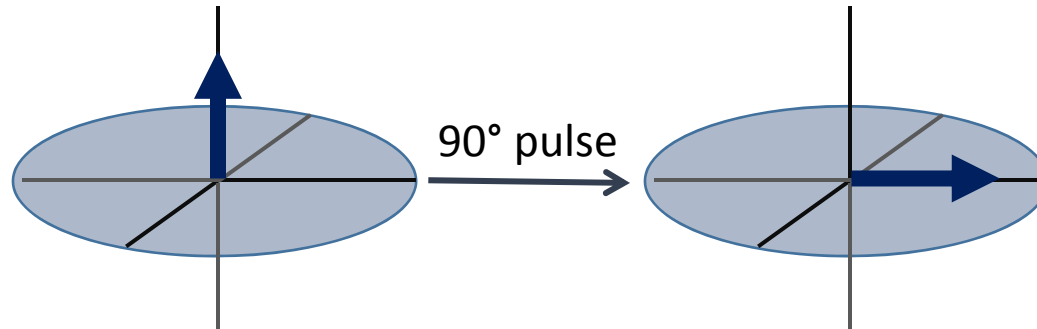


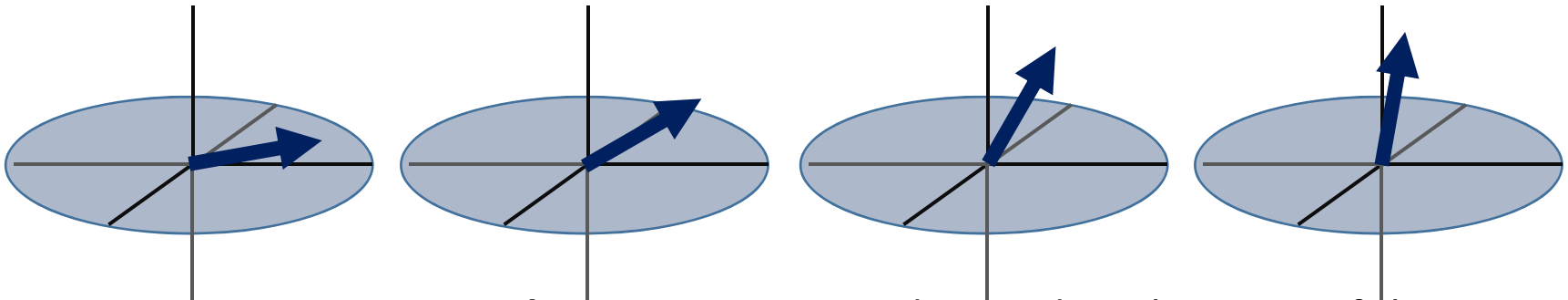
# Relaxation Measurements



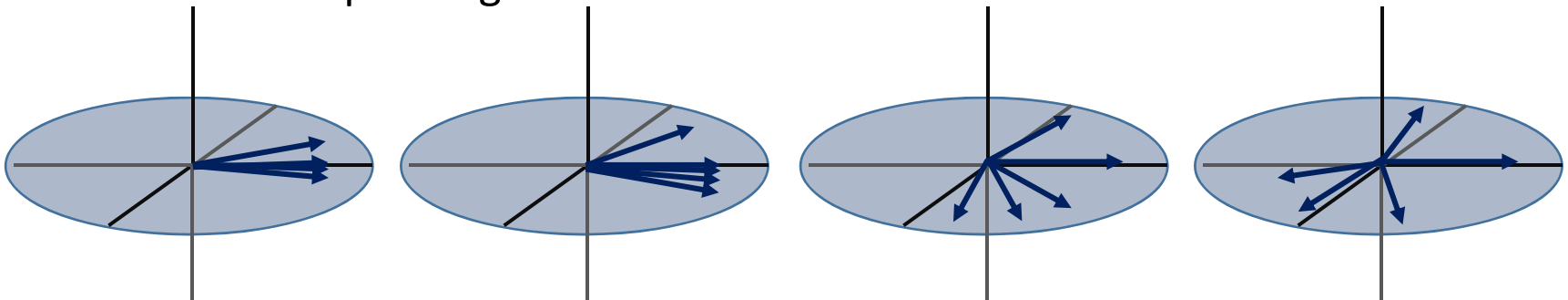
# Two Relaxation Mechanisms



**T<sub>1</sub>: Spin-lattice or longitudinal relaxation** is the average lifetime of the nuclei in the higher spin state



