PROCESSING IN TOPSPIN 3.X

TRAINING GUIDE

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- 1. Once your acquisition is complete, you need to process your data. Click on the Process button in the top line, then the Proc. Spectrum button. This will Fourier Transform your FID into a spectrum (ft), autophase (apk), and correct the baseline (abs). You can also type **efp** on the command line.
- 2. **Phasing.** Click on the Adjust Phase to enter manual phasing mode. The software will place the pivot point (red line) on the largest peak for you. If you wish to move the pivot point, click the RMB (right mouse button) where you want to *set the pivot point*. Hold the LMB (left mouse button) down on the **[0]** button and move the mouse slowly up and down. This will adjust the zero order phasing in the vicinity of the red vertical line. Correct the phasing on the peak closest to the red line an ignore the phasing elsewhere for now.
- 3. Next hole the LMB down on the **[1]** and adjust the phasing of the peaks farthest from the red line. This is the first order phase correction. Thin of the red line as the pivot on a seesaw or the fulcrum of a lever. The closer you are to the pivot point, the less adjustment you will see to the phasing. The farther you are from the pivot, the more adjustment you will see. You can move the pivot point as needed to help adjust the first order phasing.
- 4. It may take several iterations of adjusting the [0] and [1] to get your spectrum phased. Click **[R]** to reset the phasing back to the original if it gets too out of phase and start over.
- 5. To exit phasing mode, click the Return & saved phased spectrum button (resembles a computer disk with a blue arrow under it).



6. **Calibrating**. Zoom in on the peak you wish to calibrate (left click, drag, then let go). Click on the Calib. Axis button. Select the solvent or reference peak by left clicking on it and entering the desired value. Click OK.



7. Peak Picking. Click the Pick Peaks button.



- 8. Click the *Define new peak picking range* button (if not already selected). Using the LMB, drag a green box over the peaks you want to pick. DO not go below the baseline or it may pick noise. You can select multiple regions by making as many green boxes are you want.
- 9. When you are finished, click the *Return, save changes* button to exit peak picking mode.
- 10. Integration. Click the Integrate button.



- 11. Click the Define new regions using cursor (if not already selected).
- 12. Using the LMB, click where you want an integral region to begin. Drag the cursor to where you would like the region to end and let go of the LMB.
- 13. If you would like to delete an integral region, right click on the region, and select Delete Current Integral. If you want to set an integral to a specific value, right click in the region and select Calibrate Current Integral. Type in the desired value and hit ok. Remember you cannot have negative integral values
- 14. When you are finished, click the *Return, save changes* button to exit integration mode.