```
; Gradient-selected HZQC (gsHZQC) methyl-TROSY with methyl filter
; For recording 1H-13C correlations in fully protonated methyl groups
; With or without 13C polarization enhancement
; Reference: Gill, ML and Palmer, III, AG, Journal of Biomolecular NMR (2011)
XX:XXX-XXX, Figure 1
; Data processing: For each consecutive block of four data rows, add the first
to the second and the third to the fourth,
;                   then process using Rance-Kay for frequency discrimination
;$CLASS=HighRes
;$DIM=2D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

prosol relations=<triple>

#include <Avance.incl>
#include <Grad.incl>
#include <Delay.incl>

; Ensure the -DNOPOL is set if ZGOPTS is empty
#ifndef POL1
#ifndef POL2
#define NOPOL
#endif
#endif

; Unset other flags if using one of polarization schemes
#ifdef POL2
#undef POL1
#undef NOPOL
#endif

#ifdef POL1
#undef POL2
#undef NOPOL
#endif


"cnst21=o1/bf1" ; acquisition frequency should be set the same as O1P
"p11=p1*2"      ; 1H 180degree pulse at hard power
"p21=p2*2"      ; 13C 180degree pulse at hard power
```

```
"d11=10u"       ; hardware delay
"d16=250u"      ; gradient recovery delay
"d28=p21"       ; compensation for 13C 180
"d29=p1*4+8u"   ; compensation for 1H composite pulse
"TAU=3.91m"     ; 1/(2JCH), JCH=128 Hz
"TAU2=0.75m"    ; sin(2piJCH*TAU2) = 3^(-1/2)
"in0=inf1"      ; t1 increment
"d0=in0/2"      ; initial t1 delay (1/2 dwell)
"l0=td1/4"      ; number of t1 complex points
"l1=0"          ; initialize loop counter

"DELTA1=TAU/4"
"DELTA2=TAU/4-d16-p16"

#ifdef NOPOL
"DELTA3=TAU-d16-d11-p1*0.6366"
"DELTA4=TAU-p16-d16-d11-4u"
#endif

#ifdef POL1
"DELTA3=TAU/2-1*TAU2-larger(p1,p2)-p1*0.6366-p17-d16"
"DELTA4=TAU/2+1*TAU2-larger(p1,p2)"
"DELTA5=TAU/2+1*TAU2-larger(p1,p2)-p17-d16-4u"
"DELTA6=TAU/2-1*TAU2-d16-p16-d11-4u-larger(p1,p2)"
#endif

#ifdef POL2
"DELTA3=TAU-p1*0.6366"
"DELTA4=TAU-p16-d16-d11-4u"
"DELTA5=TAU/2+TAU2-p1-p17-d16"
"DELTA6=TAU/2-TAU2-p1-p17-d16-4u"
#endif



1 ze
  d11 BLKGRAD
2 30m
3 d11 do:f2 fq=cnst20(bf ppm):f1
  d11 pl9:f1
  d1 cw:f1 ph0 pl2:f2
  4u do:f1
  d11 pl1:f1 fq=cnst21(bf ppm):f1
```

```
  d11 UNBLKGRAD

#ifdef NOPOL
  ;***purge***
  (p2 ph0):f2
  4u
  p15:gp1
  d16
  ;***evolve AP to MQ***
  (p1 ph1):f1
  d16
  d11
  DELTA3
  if "l1 % 4 == 0" goto 4
  if "l1 % 4 == 1" goto 5
  if "l1 % 4 == 2" goto 6
  if "l1 % 4 == 3" goto 7
#endif

#ifdef POL1
  p15:gp1
  d16
  ;***transfer polarization from 13C to 1H***
  (p2 ph7):f2
  TAU2
  TAU2
  (p1 ph1):f1
  ;***evolve AP to MQ***
  DELTA3
  p17:gp6
  d16
  (center (p11 ph20):f1 (p21 ph7):f2 )
  4u
  p17:gp6
  d16
  DELTA5
  if "l1 % 4 == 0" goto 6
  if "l1 % 4 == 1" goto 7
  if "l1 % 4 == 2" goto 4
  if "l1 % 4 == 3" goto 5
#endif
```

```
#ifdef POL2
  p15:gp1
  d16
  ;***transfer polarization from 13C to 1H***
  (p2 ph7):f2
  DELTA5
  p17:gp6
  d16
  (p11 ph20):f1
  4u
  p17:gp7
  d16
  DELTA6
  (ralign (p1 ph1):f1 (p21 ph7):f2 )
  ;***evolve AP to MQ***
  DELTA3
  if "l1 % 4 == 0" goto 4
  if "l1 % 4 == 1" goto 5
  if "l1 % 4 == 2" goto 6
  if "l1 % 4 == 3" goto 7
#endif

    ;***create MQ magnetization***
 4  (p2 ph2):f2
    ;***J-filter***
    DELTA1
    d29
    ;***t1***
    d0
    (p21 ph20):f2
    (p1 ph10 4u p11 ph11 4u p1 ph10):f1
    ;***J-filter***
    DELTA2
    p16:gp2 ; ZQ encode gradient
    d16
    ;***create AP magnetization***
    (p2 ph6):f2
    d28
    d29
 goto 8

    ;***create MQ magnetization***
```

```
5  (p2 ph7):f2
   ;***J-filter***
   DELTA1
   d29
   (p21 ph20):f2
   ;***t1***
   d0
   (p1 ph10 4u p11 ph11 4u p1 ph10):f1
   ;***J-filter***
   DELTA2
   p16:gp3 ; DQ encode gradient
   d16
   ;***create AP magnetization***
   (p2 ph5):f2
   d28
   d29
goto 8

6  d28
   d29
   ;***create MQ magnetization***
   (p2 ph2):f2
   ;***J-filter***
   DELTA1
   (p1 ph10 4u p11 ph11 4u p1 ph10):f1
   (p21 ph20):f2
   ;***t1***
   d0
   ;***J-filter***
   d29
   DELTA2
   p16:gp2 ; ZQ encode gradient
   d16
   ;***create AP magnetization***
   (p2 ph6):f2
goto 8

