T2 determination

T2 determination is important for you to set up the proper mix time of 2D NMR parameter. **cpmgt2**, a sequence invented by Carr, Purcell, Meiboom and Gill, is used for T2 determination. To do this, please following the steps:

1. calibrate pw90, **pw=pw90** ↵
2. **cpmgt2** ↵
3. click *acqi*, turn off spin (this increase the field in homogeneity , no diffusion)
4. **dg** ↵ (see p1 and pw , p1=2 * pw90, pw=pw90)
5. **d2=0.002** ↵ (for small molecules, d2=0.01, for macromolecules, d2=0.001)
6. **bt=0.004,0.008,0.016,0.032,0.064,0.132,0.264,1,2,4,8** ↵
7. **dg dps** ↵

You will see the pulse sequence which looks like this.
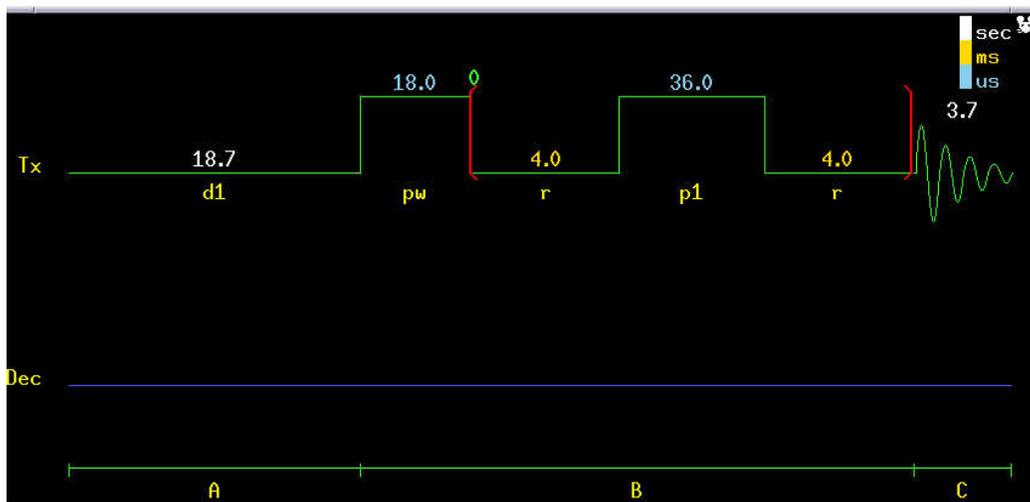
You can not get more info from the above sequence. The lower one can tell you more.
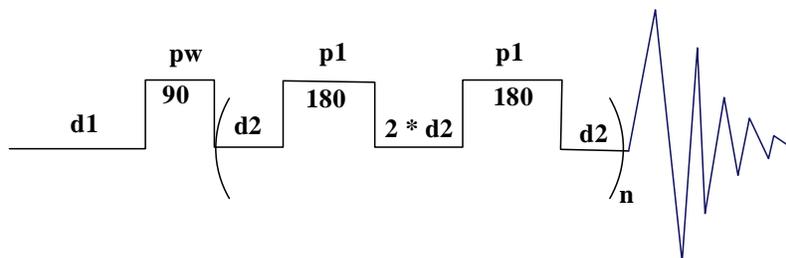
Please note that **d2** is the spin-echo cycle time.
bt is called big tau. **bt=(4*d2)*n**.
big tau (bt) shown on the above picture is the total time for T2 relaxation.

Typically, bt is arrayed for a T2 experiment. If bt is not a multiple of 4*d2, it is rounded automatically by the machine so that it is.

After you type in the **bt** data, the **dg** text window will indicate the parameter **bt** to be **arrayed**(not **0**)

ga ↵
ds(1) ↵
You should get the first spectrum. Phase it and place the *th* somewhere you like.

You can expend the spectrum and select the peaks by adjusting *th*(threshold).
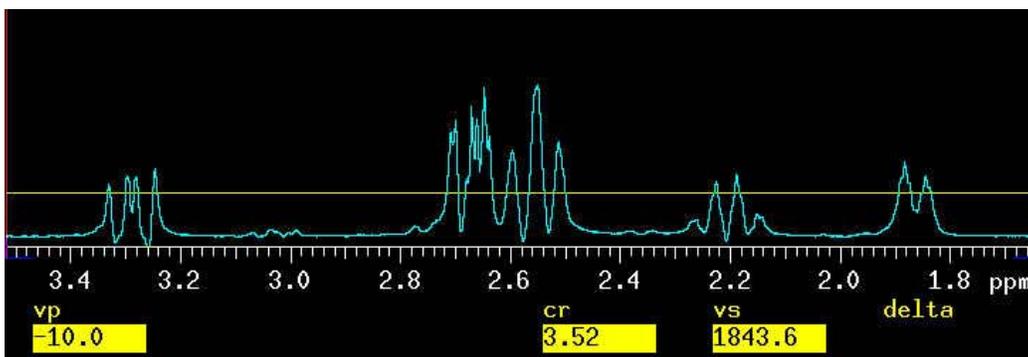
dssa ↵ you will see the following stacked spectra.
dssl ↵ you will number the stacked spectra below from bottom to the top.