**T<sub>2</sub>: Spin-spin or transverse relaxation** corresponds to a de-coherence of the transverse nuclear spin magnetization

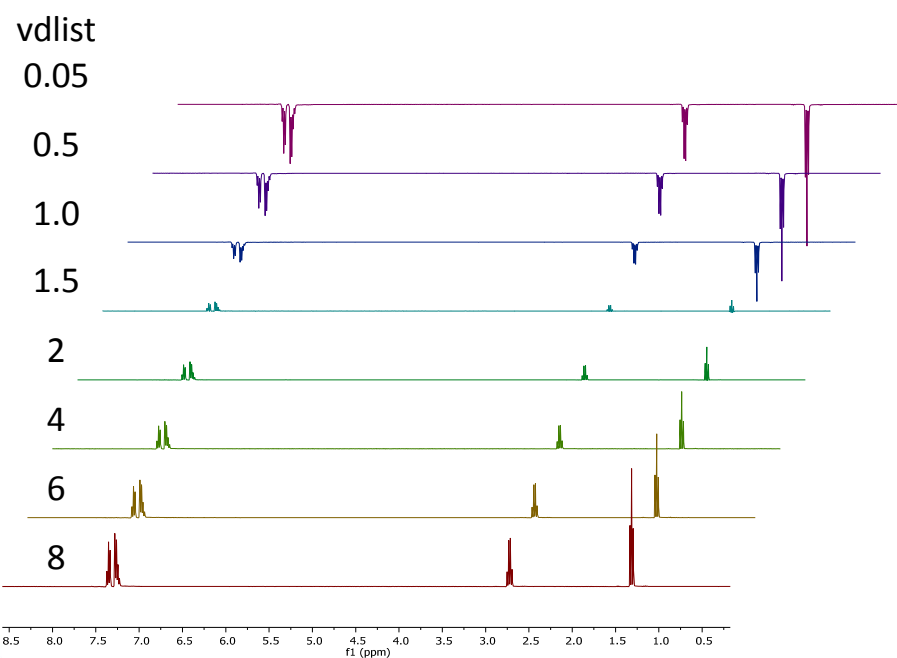
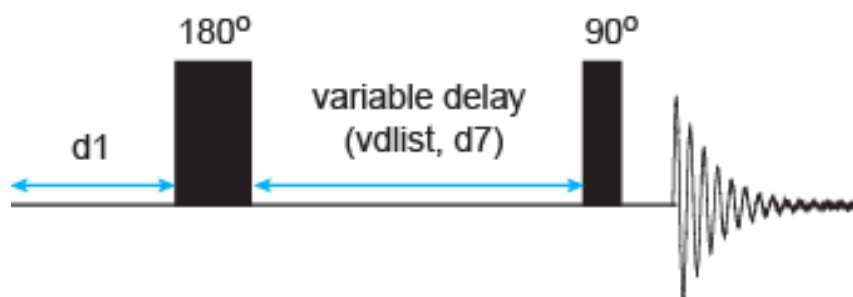


# Spin-Lattice Relaxation Time or $T_1$

- Any factor which slows molecular motion (e.g. increasing solution viscosity, aggregation, or rigidifying the molecule) shortens the spin-lattice relaxation time
- A short  $T_1$  favors sensitivity but too short can result in line broadening and degradation of resolution since  $T_2$  cannot be longer than  $T_1$
- 3 principal magnetic interactions that contribute to  $T_1$  relaxation of spin  $\frac{1}{2}$  nuclei:
  - Dipole-dipole interaction - the nucleus experiences a fluctuating field due to the motions of neighboring dipoles, unpaired electrons, or other nuclei
  - Chemical shift anisotropy - chemical shielding of the nucleus is a function of molecular orientation with respect to  $B_0$  field direction
  - Spin rotation interaction – small magnetic fields are induced at the nucleus as a molecule reorients; this field fluctuates because the motions are not uniform but proceed by a series of small jumps
- Small amounts of paramagnetic substances speed up relaxation
- Inversion recovery experiment measures  $T_1$