7  d28
   d29
   ;***create MQ magnetization***
   (p2 ph7):f2
   ;***J-filter***
```

```
    DELTA1
    (p1 ph10 4u p11 ph11 4u p1 ph10):f1
    ;***t1***
    d0
    (p21 ph20):f2
    ;***J-filter***
    d29
    DELTA2
    p16:gp3 ; DQ encode gradient
    d16
    ;***create AP magnetization***
    (p2 ph5):f2
 goto 8


#ifdef POL1
 8  DELTA4
    (center (p11 ph10):f1 (p21 ph20):f2 )
    4u
    p16:gp5 ; SQ decode gradient
    d16 pl12:f2
    d11 BLKGRAD
    DELTA6
#else
 8  4u
    p16:gp4 ; SQ decode gradient
    d16 pl12:f2
    d11 BLKGRAD
    DELTA4
#endif


    ;***detect***
    go=2 ph30 cpd2:f2
    10u do:f2
    30m wr #0 if #0 zd
    30m iu1
    lo to 2 times 4
    30m id0
    lo to 3 times l0
exit
```

```
ph0=0
ph1=0 0
ph2=0 2
ph5=0 0
ph6=2 2
ph7=2 0
ph10=0 0
ph11=1 1
ph20=0 0

#ifdef POL2
ph30=2 0
#else
ph30=0 2
#endif

;*** VARIABLES SET BY USER ***
;d1 = recycle delay
;td1 = 4 * number of complex points (e.g. for 250 t1 points, td1=1000)
;o1p = set offset to just outside of methyl region [2.0 ppm]

;p1 = 1H hard 90 @ pl1
;p2 = 13C hard 90 at pl2
;p11 = 1H hard 180 @ pl1
;p21 = 13C hard 180 @ pl2
;p15 = pulse for gz1 [1ms]
;p16 = pulse for gz2-gz5 [500us]
;p17 = pulse for gz6-gz7 [500us]

;pl0 = 120 dB
;pl1 = 1H hard power
;pl2 = 13C hard power
;pl12 = 13C broadband decoupling power
;p15 = pulse for gpz1 [1ms]
;p16 = pulse for gpz2-gpz5 [500us]
;p17 = pulse for gpz6-gpz7 [500us]

;cnst2 = number of 1/(2JCH) intervals for relaxation delay (T)
;cnst20 = water offset [4.7ppm]

;gpz1 7.5 G/cm (15%)
;gpz2 30 G/cm (60%)
```

```
;gpz3 18 G/cm (36%)
;gpz4 -22.5 G/cm (-45%)
;gpz5 22.5 G/cm (45%)
;gpz6 5 G/cm (10%)
;gpz7 -5 G/cm (-10%)

;gpnam1: SINE.100
;gpnam2: SINE.50
;gpnam3: SINE.50
;gpnam4: SINE.50
;gpnam5: SINE.50
;gpnam6: SINE.50
;gpnam7: SINE.50

; F1 frequency discrimination has been coded for echo/antiecho, thus
; FnMODE: undefined

; preprocessor flags, use ONLY ONE of the following:
; NOPOL : to purge 13C polarization, this is the default if nothing is set
;         option -DNOPOL (eda: ZGOPTNS)
; POL1  : to use 13C polarization enhancement scheme in Figure 1B
;         option -DPOL1 (eda: ZGOPTNS)
; POL2  : to use 13C polarization enhancement scheme in Figure 1C
;         option -DPOL2 (eda: ZGOPTNS)

; Data processing: For each consecutive block of four data rows,
;                  add the first to the second and the third to the fourth,
;                  then process using Rance-Kay (Echo-Antiecho) for frequency
discrimination
```

```
##TITLE= Parameter file, TOPSPIN        Version 2.1
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##NPOINTS= 658  $$ modification sequence number
##ORIGIN= Bruker BioSpin GmbH
##OWNER= mgill
$$ 2011-05-05 14:03:21.238 -0400  mgill@bh009902.nysbc.org
$$ /opt/topspin/data/mgill/nmr/RNaseH.D2O_methylTROSY_MLGILL_int/101/acqus
$$ process /opt/topspin/prog/mod/shimcntl
##$ACQT0= 1000000
##$AMP= (0..31)
100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100
100 100 100 100 100 100 100 100 100 100 100 100 100 100
##$ANAVPT= -1
##$AQSEQ= 0
##$AQ_mod= 3
##$AUNM= <au_getlinv>
##$AUTOPOS= <>
##$BF1= 700.13
##$BF2= 176.047829
##$BF3= 70.943557
##$BF4= 700.13
##$BF5= 600.13
##$BF6= 600.12
##$BF7= 600.12
##$BF8= 600.12
##$BYTORDA= 1
##$CFDGTYP= 2
##$CFRGTYP= 5
##$CHEMSTR= <none>
##$CNST= (0..63)
1 1 3 1 1 1 1 1 1 1 1 1 1 1 1 1 -0.5 1 1 4.703 2 30 20 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##$CPDPRG= <garp>
##$CPDPRG1= <>
##$CPDPRG2= <waltz16>
##$CPDPRG3= <garp>
##$CPDPRG4= <mlev>
##$CPDPRG5= <mlev>
##$CPDPRG6= <mlev>
##$CPDPRG7= <mlev>
##$CPDPRG8= <mlev>
```

```
##$CPDPRGB= <>
##$CPDPRGT= <>
##$D= (0..63)
0.0001142929 1.2 0.00345 0.0023 0.001725 0 0 0.484 0 0.07 0 1e-05 2e-05
3e-06 0 0.012 0.00025 0 0 0 0 0 0 0 0.00086207 0 0 0 2.9e-05 5.776e-05
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$DATE= 1304618560
##$DBL= (0..7)
120 120 120 120 120 120 120 120
##$DBP= (0..7)
150 150 150 150 150 150 150 150
##$DBP07= 0
##$DBPNAM0= <>
##$DBPNAM1= <>
##$DBPNAM2= <>
