# NMR Parameter Primer

This is a short reference of the Bruker parameters that are most commonly adjusted. The basic parameters are always available to you when using IconNMR, the 2D parameters will be made available in IconNMR if you require them, and the additional parameters are only made available in special cases. All of these parameters (and many, many more) are available when using a system in a manual mode.

## Quick Reference Guide

### Basic Parameters

| | |
|---|---|
| NS | Number of Scans |
| D1 | Relaxation Delay (in seconds) |
| AQ | Acquisition Time (in seconds) |
| O1P | Transmitter Frequency Offset (in ppm) |
| SW | Spectral Width (in ppm) |

### 2D Parameters

| | |
|---|---|
| 2TD | First Dimension Direct Acquire Size of FID (number of points in F2) |
| 1TD | Second Dimension Size of FID (number of points in F1) |
| 1SW | Second Dimension Spectral Width (in ppm) |
| O2P | Frequency Offset of Second Nucleus (center of Second Dimension) |

### Additional Parameters

| | |
|---|---|
| TE | Sample Temperature (in Kelvin) |
| D8 | Mixing Time (in seconds) |
| DS | Number of Dummy Scans Done |
| D19 | WATERGATE Delay (in seconds) |

# Parameter Details

## Basic Parameters

### NS - Number of Scans

This parameter indicates how many spectra will be acquired and added together to produce the final result. The number of scans should be set appropriately for the signals being acquired and in steps that account for the phase cycling of the pulse program being run.

### D1 - Relaxation Delay

This is a delay in seconds between each of the scans. It is important that this delay be long enough to accommodate the system, target, and experiment being done.

### AQ - Acquisition Time

This is the amount of time in seconds that the receiver is acquiring data points for each scan. It is important that this time be appropriate for the system, target, and experiment being done.

### O1P - Transmitter Frequency Offset

This is the center of the frequency range being acquired in the experiment.

### SW - Spectral Width

This is the breadth of the frequency range being acquired in the experiment. It is important to remember that the larger the frequency span, the smaller the time difference between each point acquired. So by increasing the spectral width, the acquisition time will be decreased, as the total number of points acquired is preserved.

## 2D Parameters

### 2TD - First Dimension Direct Acquire Size of FID

This is the number of points acquired in the direct dimension, it is intimately related to the spectral width (SW) and acquisition time (AQ).

### 1TD - Second Dimension Size of FID

This is the number of points acquired in the indirect dimension, it is intimately related to the second dimension spectral width (1SW). This parameter determines your resolution in the indirect dimension, but it must not be too large as the time required to acquire the data is strongly dependent on this parameter. Furthermore, acquiring too long in the indirect dimension will result in data points that bear no signal.

### 1SW - Second Dimension Spectral Width

This is the breadth of the frequency range being indirectly acquired.

### O2P - Frequency Offset of Second Nucleus

This is the offset for the rf being applied to the second nucleus.  It determines where the decoupling and the indirect dimension are centered.

## Additional Parameters

You may not have some (or any) of these parameters available to you initially.  Should you require a parameter not in your current profile, please talk to the staff for additional details.

### TE - Sample Temperature

Make damn sure your solvent can take it!

### D8 - Mixing Time

Most sequences with a mixing time (like NOESY and HOESY) use D8 as the variable for that mixing time, which is in seconds.  The mixing time can have a dramatic effect on the resulting spectrum, and needs to be set intelligently and with care.

### DS - Dummy Scans

These are iterations of the pulse sequence that are done, but not acquired.  The goal of dummy scans is to bring the system to a pseudo equilibrium in which there is enough repeatable signal to successfully perform the experiment without waiting for the spins to fully return to thermal equilibrium.

### D19 - WATERGATE Delay

This delay may be set to optimize the water-suppressed signal from a WATERGATE experiment.  The WATERGATE does produce additional nulls beyond those on resonance.  If these happen to fall in an area of interest, you should move them with this delay as $1/(2\nu_N)$ - where $\nu_N$ is the frequency spacing between the nulls (in Hertz).  Do not forget that this delay (like all delays) is in seconds.

# Conversion Guide

For those users that are more familiar with one vendor, this is a quick parameter matching between Bruker and Varian.

| Bruker | | Varian |
|---|---|---|
| NS | = | nt |
| D1 | = | d1 |
| AQ | = | at |
| O1P | = | tof |
| SW | ≈ | sw |
| 2TD | = | np |
| 1TD | = | np1 |
| 1SW | = | sw1 |
| O2P | = | dof |
| TE | = | temp |
| D8 | = | mixN |
| DS | = | ss |
| D18 | = | wgtau |