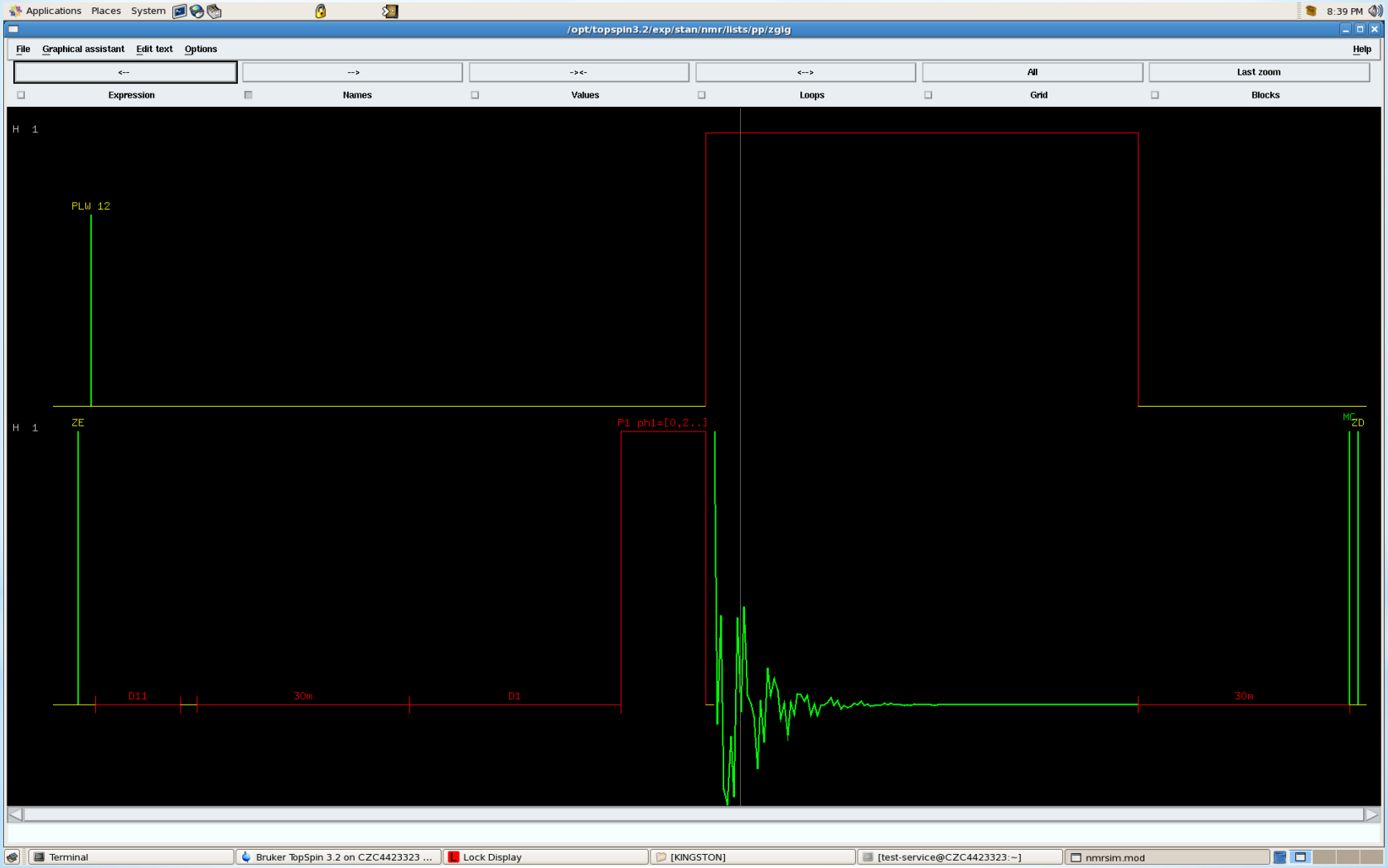
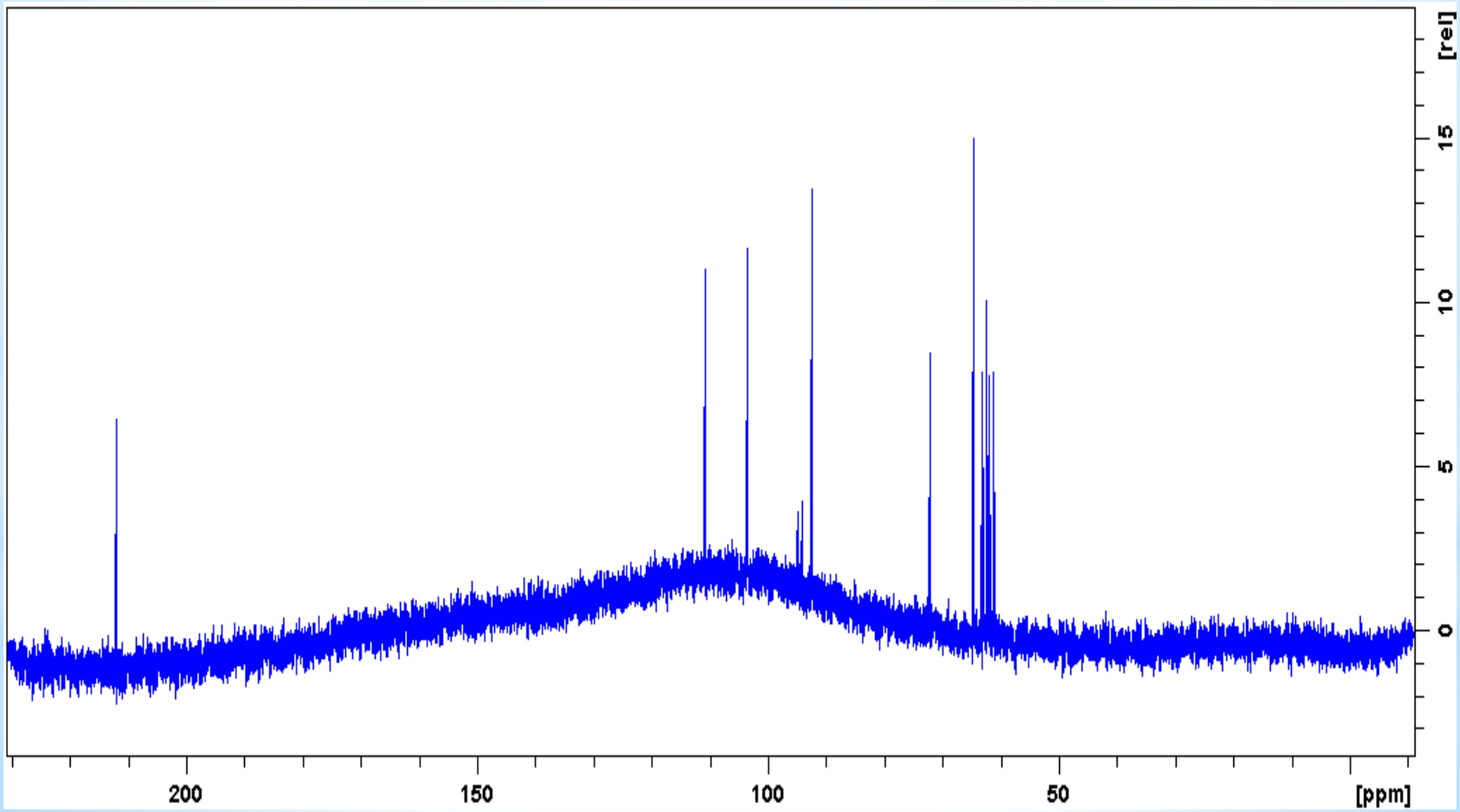
# 1.2 碳谱