##$DBPNAM3= <>
##$DBPNAM4= <>
##$DBPNAM5= <>
##$DBPNAM6= <>
##$DBPNAM7= <>
##$DBPOAL= (0..7)
0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
##$DBPOFFS= (0..7)
0 0 0 0 0 0 0 0
##$DE= 6
##$DECBNUC= <off>
##$DECIM= 16
##$DECNUC= <off>
##$DECSTAT= 4
##$DIGMOD= 1
##$DIGTYP= 8
##$DL= (0..7)
120 120 120 120 120 120 120 120
##$DP= (0..7)
150 150 150 150 150 150 150 150
##$DP07= 0
##$DPNAME0= <>
##$DPNAME1= <>
##$DPNAME2= <>
##$DPNAME3= <>
##$DPNAME4= <>
##$DPNAME5= <>
```

```
##$DPNAME6= <>
##$DPNAME7= <>
##$DPOAL= (0..7)
0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
##$DPOFFS= (0..7)
0 0 0 0 0 0 0 0
##$DQDMODE= 0
##$DR= 18
##$DS= 4
##$DSLIST= <SSSSSSSSSSSSSSS>
##$DSPFIRM= 0
##$DSPFVS= 12
##$DTYPA= 0
##$EXP= <>
##$F1LIST= <111111111111111>
##$F2LIST= <222222222222222>
##$F3LIST= <333333333333333>
##$FCUCHAN= (0..9)
0 2 1 3 0 0 0 0 0 0
##$FL1= 90
##$FL2= 90
##$FL3= 90
##$FL4= 90
##$FOV= 20
##$FQ1LIST= <freqlist>
##$FQ2LIST= <freqlist>
##$FQ3LIST= <freqlist>
##$FQ4LIST= <freqlist>
##$FQ5LIST= <freqlist>
##$FQ6LIST= <freqlist>
##$FQ7LIST= <freqlist>
##$FQ8LIST= <freqlist>
##$FRQLO3= 1894531.25
##$FRQLO3N= 0
##$FS= (0..7)
83 83 83 83 83 83 83 83
##$FTLPGN= 0
##$FW= 125000
##$FnMODE= 0
##$FnTYPE= 0
##$GP031= 0
##$GPNAM0= <SINE.100>
```

```
##$GPNAM1= <SINE.100>
##$GPNAM10= <SINE.100>
##$GPNAM11= <SINE.100>
##$GPNAM12= <SINE.100>
##$GPNAM13= <SINE.100>
##$GPNAM14= <SINE.100>
##$GPNAM15= <SINE.100>
##$GPNAM16= <SINE.100>
##$GPNAM17= <SINE.100>
##$GPNAM18= <SINE.100>
##$GPNAM19= <SINE.100>
##$GPNAM2= <SINE.50>
##$GPNAM20= <SINE.100>
##$GPNAM21= <SINE.100>
##$GPNAM22= <SINE.100>
##$GPNAM23= <SINE.100>
##$GPNAM24= <SINE.100>
##$GPNAM25= <SINE.100>
##$GPNAM26= <SINE.100>
##$GPNAM27= <SINE.100>
##$GPNAM28= <SINE.100>
##$GPNAM29= <SINE.100>
##$GPNAM3= <SINE.50>
##$GPNAM30= <SINE.100>
##$GPNAM31= <SINE.100>
##$GPNAM4= <SINE.50>
##$GPNAM5= <SINE.50>
##$GPNAM6= <SINE.50>
##$GPNAM7= <SINE.50>
##$GPNAM8= <SINE.100>
##$GPNAM9= <SINE.100>
##$GPX= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$GPY= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$GPZ= (0..31)
0 15 60 36 -45 45 10 -10 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0
##$GRDPROG= <grad_out>
##$GRPDLY= -1
##$HDDUTY= 20
##$HDRATE= 20
```

```
##$HGAIN= (0..3)
0 0 0 0
##$HL1= 400
##$HL2= 90
##$HL3= 90
##$HL4= 90
##$HOLDER= 0
##$HPMOD= (0..7)
0 0 0 0 0 0 0 0
##$HPPRGN= 0
##$IN= (0..63)
0.0002286 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001
##$INF= (0..7)
0 228.585849160409 0 0 0 0 0 0
##$INP= (0..63)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$INSTRUM= <spect>
##$L= (0..31)
16 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##$LFILTER= 200
##$LGAIN= -15
##$LINPSTP= 10
##$LOCKED= yes
##$LOCKFLD= 3588
##$LOCKGN= 116.099998474121
##$LOCKPOW= -30
##$LOCKPPM= 4.69999980926514
##$LOCNUC= <2H>
##$LOCPHAS= 209.8
##$LOCSHFT= no
##$LOCSW= 0
##$LTIME= 0.136000007390976
##$MASR= 4200
##$MASRLST= <masrlst>
##$NBL= 1
##$NC= -2
```

```
##$NLOGCH= 4
##$NS= 4
##$NUC1= <1H>
##$NUC2= <13C>
##$NUC3= <15N>
##$NUC4= <off>
##$NUC5= <off>
##$NUC6= <off>
##$NUC7= <off>
##$NUC8= <off>
##$NUCLEI= 0
##$NUCLEUS= <off>
##$O1= 1400.26
##$O2= 3515.67514513
##$O3= 8371.339726
##$O4= 0
##$O5= 0
##$O6= -99990000
##$O7= -99990000
##$O8= -99990000
##$OBSCHAN= (0..9)
0 0 0 0 0 0 0 0 0 0
##$OVERFLW= 0
##$P= (0..63)
12.13 12.44 14.5 14 28 17.16 26 52 500 25 50 24.88 2000 277 220 1000 500
500 10000 600 2500 29 76 480 680 60 55 12.13 1000 2000 120 658 0 0 0 0
0 0 0 2571 1000 2571 1714 1645 171 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1000 155
0 1500
##$PACOIL= (0..15)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$PAPS= 2
##$PARMODE= 1
##$PCPD= (0..9)
100 55 65 190 100 100 100 100 100 100
##$PHCOR= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$PHLIST= <>
##$PHP= 1
##$PH_ref= 0
##$PL= (0..63)
120 -4.5 -1 -2 120 120 120 120 120 51.31 2.122251 15.76098 12.03 120 120
4.03624 11.98 120 -4.5 8.630037 120 43.22 120 1.97 120 120 120 16.94 10.02846
```

```
