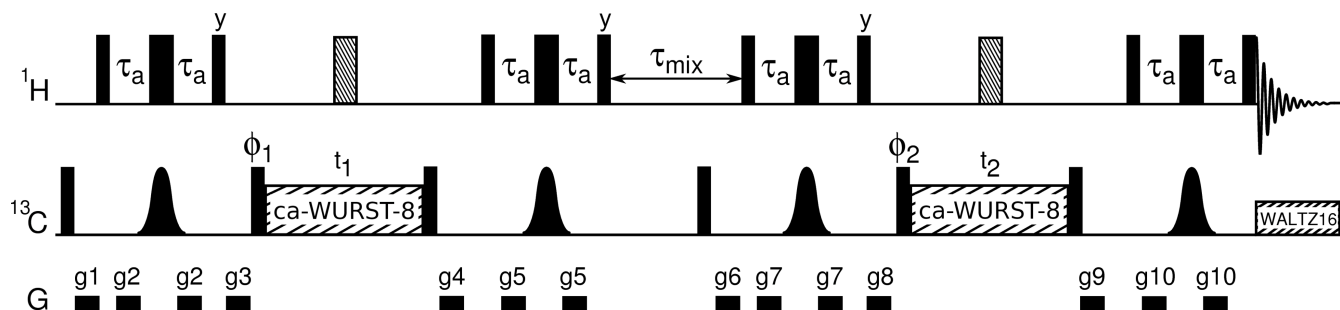


Supporting Information



Pulse scheme of 3D HSQC-NOESY-HSQC experiment used to record intra-residue Ile methyl-methyl NOEs ($H^{\delta 1}-H^{\gamma 2}$) in a highly deuterated $\alpha_7\alpha_7$ sample produced with U- ^{13}C , 1H labeled Ile. Narrow and wide rectangular pulses have flip angles of 90° and 180° , respectively. All pulses are applied along the x-axis unless indicated otherwise. Cross-hatched bars indicate composite 180° pulses of the $90_x180_y90_x$ variety (Levitt & Freeman, 1978). ^{13}C and 1H carriers are positioned at 15 and 0.8 ppm, respectively. Shaped ^{13}C pulses (1.85 ms at 800 MHz, 3.4 kHz peak field) are applied with the RE-BURP profile (Geen & Freeman, 1991) and invert only ^{13}C nuclei resonating between 10-20 ppm, without perturbation of Ile $^{13}C^\beta$ and $^{13}C^{\gamma 1}$ spins (25-40 ppm). Decoupling of $^{13}C^\beta$ and $^{13}C^{\gamma 1}$ spins during t_1/t_2 is achieved using a constant adiabaticity WURST-8 decoupling scheme (Kupce & Wagner, 1996), with a bandwidth of 15 ppm centered at 32.5 ppm (swept from 25 to 40 ppm). An additional equivalent field swept from 5 to -10 ppm (centered at -2.5 ppm) was applied as well that essentially eliminates decoupling artifacts that would otherwise manifest when only a single field centered at 32.5 ppm is applied (Kupce & Freeman, 1995; Zhang & Gorenstein, 1998). The $B_{1max}(B_{1rms})$ of the combined decoupling fields was 0.82(0.45)kHz. The phase cycle is $\phi_1=(x,-x); \phi_2=2(x),2(-x); rec=(x,-x,-x,x)$. Quadrature detection in F_1 and F_2 was accomplished by incrementing ϕ_1 and ϕ_2 , respectively, via the States-TPPI method (Marion et al., 1989). The INEPT transfer delay τ_a (extending to the center of the simultaneous $^{13}C/^1H$ 180° pulses) was set $< 1/(4 \cdot J_{CH}) \sim 1.8$ ms; a 75 ms NOE mixing time τ_{mix} was used to observe intra-residue NOEs. Pulsed-field gradients were applied along the z-axis with the

following strengths and durations (G/cm; ms): $g1 = (10; 0.5)$, $g2 = (5; 0.4)$, $g3 = (-15; 1)$, $g4 = (-18; 0.4)$, $g5 = (15; 0.8)$, $g6 = (6; 0.5)$, $g7 = (8; 0.3)$, $g8 = (7; 0.2)$, $g9 = (10; 0.5)$, $g10 = (12; 0.4)$.

References

- Geen, H., & Freeman, R. (1991) Band-selective radiofrequency pulses. *J. Magn. Reson.* 93, 93-141.
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- Kupce, E., & Wagner, G. (1996) Multisite Band-Selective Decoupling in Proteins. *J. Magn. Reson. B* 110, 309-312.
- Levitt, M., & Freeman, R. (1978) NMR population inversion using a composite pulse. *J. Magn. Reson.* 33, 473-476.
- Marion, D., Ikura, M., Tschudin, R., & Bax, A. (1989) Rapid recording of 2D NMR spectra without phase cycling. Application to the study of hydrogen exchange in proteins. *J. Magn. Reson.* 85, 393-399.
- Zhang, S. M., & Gorenstein, D. G. (1998) Bloch-Siegert shift compensated and cyclic irradiation sidebands eliminated, double-adiabatic homonuclear decoupling for C-13- and N-15-double-labeled proteins. *Journal of Magnetic Resonance* 132, 81-87.

Pulse sequence code:

```
/* Ile_cg2_cd1_noesy_800_lek.c
```

This pulse sequence will allow one to perform the following experiment:

3D C(methyl,Ile) - noesy - C(methyl,Ile) - H (methyl)

Uses three channels:

- 1) 1H - 4.73 ppm
- 2) 13C - 15.5 ppm
- 3) 15N - 119.0 ppm

Set dm = 'nnny', dmm = 'cccp' [13C decoupling during acquisition].

Set dm2 = 'nnnn', dmm2 = 'cccp'.

F1: 13C methyl

F2: 13C methyl

F3: 1H methyl

Modified from methyl_3d_noesy_600_v2.c by LEK on July 21, 2010

Sequence written to be able to observe Ile-d1 Ile-cg2 noes and given that d1's are assigned

enable the assignment of cg2's.

To calibrate:

pwc at dhpwr=63

pwc_reb at d_reb, sh_reb as a selective reburp pulse to invert between 10-20 ppm so as

to minimize the sw needed

Cb decoupling: CAWURST-8 between 40-25 ppm and 6-(-9) ppm to compensate for bs (use pbox)

*/

#include <standard.h>

```
static int  phi1[2] = {0,2},
            phi2[4] = {0,0,2,2},
            rec[4]  = {0,2,2,0};
```

```
static double d2_init=0.0, d3_init=0.0;
```

pulsesequance()

{

/* DECLARE VARIABLES */

```
char        fsat[MAXSTR],
            fscuba[MAXSTR],
            f1180[MAXSTR], /* Flag to start t1 @ halfdwell */
            f2180[MAXSTR], /* Flag to start t2 @ halfdwell */
            sh_reb[MAXSTR], /* reburp for inversion during first inept */
            c180_flg1a[MAXSTR],
```

```

c180_flg[0],
mess_flg[0],

cbdec[0];

int      phase, phase2, t2_counter, ni2, ni,
         t1_counter; /* used for states tppi in t2,t1 */

double   tau1,        /* t1 delay */
         tau2,        /* t2 delay */
         taua,        /* ~ 1/4JCH = 1.7 ms; first inept */
         mix,         /* noesy mixing time */
         pwc,         /* 90 c pulse at dhpwr */
         tsatpwr,     /* low level 1H trans.power for presat */
         dhpwr,       /* power level for high power 13C pulses on dec1 */
         sw1,         /* sweep width in f1 */
         sw2,         /* sweep width in f2 */

         d_reb,
         pwc_reb,

         dhpwr2,
         pwn,

         tpwrmess,
         dly_pg1,

         tof_me,

```

```
dpwr_cb,  
dmf_cb,  
dres_cb,
```

```
gt0,  
gt1,  
gt2,  
gt3,  
gt4,  
gt5,  
gt6,  
gt7,  
gt8,  
gt9,  
gt10,
```

```
gzlv10,  
gzlv11,  
gzlv12,  
gzlv13,  
gzlv14,  
gzlv15,  
gzlv16,  
gzlv17,  
gzlv18,  
gzlv19,  
gzlv110;
```

```
/* LOAD VARIABLES */
```

```

getstr("fsat",fsat);
getstr("f1180",f1180);
getstr("f2180",f2180);
getstr("fscuba",fscuba);
getstr("mess_flg",mess_flg);
getstr("c180_flgga",c180_flgga);
getstr("c180_flggb",c180_flggb);

getstr("sh_reb",sh_reb);
getstr("cbdec",cbdec);

taua    = getval("taua");
mix     = getval("mix");
pwc     = getval("pwc");
tpwr    = getval("tpwr");
tsatpwr = getval("tsatpwr");
dhpwr   = getval("dhpwr");
dpwr    = getval("dpwr");
phase   = (int) ( getval("phase") + 0.5);
phase2  = (int) ( getval("phase2") + 0.5);
sw1     = getval("sw1");
sw2     = getval("sw2");
ni2     = getval("ni2");
ni      = getval("ni");

d_reb   = getval("d_reb");
pwc_reb = getval("pwc_reb");

dhpwr2  = getval("dhpwr2");