zgig:反门控去耦一维碳谱



# 1.2 碳谱

zgig:反门控去耦一维碳谱



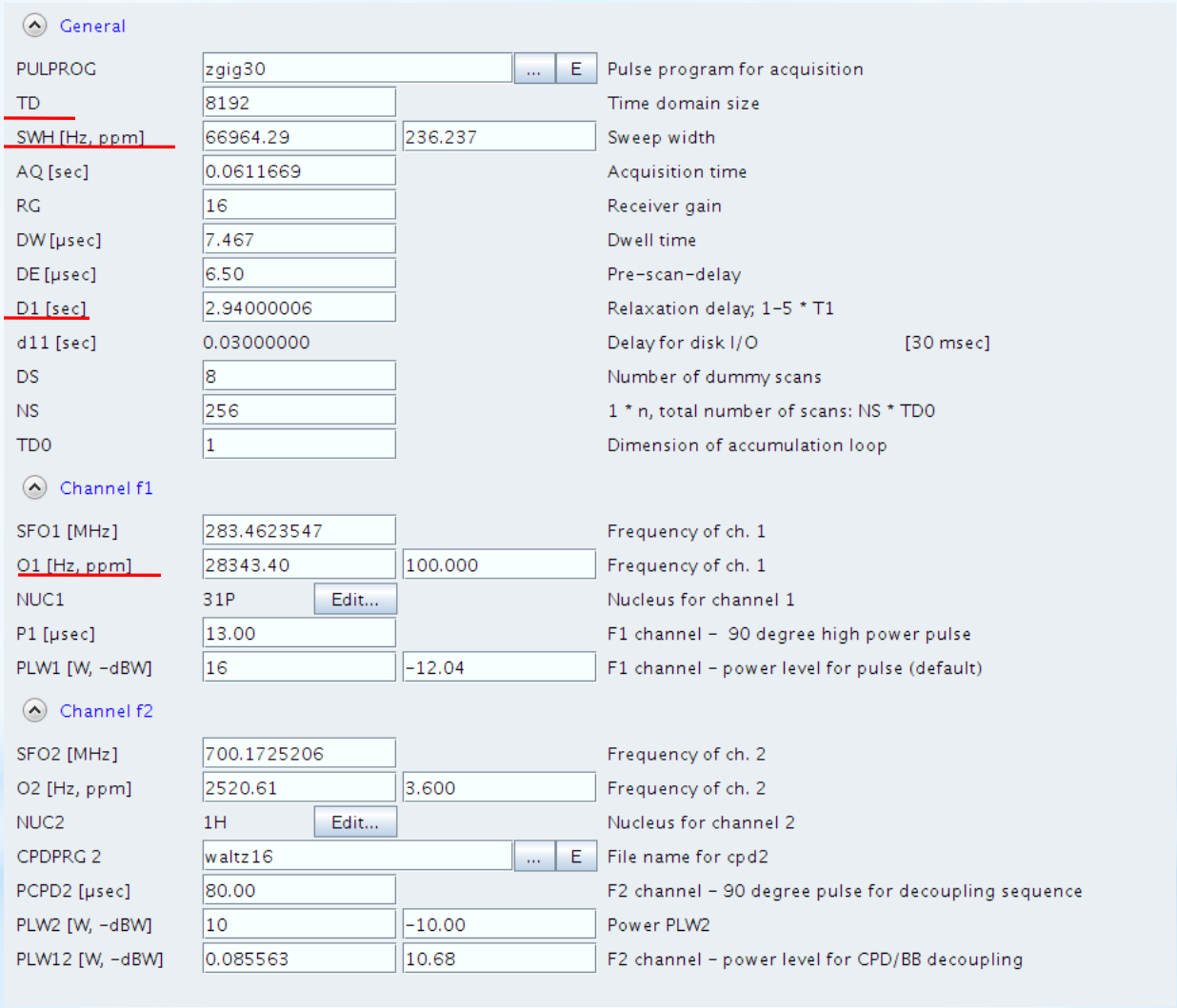
# 1.3磷谱：

| | | |
|---|---|---|
| PULPROG | zgig30 ... E | Current pulse program |
| AQ_mod | DQD | Acquisition mode |
| TD | 8192 | Size of fid |
| DS | 8 | Number of dummy scans |
| NS | 256 | Number of scans |
| TD0 | 1 | Loop count for 'td0' |
| Width | | |
| SW [ppm] | 236.2370 | Spectral width |
| SWH [Hz] | 66964.289 | Spectral width |
| AQ [sec] | 0.0611669 | Acquisition time |
| FIDRES [Hz] | 16.348703 | Fid resolution |
| FW [Hz] | 250000.000 | Filter width |
| Receiver | | |
| RG | 16 | Receiver gain |
| DW [µsec] | 7.467 | Dwell time |
| DWOV [µsec] | 0.025 | Oversampling dwell time |
| DECIM | 298.667 | Decimation rate of digital filter |
| DSPFIRM | sharp(standard) | DSP firmware filter |
| DIGTYP | DRU | Digitizer type |
| DIGMOD | digital | Digitization mode |
| DR | 21 | Digitizer resolution |
| DDR | 9 | Digital digitizer resolution |
| DE [µsec] | 6.50 | Pre-scan delay |
| HPPRGN | normal | Preamplifier gain |
| PRGAIN | high | High power preamplifier gain |
| DQDMODE | add | Digital quad detection mode |
| PH_ref [degree] | 0 | Receiver phase correction |

# 1.3磷谱:

| | | | |
|---|---|---|---|
| NUC1 | 31P | Edit... | Observe nucleus |
| O1 [Hz] | 28343.40 | | Transmitter frequency offset |
| O1P [ppm] | 100.000 | | Transmitter frequency offset |
| SFO1 [MHz] | 283.4623547 | | Transmitter frequency |
| BF1 [MHz] | 283.4340113 | | Basic transmitter frequency |
| Nucleus 2 | | | |
| NUC2 | 1H | Edit... | 2nd nucleus |
| O2 [Hz] | 2520.61 | | Frequency offset of 2nd nucleus |
| O2P [ppm] | 3.600 | | Frequency offset of 2nd nucleus |
| SFO2 [MHz] | 700.1725206 | | Frequency of 2nd nucleus |
| BF2 [MHz] | 700.1700000 | | Basic frequency of 2nd nucleus |

# 1.3磷谱：



General

| | | | |
|---|---|---|---|
| PULPROG | zgig30 ... E | | Pulse program for acquisition |
| TD | 8192 | | Time domain size |
| SWH [Hz, ppm] | 66964.29 | 236.237 | Sweep width |
| AQ [sec] | 0.0611669 | | Acquisition time |
| RG | 16 | | Receiver gain |
| DW [µsec] | 7.467 | | Dwell time |
| DE [µsec] | 6.50 | | Pre-scan-delay |
| D1 [sec] | 2.94000006 | | Relaxation delay; 1-5 * T1 |
| d11 [sec] | 0.03000000 | | Delay for disk I/O [30 msec] |
| DS | 8 | | Number of dummy scans |
| NS | 256 | | 1 * n, total number of scans: NS * TD0 |
| TD0 | 1 | | Dimension of accumulation loop |

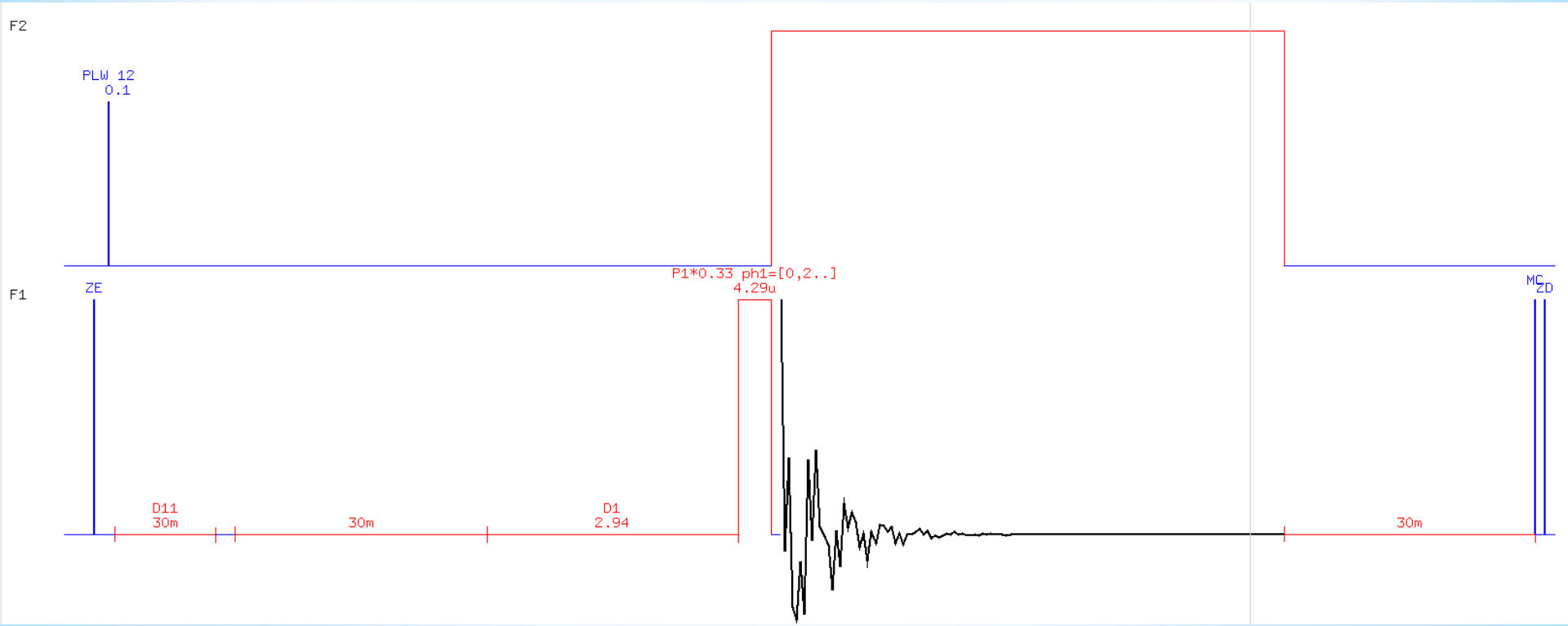
Channel f1

| | | | |
|---|---|---|---|
| SFO1 [MHz] | 283.4623547 | | Frequency of ch. 1 |
| O1 [Hz, ppm] | 28343.40 | 100.000 | Frequency of ch. 1 |
| NUC1 | 31P Edit... | | Nucleus for channel 1 |
| P1 [µsec] | 13.00 | | F1 channel - 90 degree high power pulse |
| PLW1 [W, -dBW] | 16 | -12.04 | F1 channel - power level for pulse (default) |