120 12.33571 4.864093 120 120 120 120 120 120 120 120 120 120 120 120
120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120
120
##$PLSTEP= 0.1
##$PLSTRT= -6
##$POWMOD= 0
##$PQPHASE= 0
##$PQSCALE= 0
##$PR= 3
##$PRECHAN= (0..15)
-1 3 0 4 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
##$PRGAIN= 0
##$PROBHD= <5 mm CPTXI 1H-13C/15N/2H Z-GRD Z44906/0010
>
##$PROSOL= no
##$PULPROG= <gsHZQC>
##$PW= 0
##$PYNM= <acqu.py>
##$QNP= 1
##$RD= 0
##$RECCHAN= (0..15)
-1 2 0 0 0 0 0 0 0 -1 -1 -1 -1 -1 -1 -1
##$RECPH= 0
##$RECPRE= (0..15)
-1 0 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
##$RECPRFX= (0..15)
-1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RECSEL= (0..15)
0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RG= 1024
##$RO= 0
##$ROUTWD1= (0..23)
0 64 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0
##$ROUTWD2= (0..23)
1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RPUUSED= (0..8)
0 0 0 0 0 0 0 0 0
##$RSEL= (0..9)
0 1 2 3 0 0 0 0 0 0
##$S= (0..7)
83 83 83 83 83 83 83 83
##$SEOUT= 0
```

##$SFO1= 700.13140026
##$SFO2= 176.051344675145
##$SFO3= 70.951928339726
##$SFO4= 700.13
##$SFO5= 600.13
##$SFO6= 500.13
##$SFO7= 500.13
##$SFO8= 500.13
##$SOLVENT= <H2O+D2O>
##$SP= (0..31)
1 29.22361 -0.3434496 0.5123932 -0.3434496 0.5123932 -0.3434496 0.5123932
-0.3434496 10.31412 4.43178 35.24422 4.43178 2.987138 4.536158 10.02846
10.31412 10.31412 8.948763 33.82278 17.62942 150 150 21.46449 14.3981 23.96326
10.52356 23.96326 13.85691 13.85691 0.4209064 10.55676
##$SP07= 0
##$SPECTR= 0
##$SPNAM0= <gauss>
##$SPNAM1= <Sinc1.1000>
##$SPNAM10= <Q5.1000>
##$SPNAM11= <Sinc1.1000>
##$SPNAM12= <Q5tr.1000>
##$SPNAM13= <Crp80,0.5,20.1>
##$SPNAM14= <Crp42,1.5,20.2>
##$SPNAM15= <Q3.1000>
##$SPNAM16= <Q3.1000>
##$SPNAM17= <Q3.1000>
##$SPNAM18= <Crp60_xfilt.2>
##$SPNAM19= <Squa100.1000>
##$SPNAM2= <Q5.1000>
##$SPNAM20= <Squa100.1000>
##$SPNAM21= <gauss>
##$SPNAM22= <gauss>
##$SPNAM23= <Pc9_4_120.1000>
##$SPNAM24= <Rsnob.1000>
##$SPNAM25= <Pc9_4_90.1000>
##$SPNAM26= <Reburp.1000>
##$SPNAM27= <Pc9_4_90.1000>
##$SPNAM28= <Eburp2.1000>
##$SPNAM29= <Eburp2tr.1000>
##$SPNAM3= <Q3.1000>
##$SPNAM30= <Bip720,50,20.1>
##$SPNAM31= <Crp42,1.5,20.2>

```
##$SPNAM4= <Q5.1000>
##$SPNAM5= <Q3.1000>
##$SPNAM6= <Q5tr.1000>
##$SPNAM7= <Q3.1000>
##$SPNAM8= <Q5tr.1000>
##$SPNAM9= <Q3.1000>
##$SPOAL= (0..31)
0.5 0.5 1 0.5 1 0.5 0 0.5 0 0.5 1 0.5 0 0.5 0.5 0.5 0.5 0.5 0.5 0.5
0.5 0.5 1 0.5 1 0.5 0 1 0 0.5 0.5
##$SPOFFS= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$SUBNAM0= <"">
##$SUBNAM1= <"">
##$SUBNAM2= <"">
##$SUBNAM3= <"">
##$SUBNAM4= <"">
##$SUBNAM5= <"">
##$SUBNAM6= <"">
##$SUBNAM7= <"">
##$SUBNAM8= <"">
##$SUBNAM9= <"">
##$SW= 13.9482745615658
##$SWIBOX= (0..15)
0 1 2 3 0 0 6 0 0 0 0 0 0 0 0 0
##$SW_h= 9765.625
##$SWfinal= 0
##$TD= 4096
##$TD0= 1
##$TE= 285.7
##$TE2= 300
##$TE3= 300
##$TEG= 300
##$TL= (0..7)
120 120 120 120 120 120 120 120
##$TP= (0..7)
150 150 150 150 150 150 150 150
##$TP07= 0
##$TPNAME0= <>
##$TPNAME1= <>
##$TPNAME2= <>
##$TPNAME3= <>
##$TPNAME4= <>
```

```
##$TPNAME5= <>
##$TPNAME6= <>
##$TPNAME7= <>
##$TPOAL= (0..7)
0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
##$TPOFFS= (0..7)
0 0 0 0 0 0 0 0
##$TUNHIN= 0
##$TUNHOUT= 0
##$TUNXOUT= 0
##$USERA1= <user>
##$USERA2= <user>
##$USERA3= <user>
##$USERA4= <user>
##$USERA5= <user>
##$V9= 5
##$VALIST= <valist>
##$VCLIST= <CCCCCCCCCCCCCCC>
##$VD= 0
##$VDLIST= <DDDDDDDDDDDDDDD>
##$VPLIST= <PPPPPPPPPPPPPPP>
##$VTLIST= <TTTTTTTTTTTTTTT>
##$WBST= 1024
##$WBSW= 4
##$XGAIN= (0..3)
0 0 0 0
##$XL= 0
##$YL= 0
##$YMAX_a= 5635
##$YMIN_a= -6503
##$ZGOPTNS= <-DPOL2>
##$ZL1= 120
##$ZL2= 120
##$ZL3= 120
##$ZL4= 120
##END=
```

```
; Gradient-selected HZQC (gsHZQC) methyl-TROSY with  methyl filter and ZQ
Hahn-echo relaxation delay
; For recording 1H-13C ZQ relaxation rates in fully protonated methyl groups
; With or without 13C polarization enhancement
; Reference: Gill, ML and Palmer, III, AG, Journal of Biomolecular NMR (2011)
XX:XXX-XXX, Figure 3
;$CLASS=HighRes