```

```
pwn = getval("pwn");

tpwrmess = getval("tpwrmess");
dly_pg1 = getval("dly_pg1");

tof_me = getval("tof_me");

dpwr_cb = getval("dpwr_cb");
dmf_cb = getval("dmf_cb");
dres_cb = getval("dres_cb");

gt0 = getval("gt0");
gt1 = getval("gt1");
gt2 = getval("gt2");
gt3 = getval("gt3");
gt4 = getval("gt4");
gt5 = getval("gt5");
gt6 = getval("gt6");
gt7 = getval("gt7");
gt8 = getval("gt8");
gt9 = getval("gt9");
gt10 = getval("gt10");

gzlvl0 = getval("gzlvl0");
gzlvl1 = getval("gzlvl1");
gzlvl2 = getval("gzlvl2");
gzlvl3 = getval("gzlvl3");
gzlvl4 = getval("gzlvl4");
gzlvl5 = getval("gzlvl5");
gzlvl6 = getval("gzlvl6");
```

```

gzlv17 = getval("gzlv17");
gzlv18 = getval("gzlv18");
gzlv19 = getval("gzlv19");
gzlv110 = getval("gzlv110");

/* LOAD PHASE TABLE */

settable(t1,2,phi1);
settable(t2,4,phi2);
settable(t9,4,rec);

/* CHECK VALIDITY OF PARAMETER RANGES */

if((dm[A] == 'y' || dm[B] == 'y' || dm[C] == 'y' ))
{
    printf("incorrect dec1 decoupler flags! ");
    abort(1);
}

if((dm2[A] == 'y' || dm2[B] == 'y' || dm2[C] == 'y'))
{
    printf("incorrect dec2 decoupler flags! ");
    abort(1);
}

if( tsatpwr > 6 )
{
    printf("TSATPWR too large !!! ");
    abort(1);
}

```

```

}

if( dpwr > 48 )
{
    printf("don't fry the probe, DPWR too large! ");
    abort(1);
}

if( d_reb > 54 )
{
    printf("don't fry the probe, d_reb too large! ");
    abort(1);
}

if( dpwr2 > 49 )
{
    printf("don't fry the probe, DPWR2 too large! ");
    abort(1);
}

if(gt0 > 3e-3 || gt1 > 3e-3 || gt2 > 3e-3 || gt3 > 3e-3 ||
    gt4 > 3e-3 || gt5 > 3e-3 || gt6 > 3e-3 ||
    gt7 > 3e-3 || gt8 > 3e-3 || gt9 > 3e-3)
{
    printf("gradients on for too long. Must be < 3e-3 \n");
    abort(1);
}

/* Phase incrementation for hypercomplex 2D data */

```

```

    if (phase2 == 2)
        tsadd(t2,1,4);

    if (phase == 2)
        tsadd(t1,1,4);

/* Calculate modifications to phases for States-TPPI acquisition */

    if( ix == 1) d2_init = d2 ;
    t1_counter = (int) ( (d2-d2_init)*sw1 + 0.5 );
    if(t1_counter % 2) {
        tsadd(t1,2,4);
        tsadd(t9,2,4);
    }

    if( ix == 1) d3_init = d3 ;
    t2_counter = (int) ( (d3-d3_init)*sw2 + 0.5 );
    if(t2_counter % 2) {
        tsadd(t2,2,4);
        tsadd(t9,2,4);
    }

/* Set up f2180 tau2 = t2 */

    tau2 = d3;

    if(f2180[A] == 'y') {
        tau2 += ( 1.0 / (2.0*sw2) );
    }

```

```

}

tau2 = tau2 - 4.0/PI*pwc - 4.0*pw - POWER_DELAY - 2.0e-6
      - PRG_START_DELAY - PRG_STOP_DELAY - POWER_DELAY - 4.0e-6;

if(tau2 < 0.4e-6) tau2 = 0.4e-6;
tau2 = tau2/2.0;

/* Set up f1180 tau1 = t1 */

tau1 = d2;
if(f1180[A] == 'y') {
    tau1 += ( 1.0 / (2.0*sw1) );
}

tau1 = tau1 - 4.0/PI*pwc - 4.0*pw - POWER_DELAY - 2.0e-6
      - PRG_START_DELAY - PRG_STOP_DELAY - POWER_DELAY - 4.0e-6;

if(tau1 < 0.4e-6) tau1 = 0.4e-6;
tau1 = tau1/2.0;

/* BEGIN ACTUAL PULSE SEQUENCE */

status(A);

offset(dof,DODEV);

rlpower(tsatpwr,TODEV); /* Set transmitter power for 1H presaturation */
rlpower(dhpwr,DODEV); /* Set Dec1 power for hard 13C pulses */
rlpower(dhpwr2,D02DEV); /* Set Dec2 power for 15N pulses */

/* Presaturation Period */

```

```

status(B);

if (mess_flg[A] == 'y') {

    rlpower(tpwrmess,TODEV);
    txphase(zero);
    rgpulse(dly_pg1,zero,2.0e-6,2.0e-6);
    txphase(one);
    rgpulse(dly_pg1/1.62,one,2.0e-6,2.0e-6);

    delay(4.0e-6);
    rgradient('z',gzlv10);
    delay(gt0);
    rgradient('z',0.0);
    delay(250.0e-6);

    rlpower(tsatpwr,TODEV);
}

if (fsat[0] == 'y')
{
    delay(2.0e-5);
    rgpulse(d1,zero,2.0e-6,2.0e-6); /* presat */
    rlpower(tpwr,TODEV); /* Set transmitter power for hard 1H pulses */
    delay(2.0e-5);
    if(fscuba[0] == 'y')
    {
        delay(2.2e-2);
    }
}

```

```

        rgpulse(pw, zero, 2.0e-6, 0.0);
        rgpulse(2*pw, one, 2.0e-6, 0.0);
        rgpulse(pw, zero, 2.0e-6, 0.0);
        delay(2.2e-2);
    }
}
else
{
    delay(d1);
}

rlpower(tpwr, TODEV);          /* Set transmitter power for hard 1H pulses */
txphase(zero);
dec2phase(zero);
decphase(zero);
delay(1.0e-5);

/* Begin Pulses */

status(C);

obsoffset(tof_me);

rcvroff();
delay(20.0e-6);

/* first ensure that magnetization does infact start on H and not C */

decrpulse(pwc, zero, 2.0e-6, 2.0e-6);

```

```

delay(2.0e-6);
rgradient('z',gzlvl1);
delay(gt1);
rgradient('z',0.0);
delay(250.0e-6);

decpower(d_reb); /* set power for reburp during inept */
delay(4e-6);

/* this is the real start */

rgpulse(pw,zero,0.0,0.0); /* 90 deg 1H pulse */

delay(2.0e-6);
rgradient('z',gzlvl2);
delay(gt2);
rgradient('z',0.0);
delay(100.0e-6);

delay(taua - gt2 - 102.0e-6 - WFG2_START_DELAY - 0.5*psc_reb); /* taua <=
1/4JCH */

simshaped_pulse("hard",sh_reb,2.0*pw,psc_reb,zero,zero,0.0,0.0);

txphase(one); decphase(t1);
decpower(dhpwr);

delay(2.0e-6);
rgradient('z',gzlvl2);
delay(gt2);

```

```

rgradient('z',0.0);
delay(100.0e-6);

delay(taua - gt2 - 102.0e-6 - 0.5*pwd_reb - WFG2_STOP_DELAY - POWER_DELAY);

rgpulse(pwd,one,0.0,0.0);
txphase(zero);

delay(2.0e-6);
rgradient('z',gzlvl3);
delay(gt3);
rgradient('z',0.0);
delay(200.0e-6);

decrpulse(pwd,t1,0.0,0.0);
decphase(zero);

if(c180_flg[A] == 'n') {

/* Cb decoupling on */
decpower(dpwr_cb);
decrpgon(cbdec,1.0/dmf_cb,dres_cb);
decon();
/* Cb decoupling on */

delay(tau1);

rgpulse(pwd,zero,0.0,0.0);
rgpulse(2.0*pwd,one,0.0,0.0);

```

```

rgpulse (pw, zero, 0.0, 0.0);

delay(taul);

/* Cb decoupling off */
decoff();
decprgoff();
/* Cb decoupling off */

decpower(dhpwr);

}

decrpulse (pwc, zero, 4.0e-6, 0.0);

delay(2.0e-6);
rgradient('z',gzlv14);
delay(gt4);
rgradient('z',0.0);
delay(200.0e-6);

decpower(d_reb);    /* set power for reburp during inept */

rgpulse (pw, zero, 0.0, 0.0);

delay(2.0e-6);
rgradient('z',gzlv15);
delay(gt5);
rgradient('z',0.0);
delay(100.0e-6);