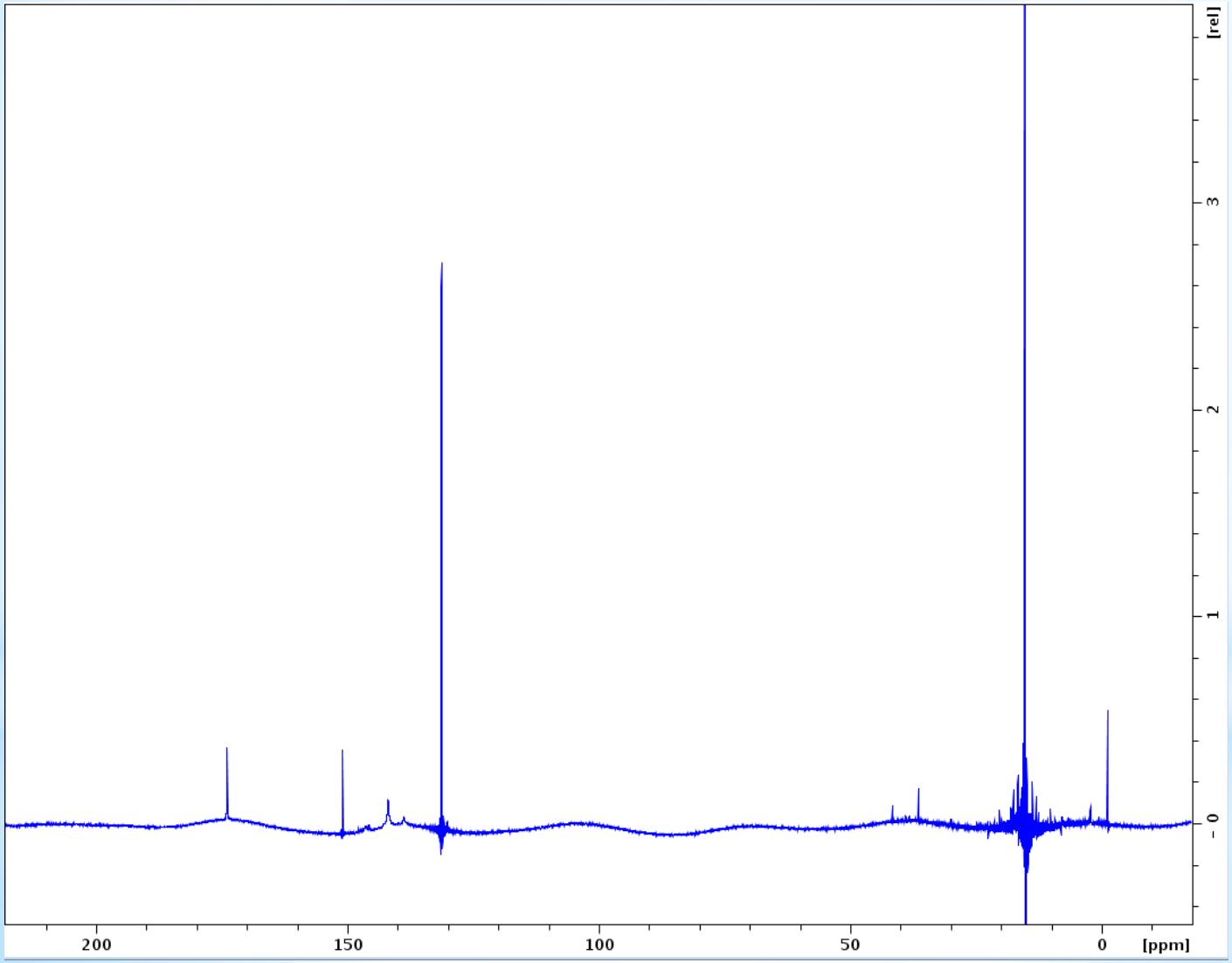
Channel f2

| | | | |
|---|---|---|---|
| SFO2 [MHz] | 700.1725206 | | Frequency of ch. 2 |
| O2 [Hz, ppm] | 2520.61 | 3.600 | Frequency of ch. 2 |
| NUC2 | 1H Edit... | | Nucleus for channel 2 |
| CPDPRG 2 | waltz16 ... E | | File name for cpd2 |
| PCPD2 [µsec] | 80.00 | | F2 channel - 90 degree pulse for decoupling sequence |
| PLW2 [W, -dBW] | 10 | -10.00 | Power PLW2 |
| PLW12 [W, -dBW] | 0.085563 | 10.68 | F2 channel - power level for CPD/BB decoupling |