;$DIM=2D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

prosol relations=<triple>

#include <Avance.incl>
#include <Grad.incl>
#include <Delay.incl>

; Ensure the -DNOPOL is set if ZGOPTS is empty
#ifndef POL1
#ifndef POL2
#define NOPOL
#endif
#endif

; Unset other flags if using one of polarization schemes
#ifdef POL2
#undef POL1
#undef NOPOL
#endif

#ifdef POL1
#undef POL2
#undef NOPOL
#endif



"cnst21=o1/bf1" ; acquisition frequency should be set the same as O1P
"p11=p1*2"      ; 1H 180degree pulse at hard power
"p21=p2*2"      ; 13C 180degree pulse at hard power
"d11=10u"       ; hardware delay
"d16=250u"      ; gradient recovery delay
```

```
"d28=p21"       ; compensation for 13C 180
"d29=p1*4+8u"   ; compensation for 1H composite pulse
"TAU=3.91m"     ; 1/(2JCH), JCH=128 Hz
"TAU2=0.75m"    ; sin(2piJCH*TAU2) = 3^(-1/2)
"in0=inf1"      ; t1 increment
"d0=in0/2"      ; initial t1 delay (1/2 dwell)
"l0=td1/4"      ; number of t1 complex points
"l1=0"          ; initialize loop counter

"DELTA1=TAU/4"
"DELTA2=(TAU/4)-p16-d16-d11"
"DELTA7=TAU*cnst2/2"
"DELTA8=(TAU*cnst2/2)-p16-d16-d11"

#ifdef NOPOL
"DELTA3=TAU-d11-p1*0.6366"
"DELTA4=TAU-p16-d16-d11"
#endif

#ifdef POL1
"DELTA3=TAU/2-1*TAU2-larger(p1,p2)-p1*0.6366-p17-d16"
"DELTA4=TAU/2+1*TAU2-larger(p1,p2)"
"DELTA5=TAU/2+1*TAU2-larger(p1,p2)-p17-d16-4u"
"DELTA6=TAU/2-1*TAU2-d16-p16-d11-4u-larger(p1,p2)"
#endif

#ifdef POL2
"DELTA3=TAU-p1*0.6366"
"DELTA4=TAU-p16-d16-d11"
"DELTA5=TAU/2+TAU2-p1-p17-d16"
"DELTA6=TAU/2-TAU2-p1-p17-d16-4u"
#endif



1 ze
  d11 BLKGRAD
2 30m
3 d11 do:f2 fq=cnst20(bf ppm):f1
  d11 pl9:f1
  d1 cw:f1 ph0 pl2:f2
  4u do:f1
  d11 pl1:f1 fq=cnst21(bf ppm):f1
```

```
  d11 UNBLKGRAD

#ifdef NOPOL
  ;***purge***
  (p2 ph0):f2
  4u
  p15:gp1
  d16
  ;***evolve AP to MQ***
  (p1 ph1):f1
  d11 BLKGRAD
  DELTA3
  if "l1 % 4 == 0" goto 4
  if "l1 % 4 == 1" goto 5
  if "l1 % 4 == 2" goto 6
  if "l1 % 4 == 3" goto 7
#endif

#ifdef POL1
  p15:gp1
  d16
  ;***transfer polarization from 13C to 1H***
  (p2 ph2):f2
  TAU2
  TAU2
  (p1 ph1):f1
  ;***evolve AP to MQ***
  DELTA3
  p17:gp6
  d16
  (center (p11 ph20):f1 (p21 ph2):f2 )
  4u
  p17:gp6
  d16
  DELTA5
  if "l1 % 4 == 0" goto 6
  if "l1 % 4 == 1" goto 7
  if "l1 % 4 == 2" goto 4
  if "l1 % 4 == 3" goto 5
#endif

#ifdef POL2
```

```
  p15:gp1
  d16
  ;***transfer polarization from 13C to 1H***
  (p2 ph2):f2
  DELTA5
  p17:gp6
  d16
  (p11 ph20):f1
  4u
  p17:gp7
  d16
  DELTA6
  (ralign (p1 ph1):f1 (p21 ph7):f2 )
  ;***evolve AP to MQ***
  DELTA3
  if "l1 % 4 == 0" goto 4
  if "l1 % 4 == 1" goto 5
  if "l1 % 4 == 2" goto 6
  if "l1 % 4 == 3" goto 7
#endif

 4  d29
    ;***create MQ magnetization***
    (p2 ph2):f2
    4u
    (p21 ph20):f2
    ;***J-filter***
    DELTA1
    4u
    ;***Relaxation delay (T/2)***
    DELTA7
    ;***t1***
    d0
    (p1 ph10 4u p11 ph11 4u p1 ph10):f1
    (p21 ph20):f2
    ;***J-filter***
    DELTA1
    d29
    ;***Relaxation delay (T/2)***
    DELTA8
    d11 UNBLKGRAD
    p16:gp2 ; ZQ encode gradient
```

```
   d16
   ;***create AP magnetization***
   (p2 ph5):f2
   8u
goto 8

5  d29
   ;***create MQ magnetization***
   (p2 ph2):f2
   4u
   ;***J-filter***
   DELTA1
   (p21 ph20):f2
   4u
   ;***Relaxation delay (T/2)***
   DELTA7
   ;***t1***
   d0
   (p1 ph10 4u p11 ph11 4u p1 ph10):f1
   ;***J-filter***
   DELTA1
   (p21 ph20):f2
   d29
   ;***Relaxation delay (T/2)***
   DELTA8
   d11 UNBLKGRAD
   p16:gp2 ; ZQ encode gradient
   d16
   ;***create AP magnetization***
   (p2 ph5):f2
   8u
goto 8

6  d29
   ;***create MQ magnetization***
   (p2 ph2):f2
   4u
   (p21 ph20):f2
   ;***Relaxation delay (T/2)***
   DELTA7
   4u
   ;***J-filter***
```

```
   DELTA1
   (p1 ph10 4u p11 ph11 4u p1 ph10):f1
   (p21 ph20):f2
   d0
   ;***Relaxation delay (T/2)***
   DELTA7
   d29
   ;***J-filter***
   DELTA2
   d11 UNBLKGRAD
   p16:gp2 ; ZQ encode gradient
   d16
   ;***create AP magnetization***
   (p2 ph5):f2
   8u
goto 8

7  d29
   ;***create MQ magnetization***
   (p2 ph7):f2
   4u