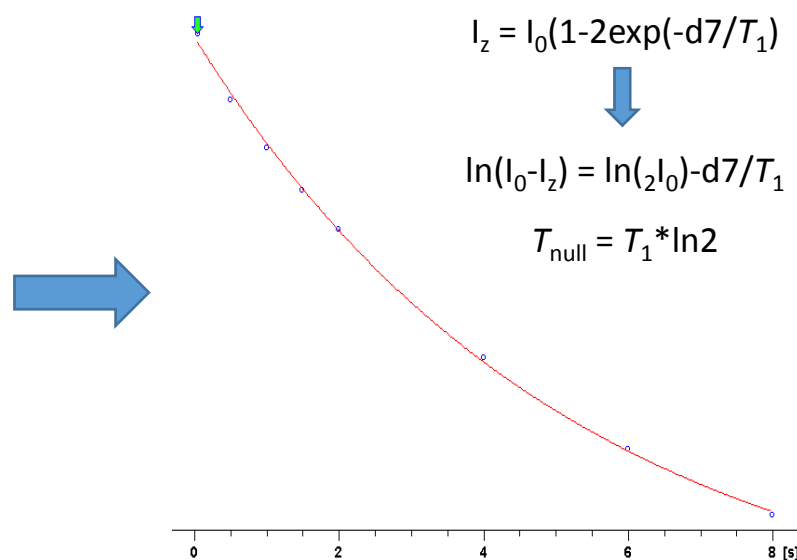


# $T_1$ Measurement: Inversion Recovery



## Parameters to note & Optimize

- To change the value of the delay, **d7**, a variable delay list must be created.
- In the acquisition parameters a VDLIST can be generated which contains values that typically cover a time range which extends past the expected  $T_1$  value.

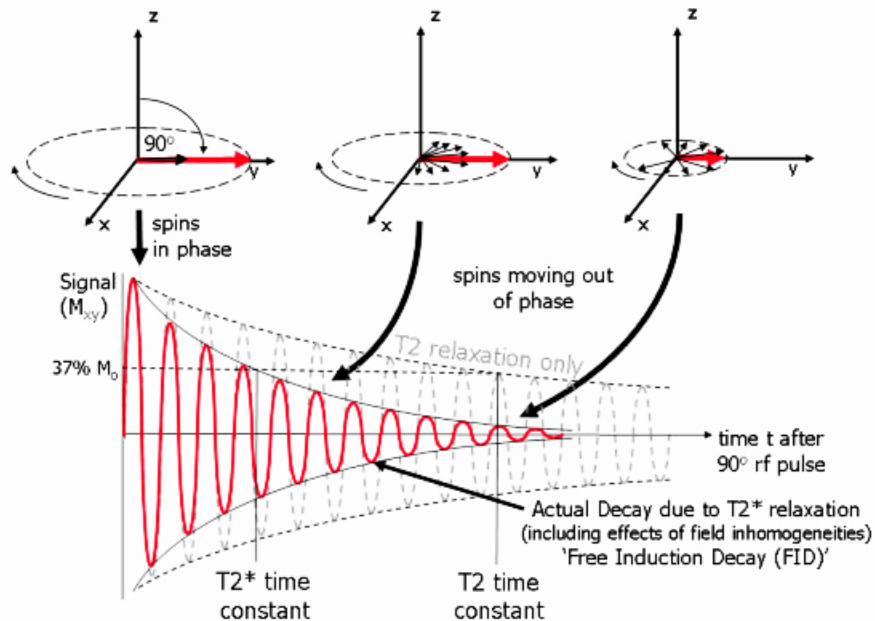
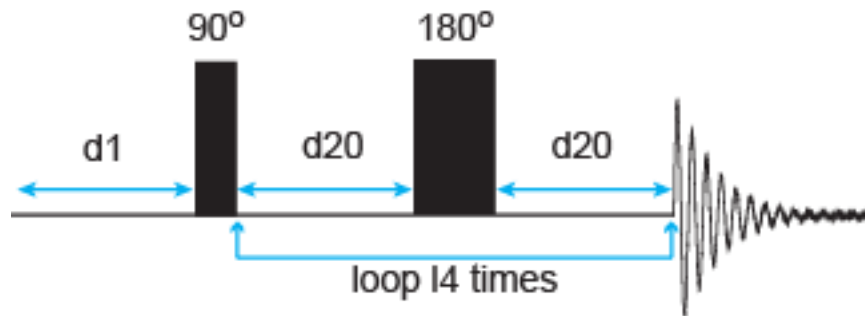