```

```

delay(taua - gt5 - 102.0e-6 - WFG2_START_DELAY - 0.5*psc_reb);    /* taua <=
1/4JCH */

simshaped_pulse("hard",sh_reb,2.0*pw,psc_reb,zero,zero,0.0,0.0);

txphase(one);

decpower(dhpwr);

delay(2.0e-6);
rgradient('z',gzlvl5);
delay(gt5);
rgradient('z',0.0);
delay(100.0e-6);

delay(taua - gt5 - 102.0e-6 - 0.5*psc_reb - WFG2_STOP_DELAY - POWER_DELAY);

rgpulse(pw,one,0.0,0.0);

txphase(zero);

delay(mix - gt6 - 352.0e-6);
decrpulse(psc,zero,0.0,0.0);

delay(2.0e-6);
rgradient('z',gzlvl6);
delay(gt6);
rgradient('z',0.0);
delay(350.0e-6);

decpower(d_reb); /* set power level for reburp */

```

```

rgpulse(pw,zero,0.0,0.0);                                /* 90 deg 1H pulse */

delay(2.0e-6);

rgradient('z',gzlv17);

delay(gt7);

rgradient('z',0.0);

delay(100.0e-6);

delay(taua - gt7 - 102.0e-6 - WFG2_START_DELAY - 0.5*psc_reb); /* taua <=
1/4JCH */

simshaped_pulse("hard",sh_reb,2.0*pw,psc_reb,zero,zero,0.0,0.0);

txphase(one); decphase(t2);

decpower(dhpwr);

delay(2.0e-6);

rgradient('z',gzlv17);

delay(gt7);

rgradient('z',0.0);

delay(100.0e-6);

delay(taua - gt7 - 102.0e-6 - 0.5*psc_reb - WFG2_STOP_DELAY - POWER_DELAY);

rgpulse(pw,one,0.0,0.0);

txphase(zero);

delay(2.0e-6);

rgradient('z',gzlv18);

```

```

delay(gt8);
rgradient('z',0.0);
delay(200.0e-6);

decrgpulse(pwc,t2,2.0e-6,0.0);
decphase(zero);

if(c180_flg[A] == 'n') {

/* Cb decoupling on */
decpower(dpwr_cb);
decprgon(cbdec,1.0/dmf_cb,dres_cb);
decon();
/* Cb decoupling on */

delay(tau2);

rgpulse(pw,zero,0.0,0.0);
rgpulse(2.0*pw,one,0.0,0.0);
rgpulse(pw,zero,0.0,0.0);

delay(tau2);

/* Cb decoupling off */
decoff();
decprgoff();
/* Cb decoupling off */

decpower(dhpwr);

```

```
}
```

```
decrpulse(pwc,zero,4.0e-6,0.0);
```

```
delay(2.0e-6);
```

```
rgradient('z',gzlv19);
```

```
delay(gt9);
```

```
rgradient('z',0.0);
```

```
delay(200.0e-6);
```

```
decpower(d_reb); /* set power for reburp during inept */
```

```
rgpulse(pw,zero,0.0,0.0);
```

```
delay(2.0e-6);
```

```
rgradient('z',gzlv110);
```

```
delay(gt10);
```

```
rgradient('z',0.0);
```

```
delay(100.0e-6);
```

```
delay(taua - gt10 - 102.0e-6 - WFG2_START_DELAY - 0.5*pwc_reb); /* taua <= 1/4JCH */
```

```
simshaped_pulse("hard",sh_reb,2.0*pw,pwc_reb,zero,zero,0.0,0.0);
```

```
delay(2.0e-6);
```

```
rgradient('z',gzlv110);
```

```
delay(gt10);
```

```
rgradient('z',0.0);
```

```

delay(100.0e-6);

delay(taua - gt10 - 102.0e-6 - 0.5*pwd_reb - WFG2_STOP_DELAY - 2.0*POWER_DELAY);

decpower(dpwr); /* Set power for decoupling */
dec2power(dpwr2); /* Set power for decoupling */

rgpulse(pwd, zero, 0.0, rof2);

/* BEGIN ACQUISITION */

status(D);

setreceiver(t9);

}

```

Varian procpa file:

```

gzlv18 1 1 32768 -32768 1 2 1 0 1 64
1 7000
0
dn2 2 2 8 0 0 2 1 8 1 64
1 "N15"
0
dco90pwr 7 1 32767 0 0 2 1 0 1 64
1 52
0
cf 7 1 32767 0 1 3 1 1 0 64
1 1
0
awc1 1 1 1 -1 0.001 3 1 1 0 64

```

```

1 0
0
array 2 2 256 0 0 2 1 1 1 64
1 "phase2,phase"
0
alock 2 2 8 0 0 2 1 0 1 64
1 "n"
5 "a" "n" "s" "u" "y"
aig 2 2 2 0 0 4 1 1 1 64
1 "ai"
2 "nm" "ai"
acqdim 7 1 10000000000 -10000000000 0 2 1 0 1 64
1 3
0
acqcycles 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 0 1 64
1 4096
0
acqstatus 7 1 32767 0 0 2 1 0 1 64
2 17 1
0
alfa 6 1 8190 -8190 0.0125 2 1 2 1 64
1 4.8125
0
ap 2 2 1023 0 0 4 1 6 1 64
1
"1:SAMPLE:date,solvent,file;1:3D
ACQUISITION:sw:1,sw1:1,sw2:1,ni:0,ni2:0,phase:0,phase2:0,at:3,np:0,ss:0,nt:0,ct
:0;1:CHANNEL
1:sfrq:3,tn,tof:1,tpwr:0,mlevpwr:0,tsatpwr:0,pw:1,pwmlev:1;1:CHANNEL
2:dfrq:3,dn,dof:1,dpwr:0,dlowpwr:0,pwx1:1,dm,dmm,dmf:0,dseq,homo;2:DELAYS:d1:3,
d2:3,d3:3,hscuba:3,mixnoe:3,mixshift:3,mixmlev:3,trim:3,jxh:1;1:FLAGS:fscuba,fm
lev,fnoesy,dp,hs;2:2D DISPLAY:sp1:1,wpl:1,sc2:0,wc2:0,rfl1:1,rfp1:1;2:DEC. &
VT:dn:2,dof:1,dm,dmm,dmf,dpwr(dpwr):0,pwxlv1:0,pwx:1,dlp(dlp):0,homo,temp(temp)
:1,satflg,satdly:3,satfrq:1,satpwr:0;2:PROCESSING:cf(nf):0,lb(lb):2,sb(sb):3,sb
s(sb):3,gf(gf):3,gfs(gf):3,awc(awc):3,lsfid(lsfid):0,phfid(phfid):1,wtfile,proc
,fn:0,math,,werr,wexp,wbs,wnt;2(ni):2D

```

```
PROCESSING:lb1(lb1):2,sb1(sb1):3,sbs1(sb1):3,gf1(gf1):3,gfs1(gf1):3,awc1(awc1):  
3,wtfile1,proc1,fn1:0;2:DISPLAY:sp:1,wp:1,vs:0,sc:0,wc:0,hzmm:2,is:2,rfl:1,rfp:  
1,th:0,ins:3,aig*,dcg*,dmg*;"
```

0

ampmode 2 2 8 0 0 2 1 0 1 64

1 "dddp"

0

arrayelemts 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 0 1 64

1 4

0

arraydim 7 1 32768 1 1 2 1 5 1 64

1 4096

0

at 1 1 14 14 14 2 1 8203 1 64

1 0.0640192500001

0

awc 1 1 1 -1 0.001 3 1 1 0 64

1 0

0

c180_flgga 2 2 8 0 0 2 1 0 1 64

1 "n"

0

axisf 4 2 4 0 0 4 1 0 1 64

1 "s"

4 "m" "n" "s" "u"

axis 4 2 4 0 0 4 1 0 1 64

1 "p"

11 "c" "d" "1" "2" "3" "h" "k" "m" "n" "p" "u"