# 1.3磷谱:

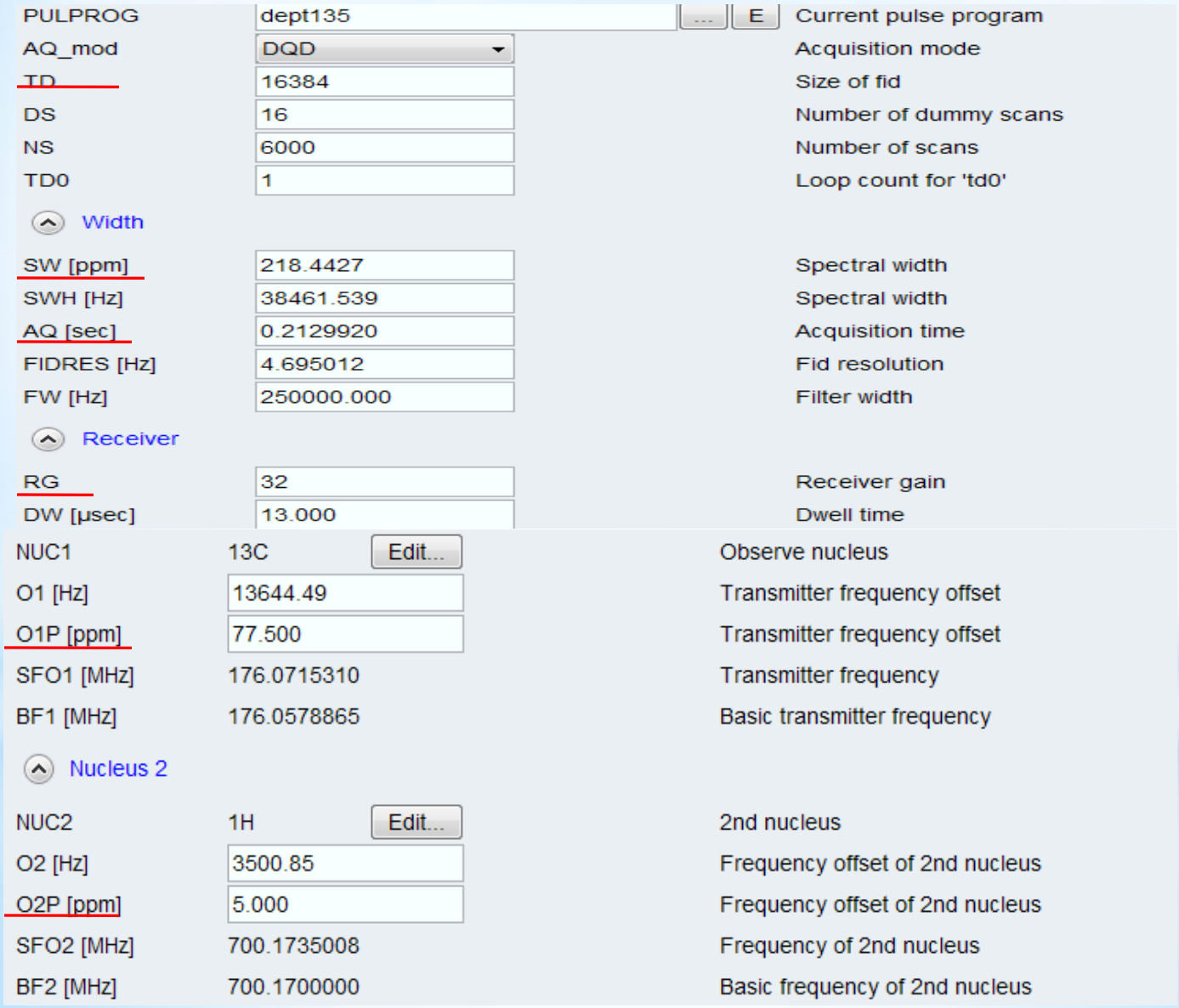


# 1.3磷谱:



# 1.4 DEPT:

所有与氢相关的碳的检测。Dept45除季碳外的所有碳都出现，为正峰；dept90只出现CH；dept135中CH,$CH_3$朝上，$CH_2$朝下；

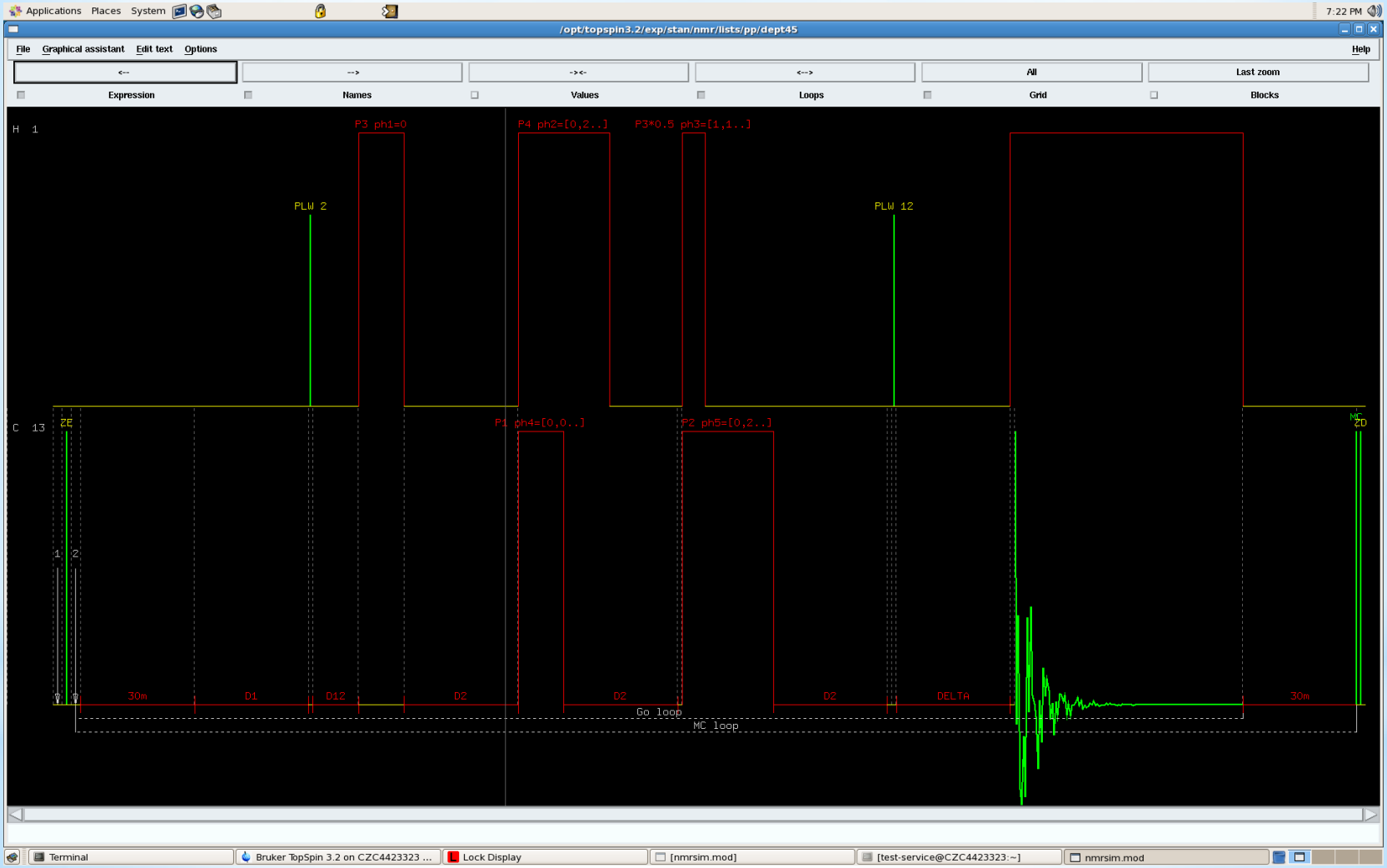


| | | | |
|---|---|---|---|
| PULPROG | dept135 | ... E | Current pulse program |
| AQ_mod | DQD | | Acquisition mode |
| TD | 16384 | | Size of fid |
| DS | 16 | | Number of dummy scans |
| NS | 6000 | | Number of scans |
| TD0 | 1 | | Loop count for 'td0' |
| Width | | | |
| SW [ppm] | 218.4427 | | Spectral width |
| SWH [Hz] | 38461.539 | | Spectral width |
| AQ [sec] | 0.2129920 | | Acquisition time |
| FIDRES [Hz] | 4.695012 | | Fid resolution |
| FW [Hz] | 250000.000 | | Filter width |
| Receiver | | | |
| RG | 32 | | Receiver gain |
| DW [µsec] | 13.000 | | Dwell time |
| NUC1 | 13C | Edit... | Observe nucleus |
| O1 [Hz] | 13644.49 | | Transmitter frequency offset |
| O1P [ppm] | 77.500 | | Transmitter frequency offset |
| SFO1 [MHz] | 176.0715310 | | Transmitter frequency |
| BF1 [MHz] | 176.0578865 | | Basic transmitter frequency |
| Nucleus 2 | | | |
| NUC2 | 1H | Edit... | 2nd nucleus |
| O2 [Hz] | 3500.85 | | Frequency offset of 2nd nucleus |
| O2P [ppm] | 5.000 | | Frequency offset of 2nd nucleus |
| SFO2 [MHz] | 700.1735008 | | Frequency of 2nd nucleus |
| BF2 [MHz] | 700.1700000 | | Basic frequency of 2nd nucleus |

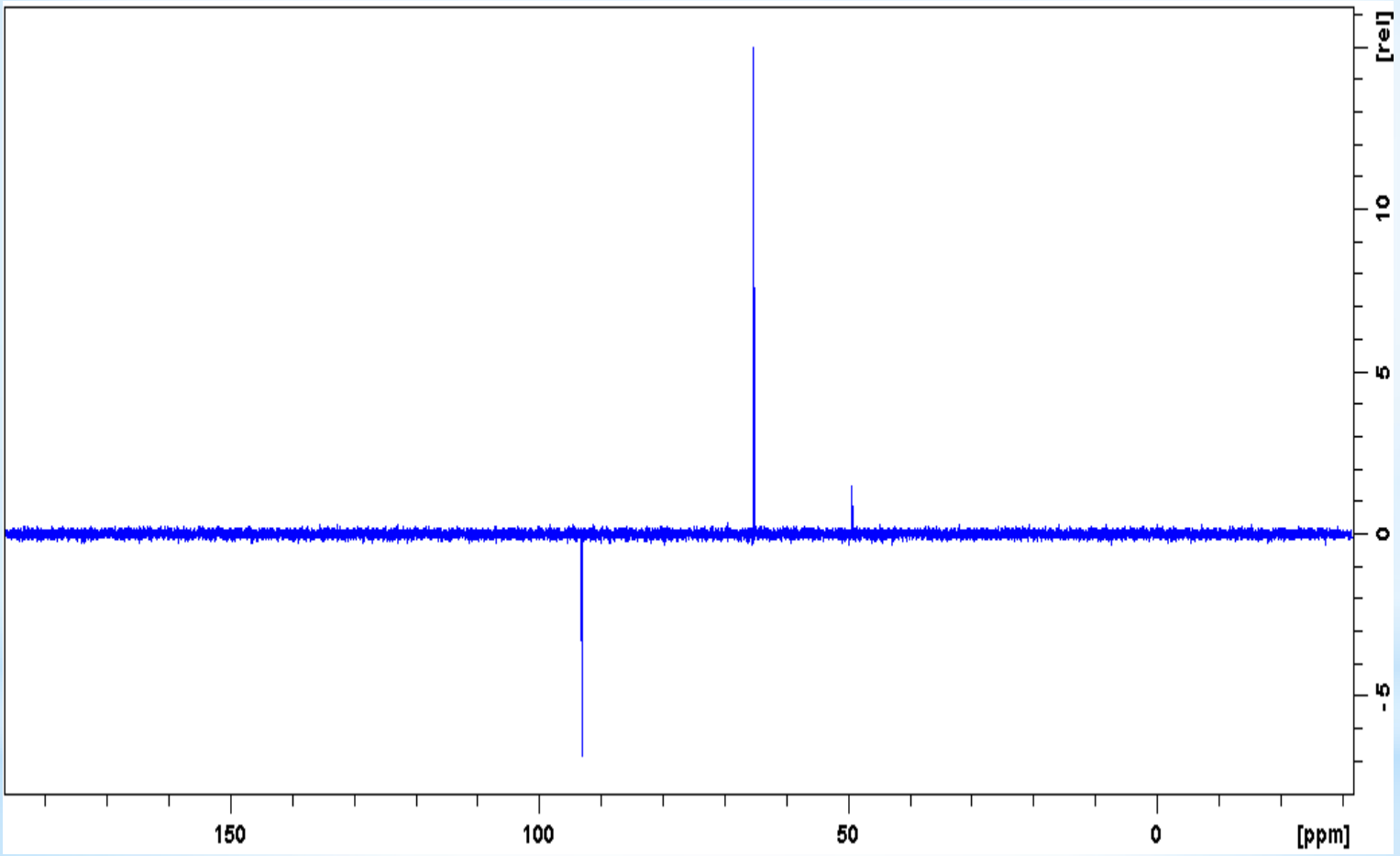
# 1.4 DEPT:

| | | | |
|---|---|---|---|
| PULPROG | dept135 ... E | | Pulse program for acquisition |
| TD | 16384 | | Time domain size |
| SWH [Hz, ppm] | 38461.54 | 218.443 | Sweep width |
| AQ [sec] | 0.2129920 | | Acquisition time |
| RG | 32 | | Receiver gain |
| DW [µsec] | 13.000 | | Dwell time |
| DE [µsec] | 18.00 | | Pre-scan-delay |
| CNST2 | 140.0000000 | | = J(XH) |
| D1 [sec] | 4.00000000 | | Relaxation delay; 1-5 * T1 |
| d2 [sec] | 0.00357143 | | 1/(2J(XH)) |
| d12 [sec] | 0.00002000 | | Delay for power switching [20 usec] |
| DELTA [sec] | 0.00001477 | | DELTA=p1*4/3.1416 |
| DS | 16 | | 8 |
| NS | 6000 | | 4 * n, total number of scans: NS * TD0 |
| TD0 | 1 | | Dimension of accumulation loop |
| Channel f1 | | | |
| SFO1 [MHz] | 176.0715310 | | Frequency of ch. 1 |
| O1 [Hz, ppm] | 13644.49 | 77.500 | Frequency of ch. 1 |
| NUC1 | 13C Edit... | | Nucleus for channel 1 |
| P1 [µsec] | 11.60 | | F1 channel - 90 degree high power pulse |
| p2 [µsec] | 23.20 | | F1 channel - 180 degree high power pulse |
| PLW1 [W, -dBW] | 100 | -20.00 | F1 channel - power level for pulse (default) |
| Channel f2 | | | |
| SFO2 [MHz] | 700.1735008 | | Frequency of ch. 2 |
| O2 [Hz, ppm] | 3500.85 | 5.000 | Frequency of ch. 2 |
| NUC2 | 1H Edit... | | Nucleus for channel 2 |
| CPDPRG 2 | waltz16 ... E | | File name for cpd2 |