   ;***Relaxation delay (T/2)***
   DELTA7
   (p21 ph20):f2
   4u
   ;***J-filter***
   DELTA1
   (p1 ph10 4u p11 ph11 4u p1 ph10):f1
   ;***t1***
   d0
   ;***Relaxation delay (T/2)***
   DELTA7
   (p21 ph20):f2
   d29
   ;***J-filter***
   DELTA2
   d11 UNBLKGRAD
   p16:gp3 ; DQ encode gradient
   d16
   ;***create AP magnetization***
   (p2 ph6):f2
   8u
```

```
 goto 8

#ifdef POL1
 8  DELTA4
    (center (p11 ph10):f1 (p21 ph20):f2 )
    4u
    p16:gp5 ; SQ decode gradient
    d16 pl12:f2
    d11 BLKGRAD
    DELTA6
#else
 8  p16:gp4 ; SQ decode gradient
    d16 pl12:f2
    d11 BLKGRAD
    DELTA4
#endif

    ;***detect***
    go=2 ph30 cpd2:f2
    10u do:f2
    30m wr #0 if #0 zd
    30m iu1
    lo to 2 times 4
    30m id0
    lo to 3 times l0
exit

ph0=0
ph1=0 0
ph2=0 2
ph5=0 0
ph6=2 2
ph7=2 0
ph10=0 0
ph11=1 1
ph20=0 0

#ifdef POL2
ph30=2 0
#else
ph30=0 2
#endif
```

```
;*** VARIABLES SET BY USER ***
;d1 = recycle delay
;td1 = 4 * number of complex points (e.g. for 250 t1 points, td1=1000)
;o1p = set offset to just outside of methyl region [2.0 ppm]

;p1 = 1H hard 90 @ pl1
;p2 = 13C hard 90 at pl2
;p11 = 1H hard 180 @ pl1
;p21 = 13C hard 180 @ pl2
;p15 = pulse for gz1 [1ms]
;p16 = pulse for gz2-gz5 [500us]
;p17 = pulse for gz6-gz7 [500us]

;pl0 = 120 dB
;pl1 = 1H hard power
;pl2 = 13C hard power
;pl12 = 13C broadband decoupling power
;p15 = pulse for gpz1 [1ms]
;p16 = pulse for gpz2-gpz5 [500us]
;p17 = pulse for gpz6-gpz7 [500us]

;cnst20 = water offset [4.7ppm]

;gpz1 7.5 G/cm (15%)
;gpz2 30 G/cm (60%)
;gpz3 18 G/cm (36%)
;gpz4 -22.5 G/cm (-45%)
;gpz5 22.5 G/cm (45%)
;gpz6 5 G/cm (10%)
;gpz7 -5 G/cm (-10%)

;gpnam1: SINE.100
;gpnam2: SINE.50
;gpnam3: SINE.50
;gpnam4: SINE.50
;gpnam5: SINE.50
;gpnam6: SINE.50
;gpnam7: SINE.50

; F1 frequency discrimination has been coded for echo/antiecho, thus
; FnMODE: undefined
```

```
; preprocessor flags, use ONLY ONE of the following:
; NOPOL : to purge 13C polarization, this is the default if nothing is set
;         option -DNOPOL (eda: ZGOPTNS)
; POL1  : to use 13C polarization enhancement scheme in Figure 1B
;         option -DPOL1 (eda: ZGOPTNS)
; POL2  : to use 13C polarization enhancement scheme in Figure 1C
;         option -DPOL2 (eda: ZGOPTNS)

; Data processing: For each consecutive block of four data rows,
;                  add the first to the second and the third to the fourth,
;                  then process using Rance-Kay (Echo-Antiecho) for frequency
discrimination
```

```
##TITLE= Parameter file, TOPSPIN        Version 2.1
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##NPOINTS= 628  $$ modification sequence number
##ORIGIN= Bruker BioSpin GmbH
##OWNER= mgill
$$ 2011-05-05 14:13:00.851 -0400  mgill@bh009902.nysbc.org
$$ /opt/topspin/data/mgill/nmr/RNaseH.D2O_methylTROSY_MQRELAX/101/acqus
$$ process /opt/topspin/prog/mod/shimcntl
##$ACQT0= 1000000
##$AMP= (0..31)
100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100
100 100 100 100 100 100 100 100 100 100 100 100 100 100
##$ANAVPT= -1
##$AQSEQ= 0
##$AQ_mod= 3
##$AUNM= <au_getlinv>
##$AUTOPOS= <>
##$BF1= 700.13
##$BF2= 176.047829
##$BF3= 70.943557
##$BF4= 700.13
##$BF5= 600.13
##$BF6= 600.12
##$BF7= 600.12
##$BF8= 600.12
##$BYTORDA= 1
##$CFDGTYP= 2
##$CFRGTYP= 5
##$CHEMSTR= <none>
##$CNST= (0..63)
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 -0.5 1 1 4.703 2 30 20 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##$CPDPRG= <garp>
##$CPDPRG1= <>
##$CPDPRG2= <waltz16>
##$CPDPRG3= <garp>
##$CPDPRG4= <mlev>
##$CPDPRG5= <mlev>
##$CPDPRG6= <mlev>
##$CPDPRG7= <mlev>
##$CPDPRG8= <mlev>
```

```
##$CPDPRGB= <>
##$CPDPRGT= <>
##$D= (0..63)
0.0001142929 1.2 0.00345 0.0023 0.001725 0 0 0.484 0 0.07 0 1e-05 2e-05
3e-06 0 0.012 0.00025 0 0 0 0 0 0 0 0.00086207 0 0 0 2.9e-05 5.776e-05
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$DATE= 1304619124
##$DBL= (0..7)
120 120 120 120 120 120 120 120
##$DBP= (0..7)
150 150 150 150 150 150 150 150
##$DBP07= 0
##$DBPNAM0= <>
##$DBPNAM1= <>
##$DBPNAM2= <>