awc2 1 1 1 -1 0.001 3 1 1 0 64

1 0

0

c13_de 3 1 14 14 14 2 1 8192 1 64
1 0.001
0
bs 7 1 32767 0 1 2 1 0 0 64
1 16
0
cbdec 2 2 8 0 0 2 1 0 1 64
1 "cb_ad"
0
c180_flgbb 2 2 8 0 0 2 1 0 1 64
1 "n"
0
celem 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 0 1 64
1 0
0
d4 3 1 14 14 14 2 1 8194 1 64
1 0
0
cr2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0
0
console 2 2 8 0 0 2 1 0 1 64
1 "inova"
0
cofrq 5 1 10000000000 -10000000000 0 2 1 0 1 64
1 10800
0
cr 1 1 10000000000 -10000000000 0 4 1 1 1 64
1 -49645.2679535

```
0
cp 2 2 1 0 0 2 1 0 1 64
1 "y"
2 "y" "n"
cr1 1 1 10000000000 -10000000000 0 4 1 3 1 64
1 -613.603499887
0
cutoff 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 0 64
1 200
0
ct 7 1 10000000000 0 1 2 1 6 1 64
1 0
0
crf 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0
0
d2 3 1 14 14 14 2 1 8194 1 64
1 0
0
d1 3 1 14 14 14 2 1 8194 1 64
1 1
0
d3 3 1 14 14 14 2 1 8194 1 64
1 0
0
date 2 2 9 0 0 2 1 1 1 64
1 "Jul 23 2010"
0
d_reb 1 1 9 9 9 2 1 8192 1 64
1 45
```

```

0
d_ibca 1 1 9 9 9 2 1 8192 1 64
1 46
0
dcg 2 2 3 0 0 4 1 1 1 64
1 ""
2 "dc" "cdc"
dcapwr 7 1 77 0 1 2 1 0 1 64
1 64
0
dm 4 2 4 0 0 2 1 0 1 64
1 "nnny"
4 "a" "n" "s" "y"
dg 2 2 1023 0 0 4 1 6 1 64
1
    "1:SAMPLE:date;1:3D
    ACQUISITION:sw:1,sw1:1,sw2:1,ni:0,ni2:0,phase:0,phase2:0,np:0,ss:0,nt:0,at:3;2:
    SPECIAL:gain,temp:1,seqfil;2:DELAYS:taua:5,mix:5,d1:3,d2:6,d3:6,dly_pg1:6,tin,v
    twait;3:CHANNEL
    1:sfrq:3,tn,tof:1,tof_me:1,tpwr:0,tsatpwr:0,tpwrmess:0,pw:2,alfa:1;3:FLAGS:fsat
    ,fscuba,f1180,f2180,mess_flg,c180_flg,c180_flg;4:CHANNEL
    3:dfrq2:3,dn2,dof2:1,dhpwr2:0,dpwr2:0,pwn:1,dm2,dmm2,dmf2,dseq2,dres2;"
0
deltaone 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 0 1 64
1 0
0
decfrq 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 0 1 64
1 -3000
0
ddseq 2 2 8 0 0 2 1 0 1 64
1 "waltz16"
0
dcodpwr 7 1 61 0 0 2 1 0 1 64

```

```

1 57
0
deltaf 1 1 100 0 0 4 1 0 1 64
1 0.00296542986425
0
delta2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0
0
deltafrq 5 1 10000000000 -10000000000 0 2 1 0 1 64
1 -19000
0
dfrq2 1 1 10000000000 0 0 2 1 9 1 64
1 81.043365
0
dfrq 5 1 10000000000 -10000000000 0 2 1 8 1 64
1 201.0911602
0
dfrq3 1 1 10000000000 0 0 2 1 9 1 64
1 122.7635575
0
dhipwr 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 0 1 64
1 63
0
dgs 2 2 1023 0 0 4 1 6 1 64
5 "1:AXIAL SHIMS:z1:0,z2:0,z3:0,z4:0,z5:0,z6:0;"
"2:NON AXIAL
SHIMS:x1:0,y1:0,xz:0,yz:0,xy:0,x2y2:0,x3:0,y3:0,xz2:0,yz2:0,zxy:0,zx2y2:0,z3x:0
,z3y:0,z2x2y2:0,z2xy:0;"
"3:NON AXIAL
SHIMS:zx3:0,zy3:0,x4:0,y4:0,z4x:0,z4y:0,z3x2y2:0,z3xy:0,,z4x2y2:0,z4xy:0,z5x:0,
z5y:0;"
"4:AUTOMATION:method,wshim,load,,spin:0,gain:0,alock,loc:0;"

```

"4:SPECIAL:temp;"

0

dg1 2 2 8 0 0 4 1 0 1 64

1

"1:DISPLAY:sp:1,wp:1,sp1(ni):1,wp1(ni):1,sp2(ni2):1,wp2(ni2):1;1:FID:sf:3,wf:3,vf:0;1:FLAGS:aig*,dgc*,pmode*(ni),dmg*,dmg1*(ni),dmg2*(ni2);2:REFERENCING:rfl:1,rfp:1,cr:1,delta:1,,rfl1(ni):1,rfp1(ni):1,cr1(ni):1,delta1(ni):1,,rfl2(ni2):1,rfp2(ni2):1,cr2(ni2):1,delta2(ni2):1;3:CHART:sc:0,wc:0,sc2(ni):0,wc2(ni):0,,hzm:2,vs:1,vp:1,th:1,ho:2,vo:2,axis,,pltmod,rplot;4(ni):DIMENSIONS:trace,plane(ni2);4:INTEGRAL:intmod,is:2,ins:3,io:0,,lvl:3,tlr:3;4(ni2):3D
OPTIONS:fiddc3d,specdc3d,ptspec3d,ntype3d,ss3d;"

0

dg2 2 2 1023 0 0 4 1 7 1 64

1

"1:CHANNEL
2:dfrq:3,dn,dof:1,dhpwr:0,dpwr:0,d_reb:0,pwc:1,pwc_reb:1,dseq,dm,dmm,dres,dressed,dmf,sh_reb,cbdec,dpwr_cb:0,dmf_cb:0,dres_cb:0;2:GRADIENTS:gt0:4,gzlvl0:0,gt1:4,gzlvl1:0,gt2:4,gzlvl2:0,gt3:4,gzlvl3:0,gt4:5,gzlvl4:0,gt5:4,gzlvl5:0,gt6:4,gzlvl6:0,gt7:4,gzlvl7:0,gt8:4,gzlvl8:0,gt9:4,gzlvl9:0,gt10:4,gzlvl10:0;3:CHANNEL
4:dfrq3:3,dn3,dof3:1,dpwr3:0,dpwr3_D:0,pwd:1,pwd1:1,ddseq,dm3,dseq3,dres3:0,ampmode;"

0

dh2pwr 7 1 77 0 1 2 1 0 1 64

1 0

0

dhpwr2 1 1 18 18 18 2 1 8192 1 64

1 -16

0

dhpwr 1 1 9 9 9 2 1 8192 1 64

1 61

0

dhp 1 1 9 9 9 2 1 8192 0 64

1 40

0

dlp 7 1 10 10 10 2 1 8194 0 64

1 10

0

dlowpwr 7 1 32767 0 0 2 1 0 1 64
1 46
0
dly_pg1 3 1 14 14 14 2 1 8192 1 64
1 0.005
0
dmg1 2 2 8 0 0 4 1 0 1 64
1 ""
4 "" "av1" "ph1" "pwr1"
dmf2 7 1 100000 1 0 2 1 2 1 64
1 3690
0
dm3 4 2 4 0 0 2 1 0 1 64
1 "nnnn"
4 "a" "n" "s" "y"
dm2 2 2 8 0 0 2 1 0 1 64
1 "nnnn"
0
dmf 7 1 11 11 11 2 1 8194 1 64
1 7299
0
dmf_cb 1 1 11 11 11 2 1 8192 1 64
1 25000
0
dmf3 7 1 2000000 1 0 2 1 2 1 64
1 7092
0
dmg 2 2 2 0 0 4 1 3 1 64
1 "ph"

```

0
dmm3 4 2 4 0 0 2 1 0 1 64
1 "c"
9 "c" "f" "g" "m" "p" "r" "u" "w" "x"
dmm2 2 2 8 0 0 2 1 0 1 64
1 "cccp"
0
dmm 4 2 4 0 0 2 1 0 1 64
1 "cccp"
9 "c" "f" "g" "m" "p" "r" "u" "w" "x"
dn 2 2 4 0 0 2 1 8 1 64
1 "C13"
0
fsat 2 2 8 0 0 2 1 0 1 64
1 "n"
0
dseq3 2 2 8 0 0 2 1 0 1 64
1 "waltz16"
0
dres2 7 1 360 1 0 2 1 0 1 64
1 90
0
dpwr 7 1 9 9 9 2 1 8194 1 64
1 40
0
dof2 5 1 16 16 16 2 1 8202 1 64
1 1671.2
0
dod 3 1 14 14 14 2 1 8194 1 64
1 0.009999999977648

```

```
0
dn3 2 2 8 0 0 2 1 8 1 64
1 "H2"
0
dof 5 1 8 8 8 2 1 8202 1 64
1 -15461.8390882
0
dotflag 2 2 8 0 0 4 1 0 1 64
1 "n"
2 "n" "y"
dof3 5 1 20 20 20 2 1 8202 1 64
1 1717
0
dp 2 2 1 0 0 2 1 0 1 64
1 "y"
2 "y" "n"
dpwr3_D 1 1 21 21 21 2 1 8192 1 64
1 -16
0
dpwr3 7 1 21 21 21 2 1 8194 1 64
1 -16
0
dpwr2 7 1 18 18 18 2 1 8194 1 64
1 -16
0
dpwrf 7 1 4095 0 1 2 1 2 0 64
1 4095
0
dpwr_cb 1 1 9 9 9 2 1 8192 1 64
```

