Quantitation in NMR:

Question: What do I need to use for a relaxation delay to obtain quantitative integrations?

Answer: It depends upon how "quantitative" you wish to get, what your excitation pulse-angle is, and on the longest T1 relaxation time in your sample.

If we define "Q" as the "quality" desired for quantitation (1.0 would mean that the steady state magnetization = the equilibrium magnetization...in reality, Q will always be < 1.0), the relationship can be given by:

$$Q = \frac{1 - e^{-Tr/T1}}{1 - \left[e^{-Tr/T1} \cdot Cos(\alpha)\right]}$$

- Tr is the repetition rate (Acquisition time + Relaxation Delay). On the Varian instrument, Tr = at + d1
- α is the excitation pulse angle. On the Varian instrument, the command "pw(α)" will set the angle to α.

An easier (more convenient) form of the above equation is:

$$Tr = -\ln\left(\frac{1 - Q}{1 - Q \cdot Cos(\alpha)}\right) \cdot T1$$

Using this equation, you can decide on the "quality" of integrations (based on relative relaxation rates), estimate the longest T1 in your sample, enter the pulse angle (the default in the standard ^1H parameters on our instruments is 30 degrees), and calculate the minimum value of Tr necessary.

Example: We want our integrated intensities to be accurate to within 95% (Q=.95), and we estimate that our T1s would be typical for a non-degassed organic sample (T1=1-3 sec.). Our excitation pulse is 30^0. Using the above equation: Q=.95, T1=3.0, $\alpha=30^0$...

$$Tr = -\ln\left(\frac{1 - .95}{1 - (.95 \cdot Cos(30))}\right) \cdot 3.0$$

This gives Tr = 3.8 Sec.

The default acquisition time is 3.0 sec (at=3.0), so the relaxation delay necessary for 95% relaxation would be 0.8 seconds.