##$DBPNAM3= <>
##$DBPNAM4= <>
##$DBPNAM5= <>
##$DBPNAM6= <>
##$DBPNAM7= <>
##$DBPOAL= (0..7)
0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
##$DBPOFFS= (0..7)
0 0 0 0 0 0 0 0
##$DE= 6
##$DECBNUC= <off>
##$DECIM= 16
##$DECNUC= <off>
##$DECSTAT= 4
##$DIGMOD= 1
##$DIGTYP= 8
##$DL= (0..7)
120 120 120 120 120 120 120 120
##$DP= (0..7)
150 150 150 150 150 150 150 150
##$DP07= 0
##$DPNAME0= <>
##$DPNAME1= <>
##$DPNAME2= <>
##$DPNAME3= <>
##$DPNAME4= <>
##$DPNAME5= <>
```

```
##$DPNAME6= <>
##$DPNAME7= <>
##$DPOAL= (0..7)
0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
##$DPOFFS= (0..7)
0 0 0 0 0 0 0 0
##$DQDMODE= 0
##$DR= 18
##$DS= 4
##$DSLIST= <SSSSSSSSSSSSSSS>
##$DSPFIRM= 0
##$DSPFVS= 12
##$DTYPA= 0
##$EXP= <>
##$F1LIST= <111111111111111>
##$F2LIST= <222222222222222>
##$F3LIST= <333333333333333>
##$FCUCHAN= (0..9)
0 2 1 3 0 0 0 0 0 0
##$FL1= 90
##$FL2= 90
##$FL3= 90
##$FL4= 90
##$FOV= 20
##$FQ1LIST= <freqlist>
##$FQ2LIST= <freqlist>
##$FQ3LIST= <freqlist>
##$FQ4LIST= <freqlist>
##$FQ5LIST= <freqlist>
##$FQ6LIST= <freqlist>
##$FQ7LIST= <freqlist>
##$FQ8LIST= <freqlist>
##$FRQLO3= 1894531.25
##$FRQLO3N= 0
##$FS= (0..7)
83 83 83 83 83 83 83 83
##$FTLPGN= 0
##$FW= 125000
##$FnMODE= 0
##$FnTYPE= 0
##$GP031= 0
##$GPNAM0= <SINE.100>
```

```
##$GPNAM1= <SINE.100>
##$GPNAM10= <SINE.100>
##$GPNAM11= <SINE.100>
##$GPNAM12= <SINE.100>
##$GPNAM13= <SINE.100>
##$GPNAM14= <SINE.100>
##$GPNAM15= <SINE.100>
##$GPNAM16= <SINE.100>
##$GPNAM17= <SINE.100>
##$GPNAM18= <SINE.100>
##$GPNAM19= <SINE.100>
##$GPNAM2= <SINE.50>
##$GPNAM20= <SINE.100>
##$GPNAM21= <SINE.100>
##$GPNAM22= <SINE.100>
##$GPNAM23= <SINE.100>
##$GPNAM24= <SINE.100>
##$GPNAM25= <SINE.100>
##$GPNAM26= <SINE.100>
##$GPNAM27= <SINE.100>
##$GPNAM28= <SINE.100>
##$GPNAM29= <SINE.100>
##$GPNAM3= <SINE.50>
##$GPNAM30= <SINE.100>
##$GPNAM31= <SINE.100>
##$GPNAM4= <SINE.50>
##$GPNAM5= <SINE.50>
##$GPNAM6= <SINE.50>
##$GPNAM7= <SINE.50>
##$GPNAM8= <SINE.100>
##$GPNAM9= <SINE.100>
##$GPX= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$GPY= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$GPZ= (0..31)
0 15 60 36 -45 45 10 -10 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0
##$GRDPROG= <grad_out>
##$GRPDLY= -1
##$HDDUTY= 20
##$HDRATE= 20
```

```
##$HGAIN= (0..3)
0 0 0 0
##$HL1= 400
##$HL2= 90
##$HL3= 90
##$HL4= 90
##$HOLDER= 0
##$HPMOD= (0..7)
0 0 0 0 0 0 0 0
##$HPPRGN= 0
##$IN= (0..63)
0.0002286 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001
##$INF= (0..7)
0 228.585849160409 0 0 0 0 0 0
##$INP= (0..63)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$INSTRUM= <spect>
##$L= (0..31)
16 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##$LFILTER= 200
##$LGAIN= -15
##$LINPSTP= 10
##$LOCKED= yes
##$LOCKFLD= 3588
##$LOCKGN= 116.099998474121
##$LOCKPOW= -30
##$LOCKPPM= 4.69999980926514
##$LOCNUC= <2H>
##$LOCPHAS= 209.8
##$LOCSHFT= no
##$LOCSW= 0
##$LTIME= 0.136000007390976
##$MASR= 4200
##$MASRLST= <masrlst>
##$NBL= 1
##$NC= -2
```

```
##$NLOGCH= 4
##$NS= 4
##$NUC1= <1H>
##$NUC2= <13C>
##$NUC3= <15N>
##$NUC4= <off>
##$NUC5= <off>
##$NUC6= <off>
##$NUC7= <off>
##$NUC8= <off>
##$NUCLEI= 0
##$NUCLEUS= <off>
##$O1= 1400.26
##$O2= 3515.67514513
##$O3= 8371.339726
##$O4= 0
##$O5= 0
##$O6= -99990000
##$O7= -99990000
##$O8= -99990000
##$OBSCHAN= (0..9)
0 0 0 0 0 0 0 0 0 0
##$OVERFLW= 0
##$P= (0..63)
12.13 12.44 14.5 14 28 17.16 26 52 500 25 50 24.88 2000 277 220 1000 500
500 10000 600 2500 29 76 480 680 60 55 12.13 1000 2000 120 658 0 0 0 0
0 0 0 2571 1000 2571 1714 1645 171 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1000 155
0 1500
##$PACOIL= (0..15)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$PAPS= 2
##$PARMODE= 1
##$PCPD= (0..9)
100 55 65 190 100 100 100 100 100 100
##$PHCOR= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$PHLIST= <>
##$PHP= 1
##$PH_ref= 0
##$PL= (0..63)
120 -4.5 -1 -2 120 120 120 120 120 51.31 2.122251 15.76098 12.03 120 120
4.03624 11.98 120 -4.5 8.630037 120 43.22 120 1.97 120 120 120 16.94 10.02846
```

```