1 33
0
dres 7 1 360 1 0 2 1 0 1 64
1 90
0
dseq 2 2 8 0 0 2 1 0 1 64
1 "waltz16"
0
dres_cb 7 1 360 1 0 2 1 0 1 64
1 9
0
dres3 7 1 360 1 0 2 1 0 1 64
1 90
0
dressed 7 1 360 1 0 2 1 0 1 64
1 2
0
dseq2 2 2 8 0 0 2 1 0 1 64
1 "waltz16"
0
fiddc3d 4 2 4 0 0 3 1 0 1 64
1 "nnn"
0
fad1 2 2 8 0 0 2 1 0 1 64
1 "y"
0
f1180 2 2 8 0 0 2 1 0 1 64
1 "y"
0
exp3D 2 2 8 0 0 2 1 0 1 64

```
1 "n"
0
exppath 2 2 8 0 0 2 1 0 1 64
1 "/usr2/guestkay/vnmrsys/exp15/acqfil"
0
f2180 2 2 8 0 0 2 1 0 1 64
1 "y"
0
f1coef 2 2 8 0 0 3 1 1 1 64
1 ""
0
f2coef 2 2 8 0 0 3 1 1 1 64
1 ""
0
fb 7 1 6 6 6 2 1 8203 0 64
1 7000
0
fad2 2 2 8 0 0 2 1 0 1 64
1 "n"
0
fmlev 4 2 4 0 0 2 1 0 1 64
1 "n"
0
filtfile 2 2 8 0 0 2 1 0 1 64
1 ""
0
filter 7 1 10000000000 0 1 2 1 2 1 64
1 54.0999984741
0
```

```
file 2 2 6 0 0 2 1 3 1 64
1 "exp"
0
flag3d 2 2 8 0 0 2 1 0 1 64
1 "y"
0
fnoesy 4 2 4 0 0 2 1 0 1 64
1 "n"
0
fn1 7 1 524288 64 -2 3 1 1 1 64
1 1024
0
fn 7 1 524288 64 -2 3 1 1 1 64
1 4096
0
fn2 7 1 524288 64 -2 3 1 1 0 64
1 0
0
fpmult1 1 1 10000000000 0 0 3 1 0 0 64
1 0
0
fpmult 1 1 10000000000 0 0 3 1 0 0 64
1 1
0
fpmult2 1 1 10000000000 0 0 3 1 0 0 64
1 0
0
gt5 3 1 14 14 14 2 1 8192 1 64
1 0.00075
0
```

gfs2 1 1 1000 -1000 0.001 3 1 1 0 64
1 0
0
gfl 1 1 100000 0 0 3 1 1 1 64
1 0.0050210384652
0
gain 1 1 60 0 2 2 1 0 1 64
1 28
0
fscuba 4 2 4 0 0 2 1 0 1 64
1 "n"
0
gf 1 1 100000 0 0 3 1 1 1 64
1 0.0171710532159
0
gfs 1 1 1000 -1000 0.001 3 1 1 1 64
1 0.003
0
gf2 1 1 100000 0 0 3 1 1 0 64
1 0
0
gfs1 1 1 1000 -1000 0.001 3 1 1 0 64
1 0
0
gt2 3 1 14 14 14 2 1 8192 1 64
1 0.0004
0
gt1 3 1 14 14 14 2 1 8192 1 64
1 0.0005

0
gt0 3 1 32768 -32768 -1 2 1 8192 1 64
1 0.0005
0
gt10 3 1 14 14 14 2 1 8192 1 64
1 0.0004
0
gt4 3 1 14 14 14 2 1 8192 1 64
1 0.0004
0
gt3 3 1 14 14 14 2 1 8192 1 64
1 0.001
0
gzlv12 1 1 32768 -32768 1 2 1 0 1 64
1 5000
0
gt9 3 1 14 14 14 2 1 8192 1 64
1 0.0005
0
gt7 3 1 14 14 14 2 1 8192 1 64
1 0.0003
0
gt6 3 1 14 14 14 2 1 8192 1 64
1 0.0005
0
gt8 3 1 14 14 14 2 1 8192 1 64
1 0.0002
0
gzlv11 1 1 32768 -32768 1 2 1 0 1 64
1 10000

0
gzlv10 1 1 32768 -32768 1 2 1 0 1 64
1 8000
0
gzlv110 1 1 32768 -32768 1 2 1 0 1 64
1 12000
0
gzlv15 1 1 32768 -32768 1 2 1 0 1 64
1 15000
0
gzlv14 1 1 32768 -32768 1 2 1 0 1 64
1 -18000
0
gzlv13 1 1 32768 -32768 1 2 1 0 1 64
1 -15000
0
gzlv16 1 1 32768 -32768 1 2 1 0 1 64
1 6000
0
gzlv17 1 1 32768 -32768 1 2 1 0 1 64
1 8000
0
satfrq 5 1 10000000000 -10000000000 0 2 1 0 1 64
1 -9970
0
phfid1 1 1 3600 -3600 0.1 3 1 0 0 64
1 0
0
lp 1 1 3600 -3600 0.1 4 1 3 1 64

1 0
0
lb2 1 1 100000 -100000 0 3 1 1 0 64
1 0
0
in 4 2 1 0 0 2 1 0 1 64
1 "n"
3 "n" "w" "y"
homo3 4 2 4 0 0 2 1 0 1 64
1 "n"
2 "n" "y"
homo 2 2 8 0 0 2 1 0 1 64
1 "n"
2 "n" "y"
ho 1 1 500 -500 0 4 1 1 1 64
1 -132.5
0
gzlv19 1 1 32768 -32768 1 2 1 0 1 64
1 10000
0
homo2 4 2 4 0 0 2 1 0 1 64
1 "n"
2 "n" "y"
hst 3 1 0.02 0 2.5e-08 2 1 2 1 64
1 0.01
0
hs 4 2 4 0 0 2 1 0 1 64
1 "nnyn"
2 "n" "y"
hscuba 3 1 14 14 14 2 1 8192 1 64

```
1 0.03
0
hzmm 1 1 10000000000 -10000000000 0 4 1 11 1 64
1 6.63085360808
0
il 2 2 1 0 0 2 1 0 1 64
1 "n"
2 "y" "n"
io 1 1 500 -500 0.1 4 1 1 1 64
1 10
0
ins2ref 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 0 64
1 1
0
ins2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 100
0
ins 3 1 8190 0 1e-07 4 1 3 1 64
1 100
0
intmod 2 2 8 0 0 4 1 0 1 64
1 "off"
3 "off" "partial" "full"
insref 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 0 64
1 1
0
investigator 2 2 8 0 0 2 1 0 1 64
1 ""
0
```

```

jxh 7 1 32767 0 0 2 1 0 1 64
1 105
0
jcc 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 0 1 64
1 75
0
is 1 1 1000000000 1e-06 0 4 1 3 1 64
1 4000
0
jnh 1 1 10000 80 0 2 1 1024 1 64
1 106
0
lb 1 1 100000 -100000 0 3 1 1 0 64
1 30
0
jxh2 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 0 1 64
1 94
0
lb1 1 1 100000 -100000 0 3 1 1 0 64
1 0.318309992552
0
load 2 2 4 0 0 2 1 3 1 64
1 "n"
2 "y" "n"
llamp 1 1 1000000000 0 0 4 1 0 0 64
200 -4.59109323856e-05 -5.19088607689e-05 -4.7053432354e-05 -5.81574313401e-05 -
5.19840832567e-05 -5.55371480004e-05 -4.04213315051e-05 -4.98456283822e-05 -
5.58155443287e-05 -5.04925847054e-05 -4.31948683399e-05 -5.39735883649e-05 -
5.19470995641e-05 -5.55918377358e-05 -4.98082154081e-05 -5.87051399634e-05 -
4.52509520983e-05 -6.75681585562e-05 4.89473904963e-07 -5.19699970027e-05 -
2.94218007184e-05 -3.88147345802e-05 -2.91328706226e-05 -6.29609421594e-05 -
5.00809728692e-05 -6.77146163071e-05 -6.38160126982e-05 -7.09096857463e-05 -
3.34689066221e-05 -6.18180274614e-05 -3.68875116692e-05 -4.17151532019e-05 -
2.72881752608e-05 -3.60187077604e-05 2.59389489656e-05 -4.47384954896e-05