# 1.4 DEPT:


Applications Places System
7:22 PM
/opt/topspin3.2/exp/stan/nmr/lists/pp/dept45
File Graphical assistant Edit text Options Help
<-- --> ->|<- <--> All Last zoom
Expression Names Values Loops Grid Blocks
H 1
P3 ph1=0
P4 ph2=[0,2..]
P3*0.5 ph3=[1,1..]
PLW 2
PLW 12
C 13
ZE
P1 ph4=[0,0..]
P2 ph5=[0,2..]
MC
2D
1 2
30m
D1
D12
D2
D2
D2
DELTA
30m
Go loop
MC loop
Terminal
Bruker TopSpin 3.2 on CZC4423323 ...
Lock Display
[nmrsim.mod]
[test-service@CZC4423323:~]
nmrsim.mod

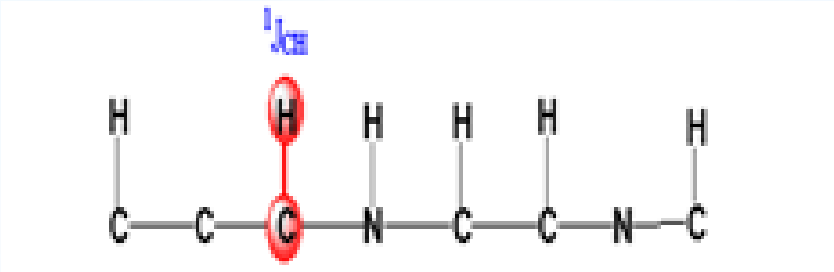
# 1.4 DEPT:



# 2.1 异核相关谱

$^{13}C$-$^{1}H$ HSQC：

异核单量子相关谱，示意图如下：



# 2.1 异核相关谱

$^{13}C$-$^{1}H$ HSQC：

| | | | |
|---|---|---|---|
| PULPROG | hsqcetgpsisp2.2 ... E | | Current pulse program |
| AQ_mod | DQD | | Acquisition mode |
| FnMODE | | Echo-Antiecho | Acquisition mode for 2D, 3D etc. |
| FnTYPE | traditional(planes) | | nD acquisition mode for 3D etc. |
| TD | 1400 | 512 | Size of fid |
| DS | 64 | | Number of dummy scans |
| NS | 16 | | Number of scans |
| TD0 | 1 | | Loop count for 'td0' |
| Width | | | |
| SW [ppm] | 12.0220 | 220.0044 | Spectral width |
| SWH [Hz] | 8417.509 | 38736.996 | Spectral width |
| IN_F [µsec] | | 25.82 | Increment for delay |
| AQ [sec] | 0.0831600 | 0.0066087 | Acquisition time |
| FIDRES [Hz] | 12.025012 | 151.316391 | Fid resolution |
| FW [Hz] | 125000.000 | | Filter width |
| Receiver | | | |
| RG | 64 | | Receiver gain |
| DW [µsec] | 59.400 | | Dwell time |
| DWOV [µsec] | 0.025 | | Oversampling dwell time |
| DECIM | 2376 | | Decimation rate of digital filter |
| DSPFIRM | sharp(standard) | | DSP firmware filter |
| DIGTYP | DRU | | Digitizer type |
| DIGMOD | digital | | Digitization mode |
| DR | 22 | | Digitizer resolution |
| DDR | 10 | | Digital digitizer resolution |
| DE [µsec] | 10.00 | | Pre-scan delay |
| NBL | 1 | | Number of blocks (of acquisition memory) |

# 2.1 异核相关谱

$^{13}C$-$^{1}H$ HSQC：

| | | | | |
|---|---|---|---|---|
| PULPROG | hsqcetgpsisp2.2 | ... E | Pulse program for acquisition | |
| TD | 1400 | | Time domain size | |
| SWH [Hz, ppm] | 8417.51 | 12.022 | Sweep width | |
| AQ [sec] | 0.0831600 | | Acquisition time | |
| RG | 64 | | Receiver gain | |
| DW [µsec] | 59.400 | | Dwell time | |
| DE [µsec] | 10.00 | | Pre-scan-delay | |
| CNST2 | 145.0000000 | | = J(XH) | |
| CNST17 | -0.5000000 | | = -0.5 for Crp60comp.4 | |
| d0 [sec] | 0.00000300 | | Incremented delay (2D) | [3 usec] |
| D1 [sec] | 0.50000000 | | Relaxation delay; 1-5 * T1 | |
| d4 [sec] | 0.00172414 | | 1/(4J)XH | |
| d11 [sec] | 0.03000000 | | Delay for disk I/O | [30 msec] |
| D16 [sec] | 0.00020000 | | Delay for homospoil/gradient recovery | |
| D24 [sec] | 0.00086207 | | 1/(8J)XH for all multiplicities | |
| DELTA [sec] | 0.00121720 | | DELTA=p16+d16+p2+d0*2-4u | |
| DELTA1 [sec] | 0.00121207 | | DELTA1=p16+d16-p1*0.78+de+8u | |
| DELTA2 [sec] | 0.00147014 | | DELTA2=d4-larger(p2,p14)/2-4u | |
| DELTA3 [sec] | 0.00055807 | | DELTA3=d24-cnst17*p24/2-p19-d16-4u | |
| DELTA4 [sec] | 0.00027014 | | DELTA4=d4-larger(p2,p14)/2-p16-d16-4u | |
| DS | 64 | | >= 16 | |
| in0 [sec] | 0.00001290 | | 1/(2 * SW(X)) = DW(X) | |
| INF1 [µsec] | 25.80 | | 1/SW(X) = 2 * DW(X) | |
| NS | 16 | | 1 * n | |
| Channel f1 | | | | |
| SFO1 [MHz] | 700.1740610 | | Frequency of ch. 1 | |
| O1 [Hz, ppm] | 4060.99 | 5.800 | Frequency of ch. 1 | |

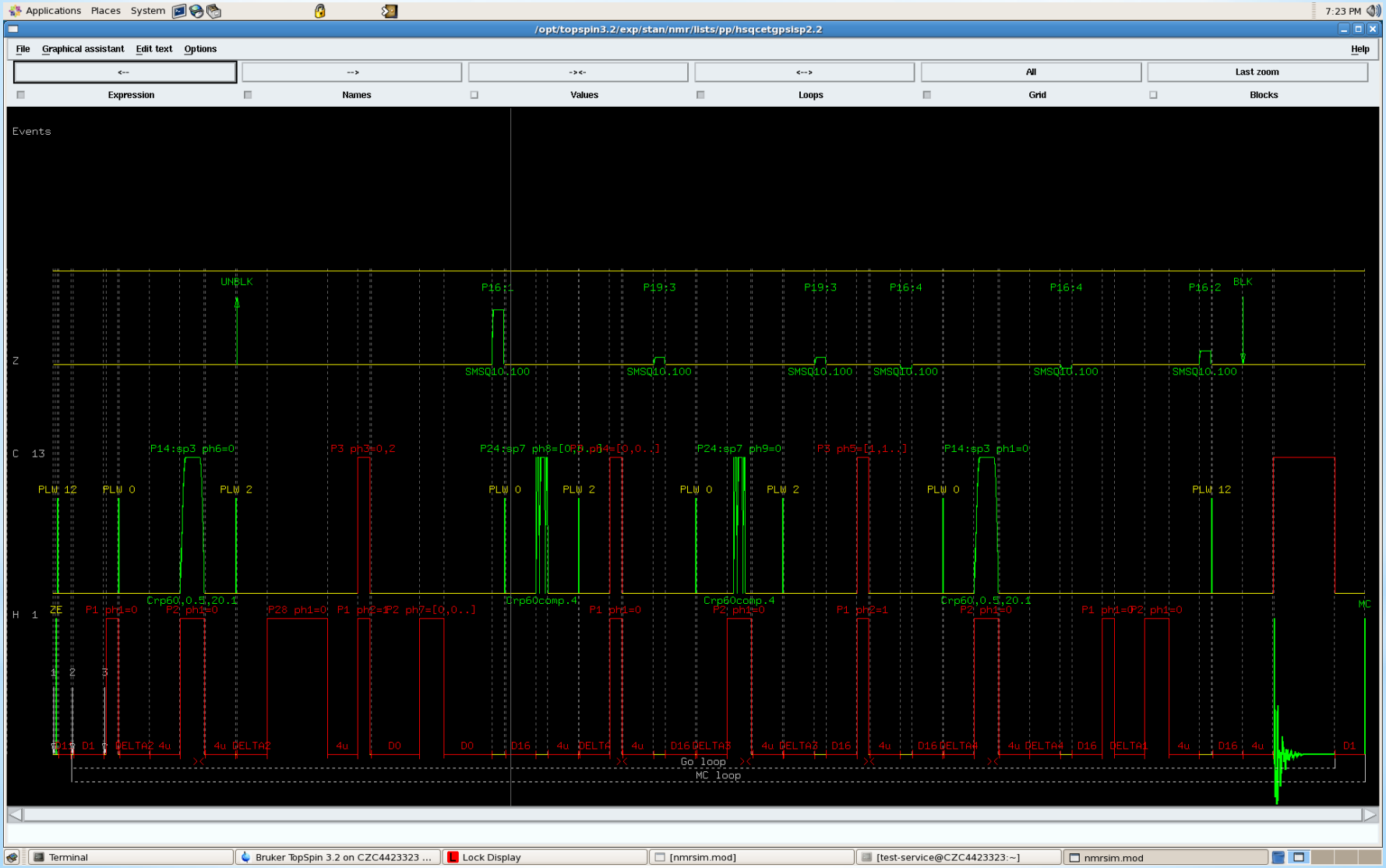
# 2.1 异核相关谱

$^{13}C$-$^{1}H$ HSQC：

```
ph1=0
ph2=1
ph3=0 2
ph4=0 0 2 2
ph5=1 1 3 3
ph6=0
ph7=0 0 2 2
ph8=0 0 2 2
ph9=0
ph31=0 2 2 0
```

