Data Processing using MestreNova

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When processing, regardless of the software you are using, you will want to always follow the same steps in the same order. Below is a checklist of the steps to follow:

- Fourier Transform
- Phase Correction
- Baseline Correction
- Spectrum Reference (optional)
- Peak Labels
- Integrations

Importing Spectra – Go to 'File/Open' or click on and select appropriate file. Note: To import a 1D spectrum you will need the FID file. To import a 2D spectrum you will need the ser file. The spectrum will automatically open already processed and with the phase corrected.

Baseline Correction – Click on 'Baseline Correction' to correct the baseline.

Spectrum Reference – Click on 'Reference' and select the peak you want to be a reference point.

Peak Labels - Click on 'Peak Picking' to obtain automatic peaks. To see a list of Peak Picking Tools and Options click on the arrow next to the icon.

Integrations – Click on 'Integration' to automatically integrate spectrum. You can manually integrate by clicking on the arrow next to the icon and selecting manual. You will then get a cursor that looks like an integration trail with a red cursor next to it. Place the red cursor on the left side of the peak to be integrated, left click and drag. To calibrate an integral, place the cursor on the desired integral and right click. Select 'Edit Integral' from the menu. Place the value in the 'Normalized' box. When finished close out the window with the box in the upper right hand corner. You can turn off the integration function by either clicking on manual again to toggle off under the integration icon or by choosing another function.

Measuring J Values – Click on 'Multiplet Analysis' to apply an automatic multiplet analysis. You can manually select peaks as well by clicking on the icon arrow and selecting 'Manual'. Place the red cursor on the left side of the peak(s), left click and drag. You can create a report by clicking on the icon arrow and selecting 'Report'. It usually places the report in the upper left hand portion of the spectrum, but you can resize and move the report anywhere you like.

Other Useful Icons –

Zoom In ⊞ - Click on icon and left click and drag in spectrum to zoom in on specific region. This icon is a toggle switch.

Full Spectrum ⊞ - Click on icon to return to original spectrum.

Increase Intensity ⊞ - Click on icon to increase the intensity of the spectrum.

Decrease Intensity ⊞ - Click on icon to decrease the intensity of the spectrum.

Crosshair ⊞ - Click on icon to toggle on and off. When on, place cursor on desired peak and it will give spectral location in ppm and Hz.

Please see Help/Contents for more detailed instructions in processing.