Tips for getting reliable quantitative information from integrals in NMR spectra

A. Data acquisition

1. Estimate the spin-lattice relaxation times (T1s) of all the relevant peaks.

2. Set **d1** to 5 times the longest T1 obtained in step 1.

3. Set **np** to a number large number, e.g. 131072.

4. Set **nt** to a large number and collect enough scans to get the S/N (signal to noise ratio) 100:1 or better.

B. Data processing

1. Set **fn** to 131072 or 262144.

2. Adjust **lb** to get the best S/N without broadening peaks too much.

3. Correct the baseline of the spectrum using **region bc cz** commands.

4. Do the integration carefully and make sure the starting and ending baselines are flat or horizontal.

5. Do the integration a few times by varying the starting and ending point of each integral, then take the average of the integrals in all trials.