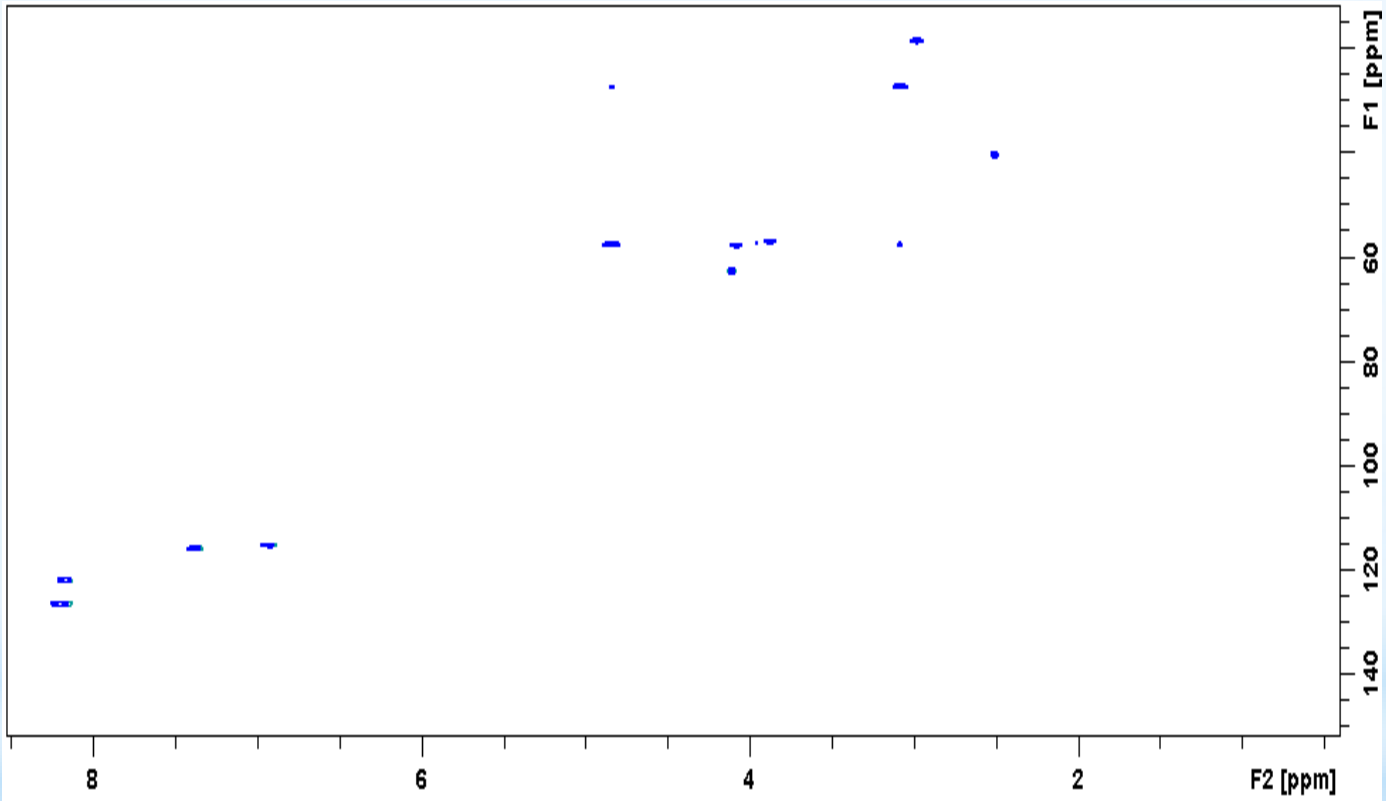
# 2.1 异核相关谱

## $^{13}C$-$^{1}H$ HSQC：



# 2.1 异核相关谱

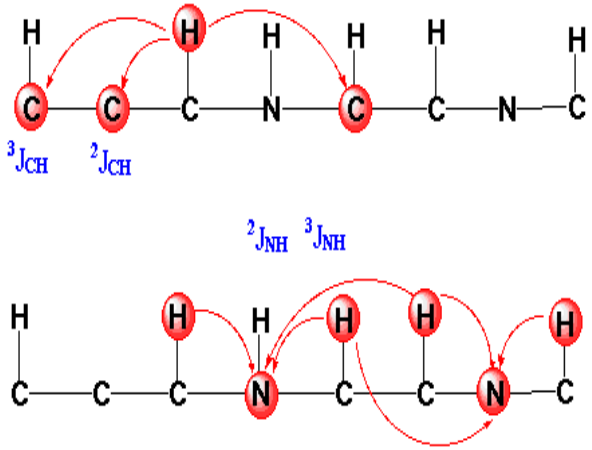
$^{13}C$-$^{1}H$ HSQC：



# 2.1 异核相关谱

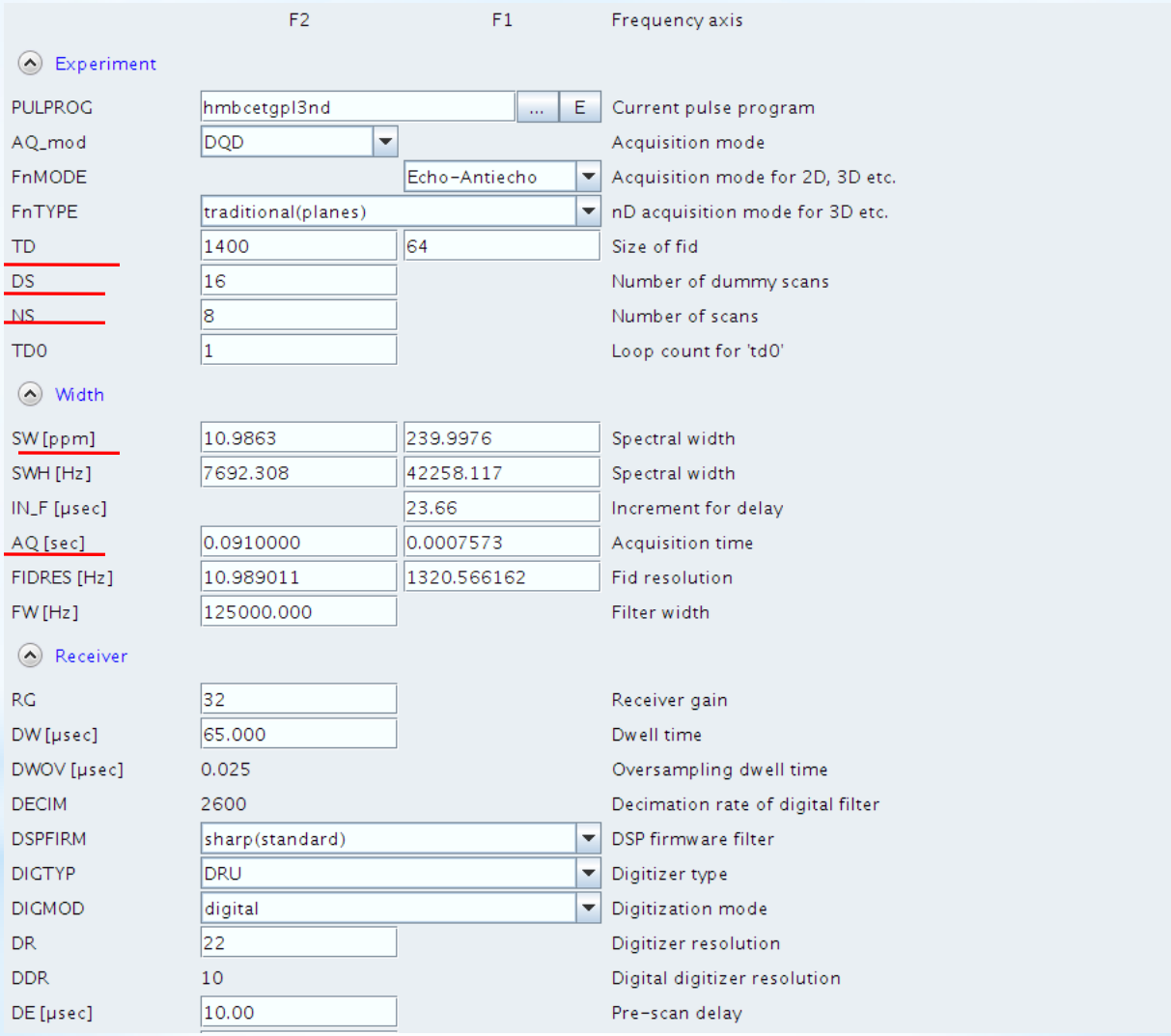
HMBC：

通过二键、三键甚至更多键相连的碳氢相关，是有机化合物结构阐述最重要的二维核磁技术，对于季碳的指认以及分子结构中各片段之间的连接方式的确认起着不可替代的作用，示意图如下：