vs	sp(ppm)	wp(ppm)	first	last	step
1037.0	0.73	5.18	1	9	1
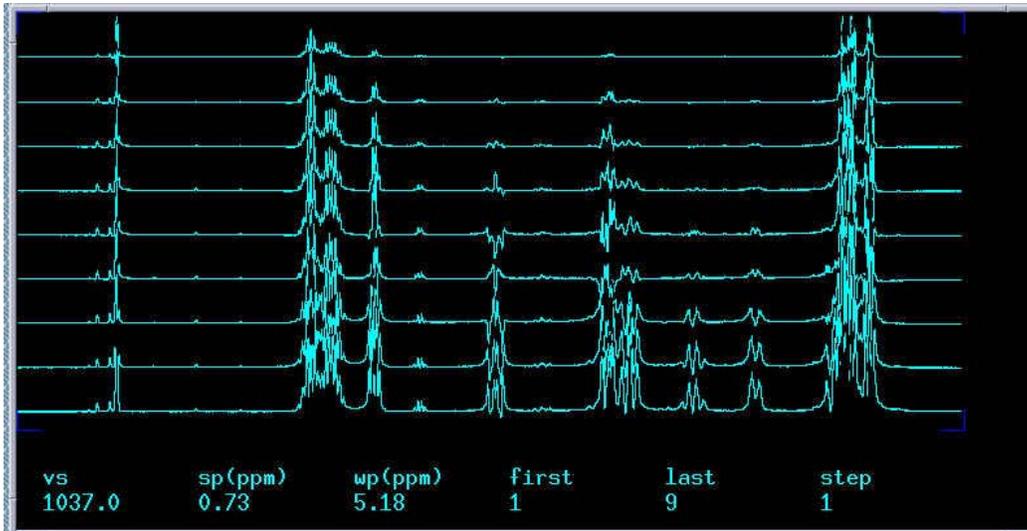
dll ↵ all the peaks above ***th*** will be listed as follows. Select the peaks you like by typying

fp(2, 6, 13, 17) ↵

t2s ↵ tells you the T2 of each peak you selected

t2 ↵ tell you the details of how T2 is calculated.

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     1        3.32962          22.8872  ⎫
     2        3.29676          26.8385  ⎪
     3        3.27894          26.0566  ⎪
     4        3.24608          29.5635  ⎪
     5        2.70751          45.7321  ⎪
     6         2.6986          50.6153  ⎪
     7        2.67855          25.2951  ⎪
     8        2.66963          57.0044  ⎪
     9        2.66017          51.4817  ⎬  Type dll
    10         2.6468          64.8351  ⎪
    11        2.63733          43.9018  ⎪
    12        2.59556          37.6492  ⎪
    13        2.54933          66.3283  ⎪
    14        2.51146           41.157  ⎪
    15        2.22463          24.1457  ⎪
    16        2.18787          27.1884  ⎪
    17        1.88155          32.6477  ⎪
    18        1.84368           26.607  ⎭
Exponential data analysis:

peak              T2              error   ⎫
   2          0.04533          0.02664    ⎪
   6          0.01385          0.008318   ⎬  Type t2s
  13          0.02325          0.005388   ⎪
  15          0.02958          0.002005   ⎪
  17          0.02573          0.004221   ⎭

peak number 2                                       Type t2
  T2 =        0.0453        error =        0.0266
        time        observed      calculated     difference
       0.008         26.840         28.662         -1.822
       0.016         23.060         23.857         -0.797
       0.032         21.780         16.453          5.327
       0.064          9.450          7.595          1.855
       0.136        -12.910          0.723        -13.633
       0.264          6.340         -0.937          7.277
       0.528         -1.070         -1.041         -0.029
       1.056         -0.160         -1.042          0.882
       2.112          0.170         -1.042          1.212

peak number 6
  T2 =        0.0139        error =        0.00832
        time        observed      calculated     difference
       0.008         50.620         53.061         -2.441
       0.016         38.010         32.649          5.361
       0.032         13.320         14.765         -1.445
       0.064        -11.960          7.356        -19.316
       0.136         17.750          6.545         11.205
       0.264         14.430          6.540          7.890
       0.528         10.960          6.540          4.420
       1.056          4.660          6.540         -1.880
       2.112          1.470          6.540         -5.070
```
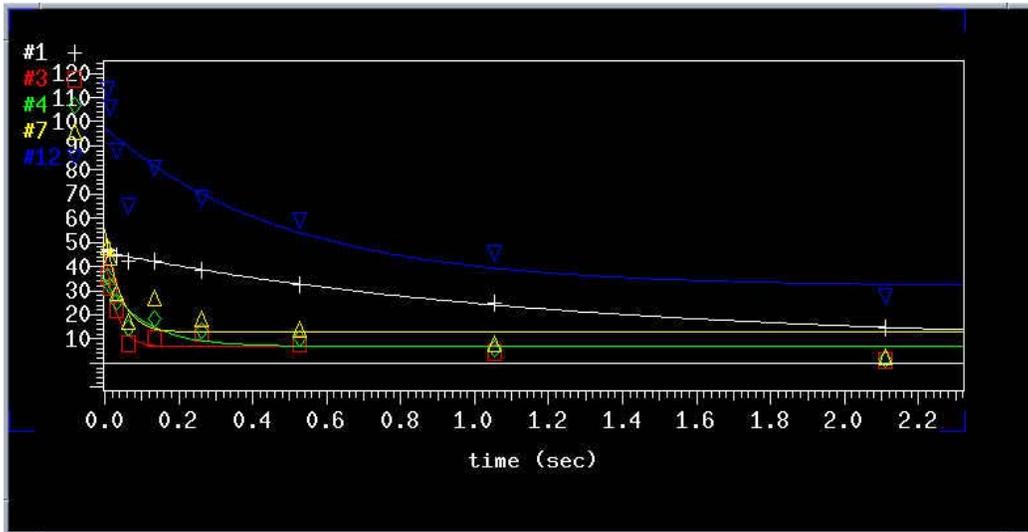
expl ↵
or **expl(2,17)** ↵ This will display the 2nd and the 17th curves.

The following is the curves of the T2 function. T2 is the constant of the equation of the curve.

If you still have problems, ask Anne-Frances. I would be happy if I can help you.