will restore the zoom to include the entire spectrum. After normalizing the integration to the first integrated peak, integrate the rest of the peaks in the same manner *including the baseline around the peak.* Your spectrum will look like the following:

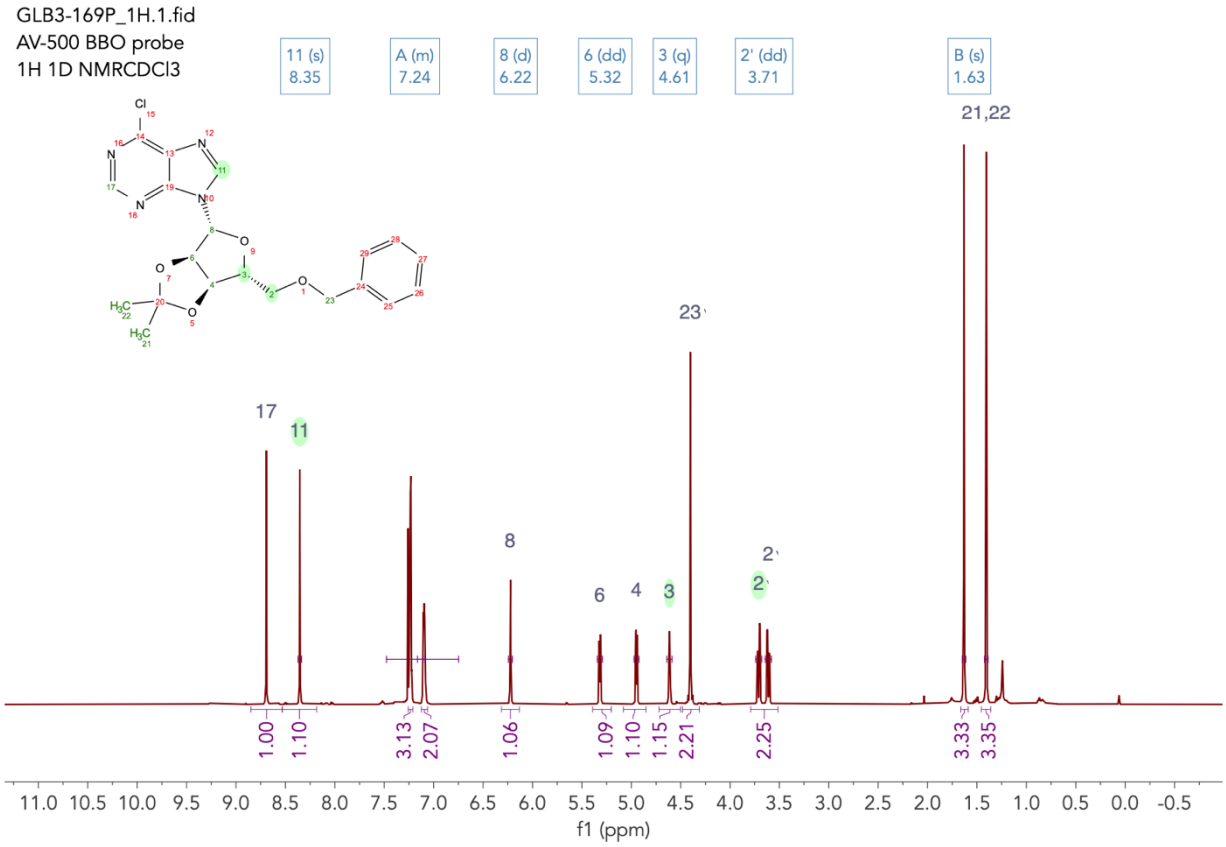


CHEM 115

S2022

Step 4: Assignment

Press **A** on your keyboard to access the assignment tool. Select or click and drag over a peak to mark it for assignment, then select the proton (or carbon-bearing the proton) you think the selected peak corresponds to. Repeat this for all product peaks. After assignment, press **J** on your keyboard to analyze peak multiplicities. Click and drag over each peak to identify its multiplicity and splitting constants (*J* values). You may now save your spectrum for later reporting. At the end of this process, your spectrum should look like the following:



CHEM 115

S2022

Step 5: Reporting

Typically, NMR data is reported as follows:

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.69 (s, 1H), 8.35 (s, 1H), 7.26 – 7.20 (m, 3H), 7.13 – 7.05 (m, 2H), 6.22 (d, *J* = 2.3 Hz, 1H), 5.32 (dd, *J* = 6.0, 2.4 Hz, 1H), 4.95 (dd, *J* = 6.0, 1.9 Hz, 1H), 4.61 (q, *J* = 2.8 Hz, 1H), 4.40 (s, 2H), 3.66 (ddd, *J* = 48.8, 10.5, 3.2 Hz, 2H), 1.63 (s, 3H), 1.41 (s, 3H).

If you have not analyzed multiplicities, you may quickly (but crudely) generate this yourself by selecting the **Auto Multiplet Analysis** button in the analysis tab in MestReNova then clicking the small button next to it labelled “Copy Multiplets” (see below). This will copy these data to your clipboard for pasting elsewhere.