# 2.1 异核相关谱

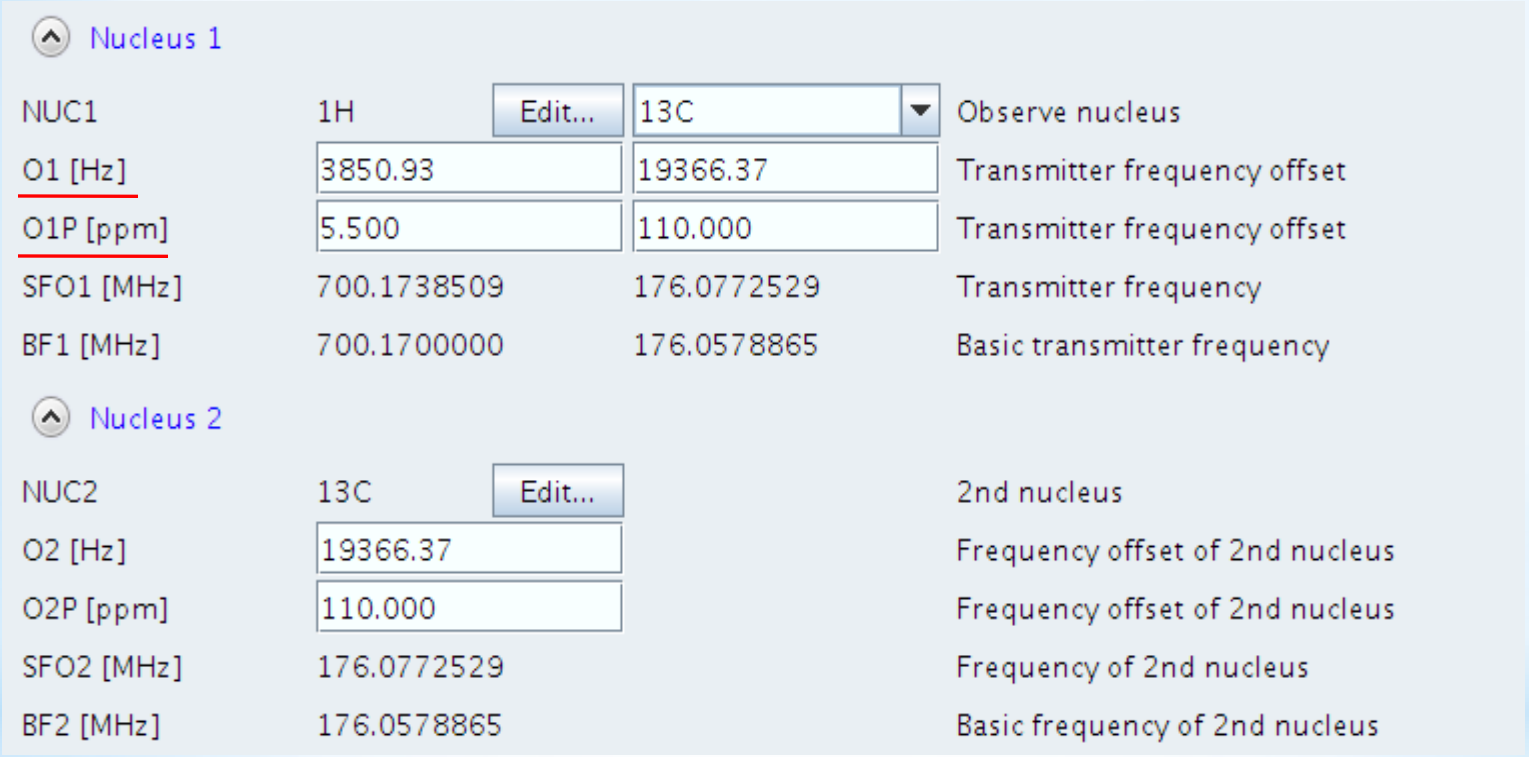
HMBC：



| | F2 | F1 | Frequency axis |
|---|---|---|---|
| **Experiment** | | | |
| PULPROG | hmbcetgpl3nd ... E | | Current pulse program |
| AQ_mod | DQD | | Acquisition mode |
| FnMODE | | Echo-Antiecho | Acquisition mode for 2D, 3D etc. |
| FnTYPE | traditional(planes) | | nD acquisition mode for 3D etc. |
| TD | 1400 | 64 | Size of fid |
| DS | 16 | | Number of dummy scans |
| NS | 8 | | Number of scans |
| TD0 | 1 | | Loop count for 'td0' |
| **Width** | | | |
| SW [ppm] | 10.9863 | 239.9976 | Spectral width |
| SWH [Hz] | 7692.308 | 42258.117 | Spectral width |
| IN_F [µsec] | | 23.66 | Increment for delay |
| AQ [sec] | 0.0910000 | 0.0007573 | Acquisition time |
| FIDRES [Hz] | 10.989011 | 1320.566162 | Fid resolution |
| FW [Hz] | 125000.000 | | Filter width |
| **Receiver** | | | |
| RG | 32 | | Receiver gain |
| DW [µsec] | 65.000 | | Dwell time |
| DWOV [µsec] | 0.025 | | Oversampling dwell time |
| DECIM | 2600 | | Decimation rate of digital filter |
| DSPFIRM | sharp(standard) | | DSP firmware filter |
| DIGTYP | DRU | | Digitizer type |
| DIGMOD | digital | | Digitization mode |
| DR | 22 | | Digitizer resolution |
| DDR | 10 | | Digital digitizer resolution |
| DE [µsec] | 10.00 | | Pre-scan delay |

# 2.1 异核相关谱

HMBC：



Nucleus 1

| | | | | |
|---|---|---|---|---|
| NUC1 | 1H | Edit... | 13C | Observe nucleus |
| O1 [Hz] | 3850.93 | | 19366.37 | Transmitter frequency offset |
| O1P [ppm] | 5.500 | | 110.000 | Transmitter frequency offset |
| SFO1 [MHz] | 700.1738509 | | 176.0772529 | Transmitter frequency |
| BF1 [MHz] | 700.1700000 | | 176.0578865 | Basic transmitter frequency |

Nucleus 2

| | | | |
|---|---|---|---|
| NUC2 | 13C | Edit... | 2nd nucleus |
| O2 [Hz] | 19366.37 | | Frequency offset of 2nd nucleus |
| O2P [ppm] | 110.000 | | Frequency offset of 2nd nucleus |
| SFO2 [MHz] | 176.0772529 | | Frequency of 2nd nucleus |
| BF2 [MHz] | 176.0578865 | | Basic frequency of 2nd nucleus |