```

2.03496692848e-05	-1.918851558e-05	-5.74051318836e-06	-6.3626881456e-05
9.63949132711e-05	5.21112997376e-05	0.000190337683307	0.000276441918686
9.71672634478e-05	0.000668614346068	0.000352685165126	0.000403929530876
0.000406486156862	0.000400811026338	0.00051202083705	5.90048330196e-05
0.000125369871967	5.6045675592e-05	0.000195721484488	0.000586495501921
0.000226417760132	0.00118924141861	0.000177095877007	0.000210481593967
9.40851459745e-05	5.80478408665e-05	0.000169042716152	0.000324096297845
0.000175537803443	0.000141080963658	3.5752873373e-05	0.00100575061515
0.000578368606512	0.000165094563272	0.000141279699164	0.000137800598168
8.40379016154e-06	1.12530606202e-05	-3.27895440932e-06	3.0927509215e-05 -
1.70599105331e-05	-8.41210021463e-06	-1.44544383147e-05	-2.41435354837e-05 -
1.77835827344e-05	-2.28232893278e-05	-5.13579152539e-06	-2.46367108048e-05 -
2.05777068913e-05	-3.80415003747e-05	-1.38831801451e-05	-2.98057329928e-05 -
2.04013631446e-05	-2.93233988486e-05	-2.68420353677e-05	-3.13568452839e-05 -
2.31144804275e-05	-4.10964639741e-05	-3.03998640447e-05	-3.85603998438e-05 -
3.66430067515e-05	-4.40820549557e-05	-2.92319782602e-05	-5.42339148524e-05 -
3.18336860801e-05	-4.89078920509e-05	-3.16614787153e-05	-4.64371987619e-05 -
3.45756561728e-05	-4.65295161121e-05	-4.06016370107e-05	-4.03111916967e-05 -
4.8075151426e-05	-4.44860561402e-05	-5.76606944378e-05	-4.60191586171e-05 -
7.60144830565e-05	-7.12518813089e-05	-5.99354461883e-05	-7.51645711716e-05 -
3.52802089765e-05	-7.59675676818e-05	-0.000122908910271	-8.37808620417e-05 -
0.000199748479645	-0.000225498559303	-0.000299852254102	-0.00137971213553
0.00225383625366	0.000222106522415	0.000117715862871	7.32263506507e-05
6.25418979325e-05	6.92917164997e-05	4.037241888e-05	5.92764699832e-05
2.83369299723e-05	5.82145476073e-05	4.53001048299e-05	5.0560112868e-05
4.75559500046e-05	5.91506395722e-05	2.9575339795e-05	3.60823432857e-05
4.28182902397e-05	9.47616263147e-06	2.82924866042e-05	1.44651085066e-05
1.84351465577e-05	2.99323119179e-06	2.02673272724e-05	1.38856275953e-05
2.39230357693e-05	1.01590594568e-05	7.77770492277e-06	1.63948388945e-05
3.4671497815e-06	9.79331070994e-06	-2.66348092737e-06	8.34015736473e-06
1.37623737828e-06	7.18825594959e-06	-1.72181694325e-06	2.76931655208e-06 -
9.34515810513e-06	1.97041913452e-06	-1.55771431309e-06	2.83783629129e-06
7.09729692971e-06	-3.37294500241e-06	8.42990687033e-07	-1.31613546728e-06
2.85011287815e-06	1.95264601643e-06	-2.35224979406e-06	5.34264290764e-06
5.38853953458e-07	3.03897081722e-06	-1.1234566955e-05	4.07221705245e-07
2.5734088922e-05	1.53106557264e-05	5.71191558265e-05	-1.89281618077e-05 -
1.01514087874e-05	-1.1526902199e-05	1.56137411977e-06	-9.10408743948e-06 -
1.6485046217e-06	-1.38697050716e-05	-1.64660582413e-06	-1.30044963953e-05 -
9.72137331701e-06	-1.18258340081e-05	-1.10163100544e-05	-2.02856863325e-05 -
1.28133751787e-06	-1.83538886631e-05	-3.99468035539e-06	-1.01575587905e-05 -
9.91281649476e-06	-1.19286560221e-05	-8.64937078404e-07	-1.60061954375e-05

0

liamp 1 1 1000000000 0 0 4 1 0 0 64

4 0 0 0 0.577882409096

0

lcpeak_ 7 1 32767 0 0 2 1 0 1 64

1 0

0

lifrq 1 1 1000000000 -1000000000 0 4 1 0 1 64

7 4184.7535823 3445.32962737 3445.32962737 2811.537666 2811.537666 2072.11371107 0

0

llfrq 1 1 1000000000 -1000000000 0 4 1 0 0 64

200	6387.48778104	6368.71945259	6356.20723363	6324.92668622	6312.41446725
	6299.90224829	6287.39002933	6268.62170088	6243.59726295	6231.08504399
	6206.06060606	6168.52394917	6156.01173021	6143.49951124	6130.98729228
	6112.21896383	6074.68230694	6049.65786901	6005.86510264	5974.58455523
	5955.81622678	5943.30400782	5924.53567937	5899.51124145	5880.742913
	5849.46236559	5836.95014663	5824.43792766	5805.66959922	5786.90127077
	5768.13294233	5755.62072336	5736.85239492	5724.34017595	5705.57184751
	5668.03519062	5643.01075269	5624.24242424	5611.73020528	5592.96187683
	5542.91300098	5524.14467253	5480.35190616	5430.3030303	5380.25415445
	5348.97360704	5311.43695015	5286.41251222	5261.38807429	5230.10752688
	5192.57086999	5142.52199413	5123.75366569	5104.98533724	5061.19257087
	4992.37536657	4911.0459433	4854.74095797	4792.17986315	4742.13098729
	4710.85043988	4692.08211144	4673.31378299	4617.00879765	4560.70381232
	4498.1427175	4473.11827957	4429.3255132	4391.7888563	4366.76441838
	4347.99608993	4316.71554252	4279.17888563	4266.66666667	4254.1544477
	4235.38611926	4185.3372434	4160.31280547	4135.28836755	4110.26392962
	4097.75171065	4085.23949169	4072.72727273	4053.95894428	4041.44672532
	4028.93450635	4010.16617791	3997.65395894	3978.8856305	3953.86119257
	3941.34897361	3928.83675464	3916.32453568	3897.55620723	3885.04398827
	3866.27565982	3853.76344086	3834.99511241	3809.97067449	3772.4340176
	3753.66568915	3741.15347019	3728.64125122	3716.12903226	3703.61681329
	3684.84848485	3672.33626588	3653.56793744	3634.79960899	3622.28739003
	3591.00684262	3572.23851417	3497.16520039	3472.14076246	3459.6285435
	3447.11632454	3428.34799609	3409.57966764	3365.78690127	3334.50635386
	3284.45747801	3259.43304008	3234.40860215	3203.12805474	3178.10361681
	3096.77419355	3021.70087977	2996.67644184	2984.16422287	2971.65200391
	2959.13978495	2940.3714565	2927.85923754	2896.57869013	2859.04203324
	2846.52981427	2834.01759531	2815.24926686	2783.96871945	2765.20039101
	2746.43206256	2727.66373412	2696.38318671	2671.35874878	2652.59042033
	2633.82209189	2615.05376344	2602.54154448	2590.02932551	2571.26099707
	2546.23655914	2521.21212121	2508.69990225	2496.18768328	2477.41935484
	2464.90713587	2452.39491691	2433.62658847	2402.34604106	2389.83382209
	2377.32160313	2339.78494624	2327.27272727	2314.76050831	2289.73607038
	2277.22385142	2264.71163245	2252.19941349	2233.43108504	2220.91886608
	2202.15053763	2189.63831867	2170.86999022	2158.35777126	2127.07722385
	2114.56500489	2083.28445748	2070.77223851	2045.74780059	1995.69892473
	1983.18670577	1970.6744868	1945.65004888	1926.88172043	1908.11339198
	1883.08895406	1864.32062561	1845.55229717	1826.78396872	1814.27174976
	1801.75953079	1776.73509286	1745.45454545	1707.91788856	1689.14956012
	1670.38123167	1657.86901271	1639.10068426	1614.07624633	1576.53958944

0

lockgain_ 1 1 48 0 1 2 1 16 1 64

1 23

0

loc_ 7 1 12 12 12 2 1 8201 0 64

1 0

0

```
lockfreq_ 5 1 160 0 1e-07 2 1 9 1 64
1 122.7618
0
lockpower_ 1 1 68 0 1 2 1 16 1 64
1 48
0
lockphase_ 1 1 360 0 1 2 1 16 1 64
1 344
0
n1 2 2 6 0 0 4 1 3 1 64
1 ""
0
method 2 2 6 0 0 2 1 3 1 64
1 "/vnmr/shimmethods/z1z2"
0
lsfrq 1 1 9.99999984307e+17 -9.99999984307e+17 0 3 1 0 0 64
1 0
0
lsfid 7 1 64000 -64000 1 3 1 0 0 64
1 0
0
lp2 1 1 3600 -3600 0.1 4 1 3 1 64
1 0
0
lp1 1 1 3600 -3600 0.1 4 1 3 1 64
1 0
0
lsfid2 7 1 64000 -64000 1 3 1 0 0 64
1 0
```

```
0
lsfid1 7 1 64000 -64000 1 3 1 0 0 64
1 0
0
macro 2 2 6 0 0 4 1 3 1 64
1 ""
0
lsfrq2 1 1 9.99999984307e+17 -9.99999984307e+17 0 3 1 0 0 64
1 0
0
lsfrq1 1 1 9.99999984307e+17 -9.99999984307e+17 0 3 1 0 0 64
1 0
0
lvl 1 1 10000000000 -10000000000 0 4 1 1 1 64
1 0.00129447644839
0
mcyc 7 1 32767 0 0 2 1 0 1 64
1 1
0
math 2 2 1 0 0 3 1 3 1 64
1 "f"
3 "d" "f" "i"
mess_flg 2 2 8 0 0 2 1 0 1 64
1 "n"
0
mixshift 3 1 14 14 14 2 1 8192 1 64
1 0
0
mixmlev 3 1 14 14 14 2 1 8192 1 64
1 0.02
```

0
mix 3 1 14 14 14 2 1 8192 1 64
1 0.075
0
mixnoe 3 1 14 14 14 2 1 8192 1 64
1 0.14
0
mlevpwr 7 1 32767 0 0 2 1 0 1 64
1 50
0
osfilt 2 2 8 0 0 2 1 0 1 64
1 "a"
5 "a" "A" "b" "B" ""
nt 7 1 1000000000 1 1 2 1 2 1 64
1 48
0
ni2 7 1 32767 0 1 2 1 0 1 64
1 32
0
n3 2 2 6 0 0 4 1 3 1 64
1 ""
0
n2 2 2 6 0 0 4 1 3 1 64
1 ""
0
ni 7 1 32767 0 0 2 1 0 1 64
1 32
0
np 7 1 524288 32 2 2 1 11 1 64