# Spin-Spin Relaxation Time or $T_2$

- $T_1 = T_2$  when molecular tumbling is fast compared with the Larmor frequency; this is the condition for small molecules.
- Mechanisms of spin-spin relaxation:
  - Chemical exchange
  - Scalar spin-spin coupling if modulated at a 'suitable rate'; these are detectable when a  $^1\text{H}$  is coupled to a quadrupolar nuclei such as  $^{14}\text{N}$ ,  $^{35}\text{Cl}$ , or  $^{37}\text{Cl}$
- In a frozen sample, line broadening increases as the result of static dipole-dipole interactions.
- $T_2^*$  describes the magnetization ( $M_y$ ) decay resulting from  $B_0$  inhomogeneity.



# $T_2$ Measurement: CPMG Experiment



```
;cpmg1d
;1D experiment with T2 filter using Carr-Purcell-
Meiboom-Gill sequence
```

```
"p2=p1*2"
"d11=30m"
```

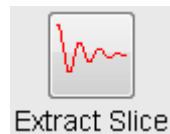
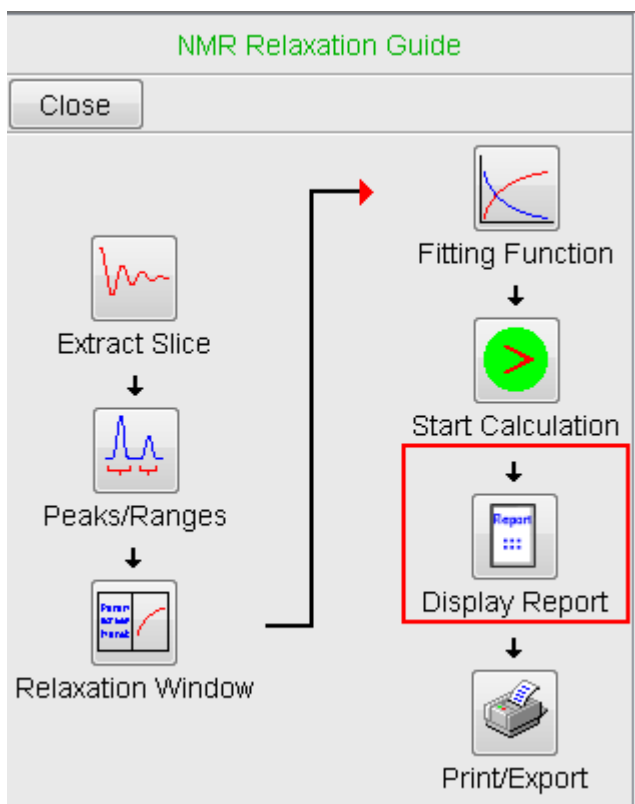
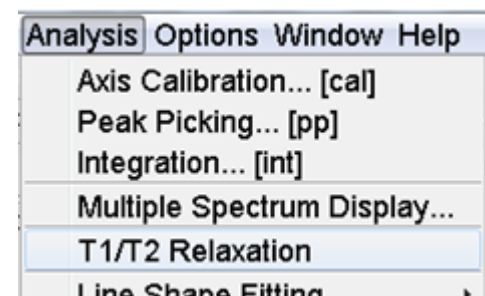
```
1 ze
2 30m
d1
p1 ph1
3 d20
p2 ph2
d20
lo to 3 times l4
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 0 2 2 1 1 3 3
ph2=1 3 1 3 0 2 0 2
ph31=0 0 2 2 1 1 3 3
```

```
; d20: fixed echo time to allow elimination of J-mod.
effects
; d20 should be << 1/J ,but > (50 * P2) [1-2 msec]
;l4: loop for T2 filter [4 - 20]
```