# 2.1 异核相关谱

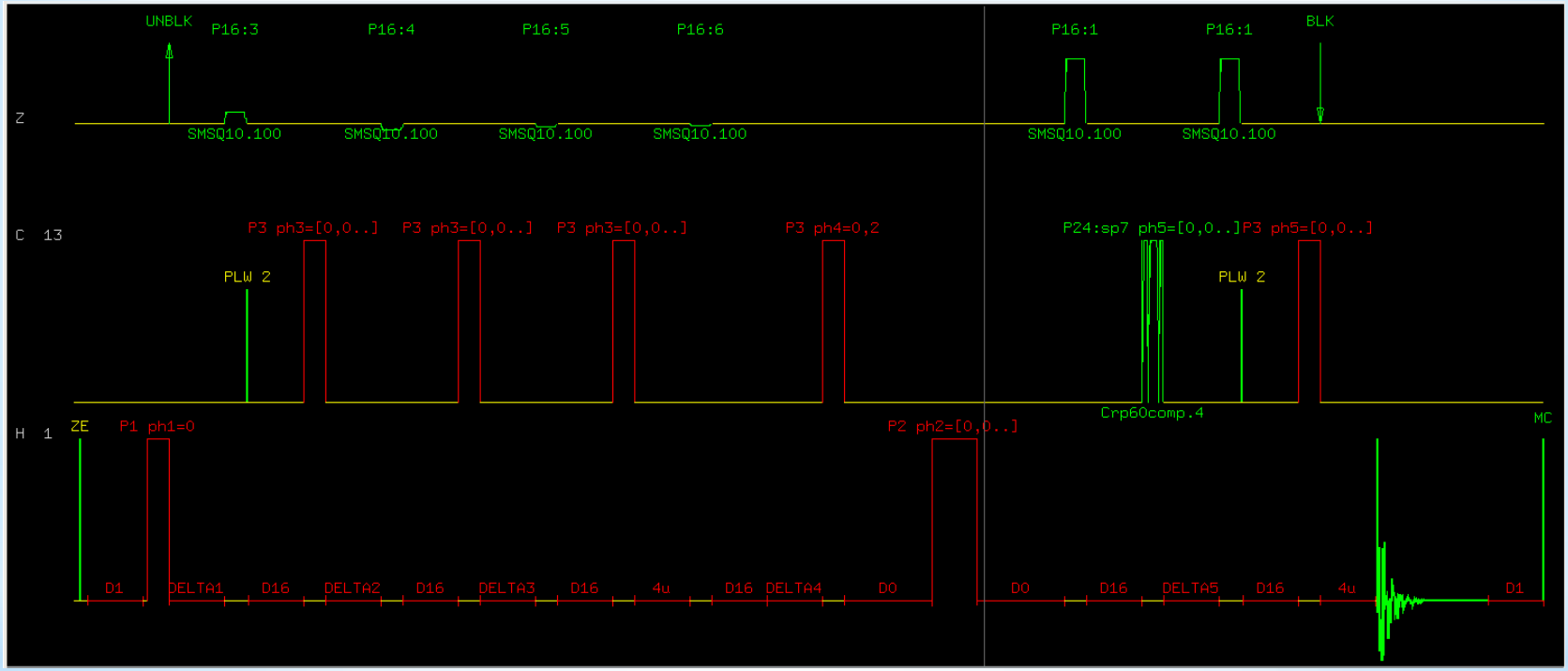
HMBC：

| | | | |
|---|---|---|---|
| PULPROG | hmbcetgpl3nd ... E | | Pulse program for acquisition |
| TD | 1400 | | Time domain size |
| SWH [Hz, ppm] | 7692.31 | 10.9863 | Sweep width |
| AQ [sec] | 0.0910000 | | Acquisition time |
| RG | 32 | | Receiver gain |
| DW [µsec] | 65.000 | | Dwell time |
| DE [µsec] | 10.00 | | Pre-scan-delay |
| CNST6 | 120.0000000 | | = 1J(XH)min |
| CNST7 | 170.0000000 | | = 1J(XH)max |
| CNST13 | 8.0000000 | | = J(XH) long range |
| cnst30 | 0.598112 | | cnst30=(1-sfo2/sfo1)/(1+sfo2/sfo1) |
| d0 [sec] | 0.00000300 | | Incremented delay (2D) [3 usec] |
| D1 [sec] | 2.00000000 | | Relaxation delay; 1-5 * T1 |
| d6 [sec] | 0.06250000 | | Delay for evolution of long range couplings (1/2Jlr) |
| D16 [sec] | 0.00020000 | | Delay for homospoil/gradient recovery |
| DELTA1 [sec] | 0.00284858 | | DELTA1=1s/(2 * (cnst6 + 0.07 * (cnst7-cnst6) ) ) -p16-d16 |
| DELTA2 [sec] | 0.00224828 | | DELTA2=1s/(cnst7 + cnst6) -p16-d16 |
| DELTA3 [sec] | 0.00180300 | | DELTA3=1s/(2 * (cnst7 - 0.07 * (cnst7-cnst6) ) ) -p16-d16 |
| DELTA4 [sec] | 0.06129600 | | DELTA4=d6-p16-d16-4u |
| DELTA5 [sec] | 0.00002110 | | DELTA5=p2+d0*2 |
| DS | 16 | | 16 |
| in0 [sec] | 0.00001180 | | 1/(2 * SW(X)) = DW(X) |
| INF1 [µsec] | 23.60 | | 1/SW(X) = 2 * DW(X) |
| NS | 8 | | 2 * n |
| Channel f1 | | | |
| SFO1 [MHz] | 700.1738509 | | Frequency of ch. 1 |
| O1 [Hz, ppm] | 3850.93 | 5.500 | Frequency of ch. 1 |

# 2.1 异核相关谱

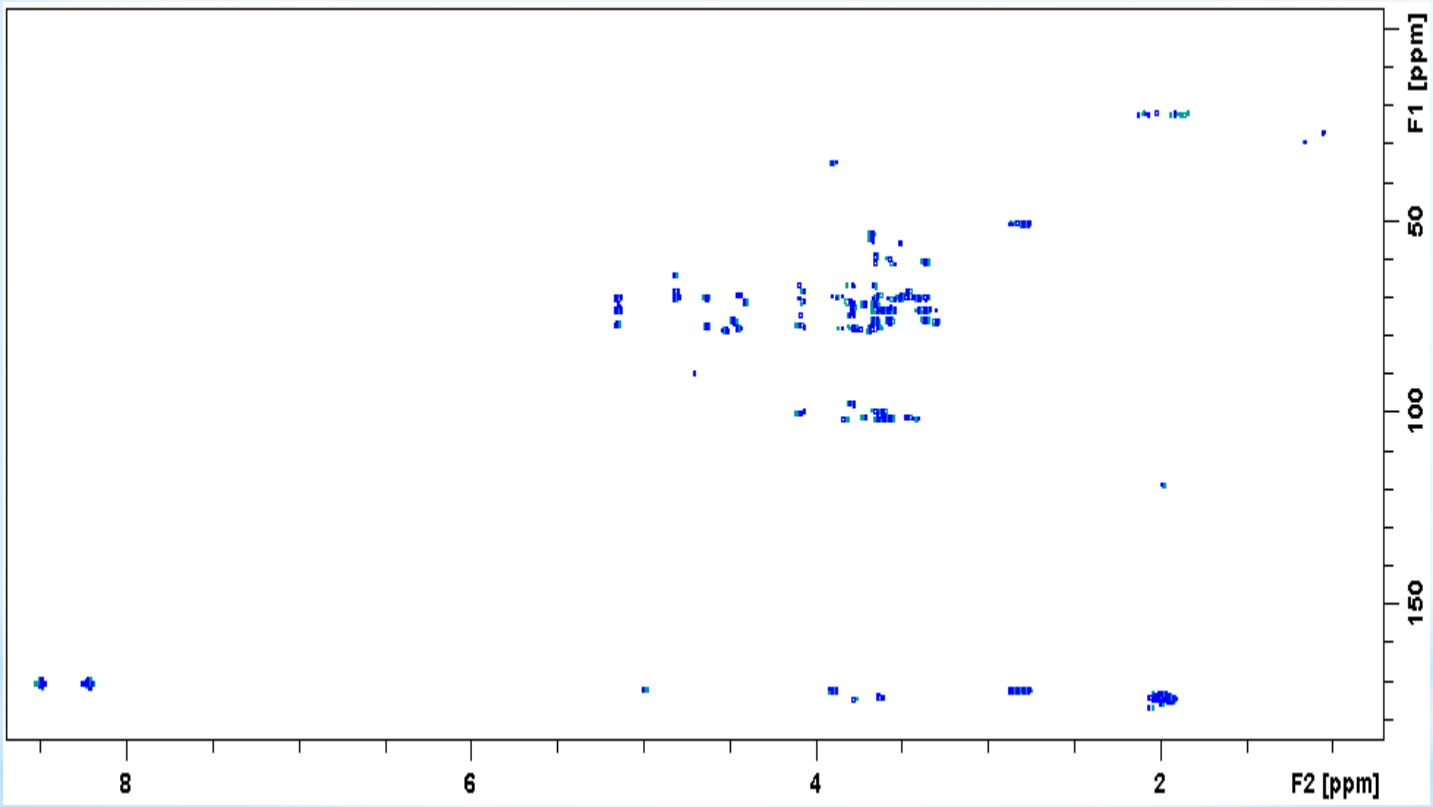
HMBC：

对应的脉冲序列如下图所示：



# 2.1 异核相关谱

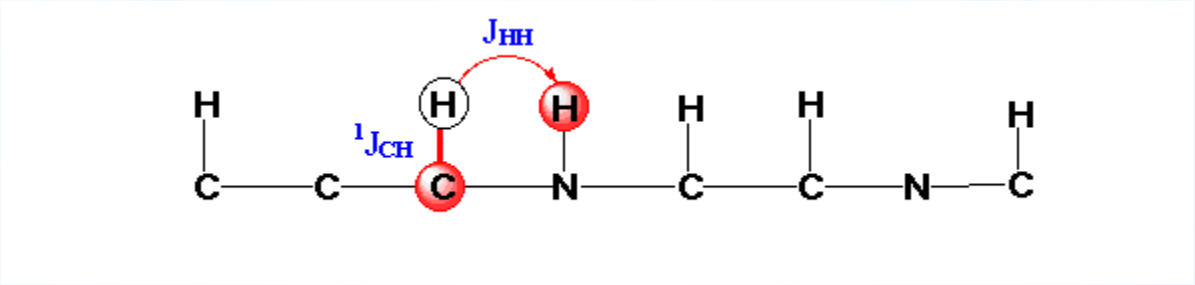
HMBC：



# 2.1 异核相关谱

H2BC：

选择性检测二键相连的碳氢相关



# 2.1 异核相关谱

H2BC：

| | | | |
|---|---|---|---|
| PULPROG | h2bcetgpl3 ... E | | Current pulse program |
| AQ_mod | DQD | | Acquisition mode |
| FnMODE | | Echo-Antiecho | Acquisition mode for 2D, 3D etc. |
| FnTYPE | traditional(planes) | | nD acquisition mode for 3D etc. |
| TD | 1400 | 64 | Size of fid |
| DS | 16 | | Number of dummy scans |
| NS | 8 | | Number of scans |
| TD0 | 1 | | Loop count for 'td0' |
| Width | | | |
| SW [ppm] | 10.9863 | 239.9976 | Spectral width |
| SWH [Hz] | 7692.308 | 42258.117 | Spectral width |
| IN_F [µsec] | | 23.66 | Increment for delay |
| AQ [sec] | 0.0910000 | 0.0007573 | Acquisition time |
| FIDRES [Hz] | 10.989011 | 1320.566162 | Fid resolution |
| FW [Hz] | 125000.000 | | Filter width |
| Receiver | | | |
| RG | 32 | | Receiver gain |
| DW [µsec] | 65.000 | | Dwell time |
| DWOV [µsec] | 0.025 | | Oversampling dwell time |
| DECIM | 2600 | | Decimation rate of digital filter |
| DSPFIRM | sharp(standard) | | DSP firmware filter |
| DIGTYP | DRU | | Digitizer type |
| DIGMOD | digital | | Digitization mode |
| DR | 22 | | Digitizer resolution |
| DDR | 10 | | Digital digitizer resolution |
| DE [µsec] | 10.00 | | Pre-scan delay |
| NBL | 1 | | Number of blocks (of acquisition memory) |