1 1538
0
notebook 2 2 8 0 0 2 1 0 1 64
1 ""
0
oscoef 7 1 49999 3 2 2 1 1 0 64
1 31
0
ntype3d 4 2 4 0 0 3 1 0 1 64
1 "nn"
0
osfb 1 1 100000 0 0 2 1 1 0 64
1 0
0
page 2 2 8 0 0 2 1 0 1 64
1 ""
0
oversamp 7 1 68 0 1 2 1 9 1 64
1 20
0
oslsfrq 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 1 0 64
1 0
0
p1 6 1 13 13 13 2 1 8194 1 64
1 0
0
pad 3 1 14 14 14 2 1 8194 1 64
1 0
0
phase 7 1 4 0 1 2 1 0 1 64

2 1 2
0
parversion 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 4 1 64
1 5.1
0
parstyle_ 2 2 8 0 0 4 1 0 1 64
1 "ppa"
0
path3d 2 2 8 0 0 4 1 0 1 64
1 "/home/guest/vnmrsys/exp8/datadir3d"
0
phfid 1 1 3600 -3600 0.1 3 1 0 0 64
1 0
0
phase2 7 1 4 0 1 2 1 0 1 64
2 1 2
0
r3 1 1 1e+18 -1e+18 0 4 1 1 1 64
1 99.3962666667
0
pw 6 1 13 13 13 2 1 8194 1 64
1 7.55
0
priority 7 1 32768 0 1 2 1 0 1 64
1 5
0
pltmod 2 2 8 0 0 4 1 0 1 64
1 "off"
5 "off" "fixed" "full" "variable" "user"

```

pkpick_ 2 2 8 0 0 4 1 0 1 64
1 ""
0
phfid2 1 1 3600 -3600 0.1 3 1 0 0 64
1 0
0
plane 2 2 8 0 0 4 1 0 1 64
1 "f1f3"
6 "f1f3" "f3f1" "f2f3" "f3f2" "f1f2" "f2f1"
preacq 6 1 13 13 13 2 1 8192 0 64
1 0
0
pmode 2 2 8 0 0 3 1 0 1 64
1 "partial"
0
presat 3 1 14 14 14 2 1 8192 1 64
1 1.5
0
proc2 2 2 8 0 0 3 1 1 1 64
1 "ft"
0
proc 2 2 10 0 0 3 1 1 1 64
1 "ft"
0
probe_ 2 2 8 0 0 2 1 8 1 64
1 ""
0
proc1 2 2 10 0 0 3 2 1 1 64
1 "ft"
0

```

```
pslabel 2 2 8 0 0 2 1 11 1 64
1 "Ile_cg2_cd1_noesy_800_lek"
0
procdim 7 1 10000000000 -10000000000 0 3 1 0 1 64
1 0
0
ptspec3d 4 2 4 0 0 3 1 0 1 64
1 "nnn"
0
pwd1 6 1 13 13 13 2 1 8192 1 64
1 0
0
pwco_sh 2 2 8 0 0 2 1 0 1 64
1 "herm180_17p6_750"
0
pwc 6 1 13 13 13 2 1 8192 1 64
1 12.8
0
pw90 6 1 13 13 13 2 1 8194 1 64
1 8.2
0
pwc_reb 6 1 13 13 13 2 1 8192 1 64
1 1850
0
pwd 6 1 13 13 13 2 1 8192 1 64
1 0
0
pwcod 6 1 13 13 13 2 1 8192 1 64
1 234
```

0

pwx2 6 1 13 13 13 2 1 8192 1 64

1 0

0

pwn15 6 1 200 0 0.025 2 1 1024 1 64

1 36.5

0

pwn 6 1 13 13 13 2 1 8192 1 64

1 0

0

pwx1 6 1 13 13 13 2 1 8192 1 64

1 36

0

r1 1 1 1e+18 -1e+18 0 4 1 1 1 64

1 0.0013333

0

pxcodec 6 1 13 13 13 2 1 8192 1 64

1 0

0

r2 1 1 1e+18 -1e+18 0 4 1 1 1 64

1 182.142857143

0

rfl 1 1 10000000000 -10000000000 0 4 1 1 1 64

1 49676.2000596

0

reffrq1 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64

1 499.6974483

0

r7 1 1 1e+18 -1e+18 0 4 1 1 1 64

1 0

0
r5 1 1 1e+18 -1e+18 0 4 1 1 1 64
1 0.032
0
r4 1 1 1e+18 -1e+18 0 4 1 1 1 64
1 0.0182848
0
r6 1 1 1e+18 -1e+18 0 4 1 1 1 64
1 0
0
reffrq 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 799.7630899
0
ref 5 1 10000000000 -10000000000 0 3 1 0 1 64
1 0
0
refpos2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 0 64
1 0
0
refpos 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0
0
reffrq2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 499.6974483
0
refpos1 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 0 64
1 0
0
refsource2 2 2 8 0 0 4 1 0 1 64

```

1 "sfrq"
0
refsource1 2 2 8 0 0 4 1 0 1 64
1 "sfrq"
0
rfband 4 2 4 0 0 2 1 0 1 64
1 "cccc"
3 "c" "h" "l"
rp 1 1 3600 -3600 0.1 4 1 3 1 64
1 -134.454676097
0
rfp1 1 1 10000000000 -10000000000 0 4 1 1 1 64
1 4342.68017578
0
rfl2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0
0
rfl1 1 1 10000000000 -10000000000 0 4 1 1 1 64
1 6565.28671875
0
rfp 1 1 10000000000 -10000000000 0 4 1 1 1 64
1 0
0
rof1 6 1 13 13 13 2 1 8194 1 64
1 0
0
rfp2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0
0
rof2 6 1 13 13 13 2 1 8194 1 64

```

```
1 1
0
samplename 2 2 8 0 0 2 1 0 1 64
1 ""
0
rp2 1 1 3600 -3600 0.1 4 1 3 1 64
1 0
0
rp1 1 1 3600 -3600 0.1 4 1 3 1 64
1 0
0
sample 2 2 8 0 0 2 1 0 1 64
1 "lysh2o"
0
satflg 2 2 8 0 0 2 1 0 1 64
1 "y"
0
tpwr 7 1 17 17 17 2 1 8194 1 64
1 63
0
sp2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0
0
seqfil 2 2 8 0 0 2 1 11 1 64
1 "Ile_cg2_cd1_noesy_800_lek"
0
sb2 1 1 1000 -1000 0.001 3 1 1 0 64
1 0
0
```

```
sb 1 1 1000 -1000 0.001 3 1 0 0 64
1 0.140572652221
0
saveglobal_ 2 2 8 0 0 3 1 0 1 64
15 "probe"
"lcpeak"
"loc"
"lockpower"
"lockgain"
"lockphase"
"lockfreq"
"z0"
"lkof"
"vloc"
"vrack"
"vzone"
"vproto"
"pkpick"
"parstyle"
0
satpwr 1 1 9.99999984307e+17 -9.99999984307e+17 0 2 1 0 1 64
1 12
0
sb1 1 1 1000 -1000 0.001 3 1 1 1 64
1 0.0154493479058
0
sc 1 1 1 1 1 4 1 8195 1 64
1 0
0
sbs1 1 1 1000 -1000 0.001 3 1 1 1 64
```

```

1 -0.00463480316103
0
sbs 1 1 1000 -1000 0.001 3 1 1 0 64
1 -0.0195756480098
0
sbs2 1 1 1000 -1000 0.001 3 1 1 0 64
1 0
0
sc2 1 1 3 3 3 4 1 8195 1 64
1 0
0
scf 1 1 1 0 0 2 1 0 1 64
1 0.45
0
shims 2 2 8 0 0 2 1 0 1 64
1 ""
0
sfrq 1 1 10000000000 0 0 2 1 11 1 64
1 799.7194143
0
sf1 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0
0
sf 1 1 8190 0 1e-07 4 1 3 1 64
1 0
0
sf2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0
0

```

```
sh_reb 2 2 8 0 0 2 1 0 1 64
1 "reb_on"
0
shape 2 2 8 0 0 2 1 0 1 64
1 "herm180_trc"
0
sp 1 1 1000000000 -1000000000 0 4 1 3 1 64
1 -49670.3348194
0
solvent 2 2 6 0 0 2 1 11 1 64
1 "d2o"
0
sn 1 1 1e+18 -1e+18 0 3 1 1 1 64
1 0
0
sp1 1 1 1000000000 -1000000000 0 4 1 3 1 64
1 -2222.60654297
0
temp 1 1 200 -150 0.1 2 1 8 1 64
1 50
0
ssntaps 7 1 2500 0 1 3 1 0 0 64
1 121
0
ss3d 2 2 8 0 0 3 1 0 1 64
1 ""
3 "" "lfs" "zfs"
spin 1 1 32000000 0 0.1 2 1 0 0 64
1 0
0
```

```

specdc3d 4 2 4 0 0 3 1 0 1 64
1 "nnn"
0
ss 7 1 32767 -32768 0 2 1 0 1 64
1 16
0
ssfilter 1 1 50000 10 0.1 3 1 0 1 64
1 50
0
sslsfrq 1 1 9.99999984307e+17 -9.99999984307e+17 0 3 1 0 0 64
1 0
0
sw1 1 1 5000000 1 -2.5e-08 2 1 0 1 64
1 2000
0
sspul 2 2 8 0 0 2 1 0 1 64
1 "n"
0
ssorder 7 1 20 1 1 3 1 0 0 64
1 7
0
sw 1 1 5 5 5 2 1 8203 1 64
1 12012.012012
0
taua 3 1 14 14 14 2 1 8192 1 64
1 0.0018
0
sw2 1 1 5000000 1 -1.25e-08 2 1 0 1 64
1 2000

