Laborhelfer
Für Euch.

Mestrenova guide

Import NMR-data

- Drag and drop your zip-file or folder into the Mestrenova screen
- **or** go to the top menu and select: File > Open... > Select your zip-file

Phase and reference your spectrum

 Automatic Phase Correction

If the baseline and signals look all waivy, you can click on the Automatic Phase Correction icon and either

- press **Automatic...**
- **or**, if this is not sufficient, press **Manual Correction** (Shortcut: Shift+P), and drag on the blue area. Play around with holding the right or the left mouse button, until your baseline is flat

 Automatic Phase Correction

If you want to flatten your baseline, press the Baseline Correction icon and

1. press **Baseline Correction...** (Shortcut: B)
2. Select a method (I recommend the **Whittaker Smoother**) and press Ok

 Reference

The next step is to pick a reference signal for your spectrum. Usually, you pick the TMS-signal which is supposed to be on the far right of your spectrum. If you have silicon in your compound, or if the TMS-signal is not visible, you can also do the following with a solvent peak.

1. Press **Z** and zoom into the TMS-signal at about 0 ppm
2. press **L** or select the Reference icon and click **Reference**
3. Hover over the signal. A red crossbar should appear, click the peak of your TMS-signal.

4. At "New Shift: " type in 0 ppm **or** go to "Solvents>>" and select "TMS"(If you reference on a solvent signal, pick your respective solvent here). Press Ok

Process your data

 Peak Picking

Now, as the spectrum has been calibrated, we need to process our data. The first step is to pick all relevant peaks.

1. If you have a very clean spectrum, go to the Peak Picking icon and click on "Automatic" (not recommended)
2. Else, press the icon and select **Peak by Peak** (Shortcut: Cmd+K)
3. Select the peaks you want to pick. If you have to zoom into an area, press **Z**, zoom onto the area, press **Cmd+K**, pick the peaks, press **F** and repeat for the remaining peaks.
4. If you want to delete a peak, press the icon and select **Delete Manually** (Shortcut: Shift+Cmd+K) and drag over the peaks you want to delete

 Integration

The next step is to integrate the signals.

1. Zoom into the respective area (**Z**)
2. Click on the Integration icon and select **Manual** (Shortcut: I)
3. Drag over the signal you want to integrate and continue for all relevant signals
4. To calibrate the integrals, right-click the integration bar (above the ppm-scale) and click **Edit Integral...**
5. Now you can either set the value for the integral you selected (change **Normalized** value to e.g. 3 for a methyl group) or change the total value for all integrals (change **Total** value to the total amount of hydrogens in your compound, e.g. 8 if your compound is toluene)
6. If you want to get rid of the integration curve above your signals, click the Integration icon and deselect **Integral curves**

Select multiplets

Usually, you have to list the coupling value of every multiplet in your spectrum.

1. Click on the Mulitplet icon and select **Manual** (Shortcut: J)
2. Drag over all multiplet peaks
3. If you have two overlapping multiplets, you can select/ deselect a multiplet peak by clicking on the Multiplet icon and selecting **Add Multiplet Peak**. Now you can select/ deselect the multiplet peaks until you get the multiplets right.

Export your data

Export the whole spectra

You will always export what is visible in your window. If you want to export the whole spectrum, press **F** and zoom into the relevant area (**Z**)

- Select your spectra, press **Cmd+c** and paste it into your Word-document or similar
- **or** go to the top menu, go to **File**>Export to pdf...

List data

If you want to have a list of your NMR data, go to the top menu and go to

1. **View**>Tables...
2. Select the data you want to list under the **NMR** area
3. For example, check **Multiplets** and **Peaks** and press Ok
4. Export the tables by clicking **Copy Multiplets/ Peaks**