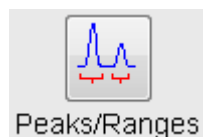


# $T_1$ & $T_2$ Relaxation Analysis



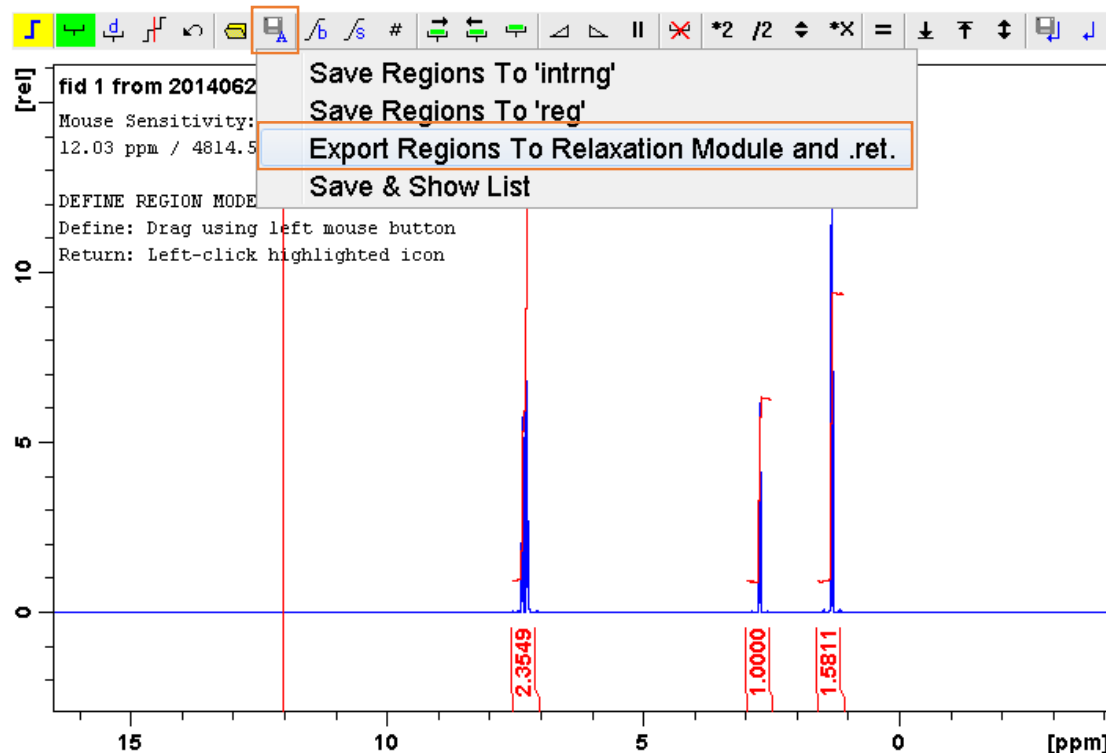
Extract Slice

- 1<sup>st</sup> popup select "FID", 2<sup>nd</sup> popup enter a value of "1"
- This will process all slices based on the first slice.



Peaks/Ranges

- Select "Manual Integration" and integrate regions of interest.
- Once regions are selected, save integrals to the relaxation module through the "Save Region as..." icon (see below).



# $T_1$ & $T_2$ Relaxation Analysis



Relaxation Window



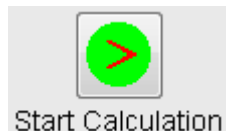
- Will extract integrals and plot for fitting.



Fitting Function




- Select the appropriate function ( $T_1$  or  $T_2$ ) to use in the fit.