```

0
time_submitted_local 2 2 8 0 0 2 1 0 1 64
1 "20100723T182415X06PM%##%"
0
time_processed 2 2 8 0 0 3 1 0 1 64
1 ""
0
th2d 1 1 1 1e-18 0 4 1 17 1 64
1 0.8
0
th 1 1 10000000000 0 0 4 1 1 1 64
1 121.937713623
0
time_complete 2 2 8 0 0 2 1 0 1 64
1 "20100723T182415"
0
time_saved 2 2 8 0 0 2 1 0 1 64
1 ""
0
time_run 2 2 8 0 0 2 1 0 1 64
1 "20100723T182415"
0
time_submitted 2 2 8 0 0 2 1 0 1 64
1 "20100723T182415"
0
tn 2 2 4 0 0 2 1 8 1 64
1 "H1"
0
tin 2 2 1 0 0 2 1 2 1 64
1 "y"

```
3 "n" "w" "y"
time_svfddate 2 2 8 0 0 2 1 0 1 64
1 "20100723T182415"
0
tlt 1 1 10000000000 -10000000000 0 4 1 1 1 64
1 -0.00106104693032
0
tof 5 1 7 7 7 2 1 8202 1 64
1 -292
0
tnsat 4 2 4 0 0 2 1 0 1 64
1 "y"
0
tof_me 5 1 10000000000 -10000000000 0 2 1 0 1 64
1 -3594.84118106
0
y1 7 1 19 19 19 2 1 8192 1 64
1 1303
0
wp 1 1 5000000 0 0 4 1 11 1 64
1 11994.4162913
0
vs2d 1 1 10000000000 1e-06 0 4 1 3 1 64
1 3188945.09581
0
vloc_ 2 2 8 0 0 2 1 8 1 64
1 "A0"
0
trim 3 1 14 14 14 2 1 8192 1 64
```

1 0.0005
0
tpwrmess 1 1 17 17 17 2 1 8192 1 64
1 53
0
tpwrf 7 1 4095 0 1 2 1 2 0 64
1 4095
0
trace 2 2 2 0 0 4 1 3 1 64
1 "f1"
3 "f1" "f2" "f3"
tsatpwr 1 1 17 17 17 2 1 8192 1 64
1 0
0
vf 1 1 10000000000 0 0 4 1 3 1 64
1 11992.7179577
0
vpfi 1 1 500 -500 0 4 1 0 1 64
1 0
0
vp 7 1 500 -500 0.1 4 1 3 1 64
1 50
0
vo 1 1 500 -500 0 4 1 1 1 64
1 0
0
vpf 1 1 500 -500 0 4 1 0 1 64
1 16.1448614824
0
vrack_ 7 1 5 1 0 2 1 0 1 64

1 1
0
vproto_ 2 2 8 0 0 2 1 0 1 64
1 ""
0
vs 1 1 10000000000 1e-06 0 4 1 3 1 64
1 454697.639932
0
wc2 1 1 4 4 4 4 1 8195 1 64
1 155
0
vzone_ 7 1 15 1 0 2 1 0 1 64
1 1
0
vtc 1 1 255 0 1 2 1 2 1 64
1 0
0
vsproj 1 1 10000000000 1e-06 0 4 1 3 1 64
1 3188945.09581
0
vtwait 3 1 14 14 14 2 1 8194 1 64
1 180
0
wc 1 1 2 2 2 4 1 8203 1 64
1 250
0
wbs 2 2 6 0 0 3 1 3 1 64
1 ""
0

```

wf 1 1 8190 0 1e-07 4 1 3 1 64
1 0.0640769250001
0
werr 2 2 6 0 0 3 1 3 1 64
1 ""
0
wdone 2 2 8 0 0 3 1 0 1 64
1 "acqdone"
0
wexp 2 2 6 0 0 3 1 3 1 64
1 "svf('pcnohmqc1120') "
0
wf2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0
0
wf1 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 0.256
0
wnt 2 2 6 0 0 3 1 3 1 64
1 ""
0
x2y2 7 1 19 19 19 2 1 8192 1 64
1 3749
0
wtfile 2 2 15 0 0 3 1 1 1 64
1 ""
0
wp2 1 1 9.99999984307e+17 -9.99999984307e+17 0 4 1 0 1 64
1 2000
0

```

```
wp1 1 1 100000 0 0 4 1 3 1 64
1 2000
0
wshim 4 2 4 0 0 2 1 1 1 64
1 "n"
15 "e" "f" "g" "n" "s" "0" "1" "2" "3" "4" "5" "6" "7" "8" "9"
wtfile2 2 2 8 0 0 3 1 1 1 64
1 ""
0
wtfile1 2 2 15 0 0 3 2 1 1 64
1 ""
0
x1 7 1 19 19 19 2 1 8192 1 64
1 -8330
0
xdiag 1 1 1e+18 0 0 4 1 17 1 64
1 0
0
x4 7 1 19 19 19 2 1 8192 1 64
1 1615
0
x3 7 1 19 19 19 2 1 8192 1 64
1 -157
0
xz 7 1 19 19 19 2 1 8192 1 64
1 1785
0
xy 7 1 19 19 19 2 1 8192 1 64
1 2534
```

0
 xz2 7 1 19 19 19 2 1 8192 1 64
 1 -3233
 0
 z3x 7 1 19 19 19 2 1 8192 1 64
 1 -722
 0
 z2 7 1 19 19 19 2 1 8192 1 64
 1 -762
 0
 yz2 7 1 19 19 19 2 1 8192 1 64
 1 -731
 0
 y4 7 1 19 19 19 2 1 8192 1 64
 1 3108
 0
 y3 7 1 19 19 19 2 1 8192 1 64
 1 315
 0
 yz 7 1 19 19 19 2 1 8192 1 64
 1 1729
 0
 z1 7 1 19 19 19 2 1 8192 1 64
 1 -95
 0
 z0_ 1 1 19 19 19 2 1 8208 1 64
 1 -12067
 0
 z1c 7 1 19 19 19 2 1 8192 1 64
 1 -1044

0
 z2xy 7 1 19 19 19 2 1 8192 1 64
 1 620
 0
 z2x2y2 7 1 19 19 19 2 1 8192 1 64
 1 -4618
 0
 z2c 7 1 19 19 19 2 1 8192 1 64
 1 196
 0
 z2x3 7 1 19 19 19 2 1 8192 1 64
 1 0
 0
 z3 7 1 19 19 19 2 1 8192 1 64
 1 4303
 0
 z2y3 7 1 19 19 19 2 1 8192 1 64
 1 0
 0
 z3c 7 1 19 19 19 2 1 8192 1 64
 1 0
 0
 z5 7 1 19 19 19 2 1 8192 1 64
 1 22639
 0
 z4x 7 1 19 19 19 2 1 8192 1 64
 1 -1450
 0
 z3y 7 1 19 19 19 2 1 8192 1 64

1 16138
 0
 z3x3 7 1 19 19 19 2 1 8192 1 64
 1 0
 0
 z3x2y2 7 1 19 19 19 2 1 8192 1 64
 1 5225
 0
 z3xy 7 1 19 19 19 2 1 8192 1 64
 1 -16178
 0
 z4 7 1 19 19 19 2 1 8192 1 64
 1 -11645
 0
 z3y3 7 1 19 19 19 2 1 8192 1 64
 1 0
 0
 z4c 7 1 19 19 19 2 1 8192 1 64
 1 0
 0
 z4xy 7 1 19 19 19 2 1 8192 1 64
 1 -2696
 0
 z4x2y2 7 1 19 19 19 2 1 8192 1 64
 1 -1027
 0
 z4y 7 1 19 19 19 2 1 8192 1 64
 1 -11164
 0
 z7 7 1 19 19 19 2 1 8192 1 64

1 0

0

z5y 7 1 19 19 19 2 1 8192 1 64

1 -7429

0

z5x 7 1 19 19 19 2 1 8192 1 64

1 -6555

0

z6 7 1 19 19 19 2 1 8192 1 64

1 -9036

0

zx2y2 7 1 19 19 19 2 1 8192 1 64

1 -2017

0

z8 7 1 19 19 19 2 1 8192 1 64

1 0

0

zxy 7 1 19 19 19 2 1 8192 1 64

1 8060

0

zx3 7 1 19 19 19 2 1 8192 1 64

1 10341

0

zy3 7 1 19 19 19 2 1 8192 1 64

1 824

0