Start Calculation



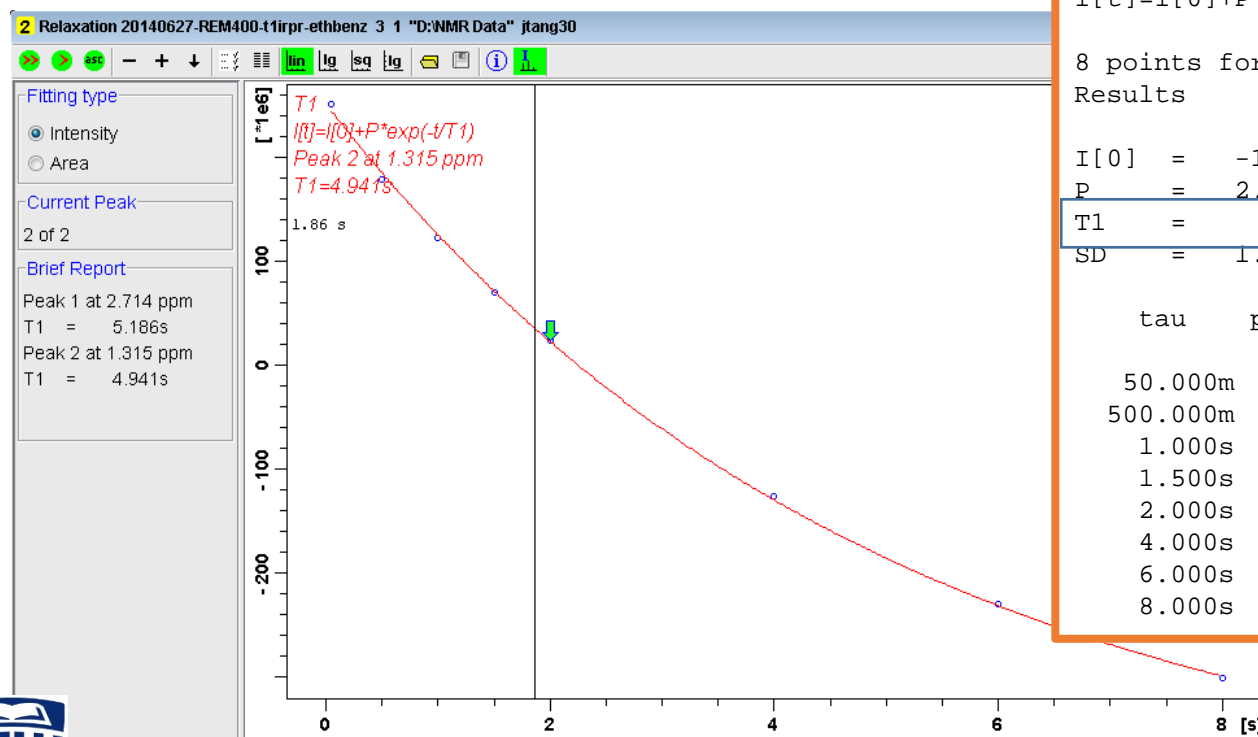
- Calculates relaxation parameter for single site. Click  for all sites.



Display Report



- Creates a relaxation report.



## Relaxation Report

$$I[t] = I[0] + P \cdot \exp(-t/T_1)$$

8 points for Peak 1, Peak Point at 2.714 ppm  
 Results Comp. 1

$$I[0] = -1.488e+000$$

$$P = 2.335e+000$$

$$T_1 = 5.186s$$

$$SD = 1.790e-002$$

tau	ppm	integral	intensity
50.000m	2.714	2.5114e+009	1.0285e+008
500.000m	2.714	1.7393e+009	7.2504e+007
1.000s	2.714	1.1713e+009	5.0455e+007
1.500s	2.714	6.5604e+008	3.0787e+007
2.000s	2.714	1.8077e+008	1.2362e+007
4.000s	2.714	-1.3507e+009	-4.725e+007
6.000s	2.714	-2.4432e+009	-8.9516e+007
8.000s	2.714	-3.2185e+009	-1.2001e+008