120 12.33571 4.864093 120 120 120 120 120 120 120 120 120 120 120 120 120
120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120
120
##$PLSTEP= 0.1
##$PLSTRT= -6
##$POWMOD= 0
##$PQPHASE= 0
##$PQSCALE= 0
##$PR= 3
##$PRECHAN= (0..15)
-1 3 0 4 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
##$PRGAIN= 0
##$PROBHD= <5 mm CPTXI 1H-13C/15N/2H Z-GRD Z44906/0010
>
##$PROSOL= no
##$PULPROG= <gsHZQC_HEZQ>
##$PW= 0
##$PYNM= <acqu.py>
##$QNP= 1
##$RD= 0
##$RECCHAN= (0..15)
-1 2 0 0 0 0 0 0 0 -1 -1 -1 -1 -1 -1 -1
##$RECPH= 0
##$RECPRE= (0..15)
-1 0 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
##$RECPRFX= (0..15)
-1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RECSEL= (0..15)
0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RG= 1024
##$RO= 0
##$ROUTWD1= (0..23)
0 64 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0
##$ROUTWD2= (0..23)
1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RPUUSED= (0..8)
0 0 0 0 0 0 0 0 0
##$RSEL= (0..9)
0 1 2 3 0 0 0 0 0 0
##$S= (0..7)
83 83 83 83 83 83 83 83
##$SEOUT= 0
```

```
##$SFO1= 700.13140026
##$SFO2= 176.051344675145
##$SFO3= 70.951928339726
##$SFO4= 700.13
##$SFO5= 600.13
##$SFO6= 500.13
##$SFO7= 500.13
##$SFO8= 500.13
##$SOLVENT= <H2O+D2O>
##$SP= (0..31)
1 29.22361 -0.3434496 0.5123932 -0.3434496 0.5123932 -0.3434496 0.5123932
-0.3434496 10.31412 4.43178 35.24422 4.43178 2.987138 4.536158 10.02846
10.31412 10.31412 8.948763 33.82278 17.62942 150 150 21.46449 14.3981 23.96326
10.52356 23.96326 13.85691 13.85691 0.4209064 10.55676
##$SP07= 0
##$SPECTR= 0
##$SPNAM0= <gauss>
##$SPNAM1= <Sinc1.1000>
##$SPNAM10= <Q5.1000>
##$SPNAM11= <Sinc1.1000>
##$SPNAM12= <Q5tr.1000>
##$SPNAM13= <Crp80,0.5,20.1>
##$SPNAM14= <Crp42,1.5,20.2>
##$SPNAM15= <Q3.1000>
##$SPNAM16= <Q3.1000>
##$SPNAM17= <Q3.1000>
##$SPNAM18= <Crp60_xfilt.2>
##$SPNAM19= <Squa100.1000>
##$SPNAM2= <Q5.1000>
##$SPNAM20= <Squa100.1000>
##$SPNAM21= <gauss>
##$SPNAM22= <gauss>
##$SPNAM23= <Pc9_4_120.1000>
##$SPNAM24= <Rsnob.1000>
##$SPNAM25= <Pc9_4_90.1000>
##$SPNAM26= <Reburp.1000>
##$SPNAM27= <Pc9_4_90.1000>
##$SPNAM28= <Eburp2.1000>
##$SPNAM29= <Eburp2tr.1000>
##$SPNAM3= <Q3.1000>
##$SPNAM30= <Bip720,50,20.1>
##$SPNAM31= <Crp42,1.5,20.2>
```

```
##$SPNAM4= <Q5.1000>
##$SPNAM5= <Q3.1000>
##$SPNAM6= <Q5tr.1000>
##$SPNAM7= <Q3.1000>
##$SPNAM8= <Q5tr.1000>
##$SPNAM9= <Q3.1000>
##$SPOAL= (0..31)
0.5 0.5 1 0.5 1 0.5 0 0.5 0 0.5 1 0.5 0 0.5 0.5 0.5 0.5 0.5 0.5 0.5
0.5 0.5 1 0.5 1 0.5 0 1 0 0.5 0.5
##$SPOFFS= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$SUBNAM0= <"">
##$SUBNAM1= <"">
##$SUBNAM2= <"">
##$SUBNAM3= <"">
##$SUBNAM4= <"">
##$SUBNAM5= <"">
##$SUBNAM6= <"">
##$SUBNAM7= <"">
##$SUBNAM8= <"">
##$SUBNAM9= <"">
##$SW= 13.9482745615658
##$SWIBOX= (0..15)
0 1 2 3 0 0 6 0 0 0 0 0 0 0 0 0
##$SW_h= 9765.625
##$SWfinal= 0
##$TD= 4096
##$TD0= 1
##$TE= 285.7
##$TE2= 300
##$TE3= 300
##$TEG= 300
##$TL= (0..7)
120 120 120 120 120 120 120 120
##$TP= (0..7)
150 150 150 150 150 150 150 150
##$TP07= 0
##$TPNAME0= <>
##$TPNAME1= <>
##$TPNAME2= <>
##$TPNAME3= <>
##$TPNAME4= <>
```

```
##$TPNAME5= <>
##$TPNAME6= <>
##$TPNAME7= <>
##$TPOAL= (0..7)
0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
##$TPOFFS= (0..7)
0 0 0 0 0 0 0 0
##$TUNHIN= 0
##$TUNHOUT= 0
##$TUNXOUT= 0
##$USERA1= <user>
##$USERA2= <user>
##$USERA3= <user>
##$USERA4= <user>
##$USERA5= <user>
##$V9= 5
##$VALIST= <valist>
##$VCLIST= <CCCCCCCCCCCCCCC>
##$VD= 0
##$VDLIST= <DDDDDDDDDDDDDDD>
##$VPLIST= <PPPPPPPPPPPPPPP>
##$VTLIST= <TTTTTTTTTTTTTTT>
##$WBST= 1024
##$WBSW= 4
##$XGAIN= (0..3)
0 0 0 0
##$XL= 0
##$YL= 0
##$YMAX_a= 5668
##$YMIN_a= -6698
##$ZGOPTNS= <-DPOL2>
##$ZL1= 120
##$ZL2= 120
##$ZL3= 120
##$ZL4= 120
##END=
```

```
; Gradient-selected HZQC (gsHZQC) methyl-TROSY with methyl filter and DQ
Hahn-echo relaxation delay
; For recording 1H-13C DQ relaxation rates in fully protonated methyl groups
; With or without 13C polarization enhancement
; Reference: Gill, ML and Palmer, III, AG, Journal of Biomolecular NMR (2011)
XX:XXX-XXX, Figure 3
;$CLASS=HighRes
;$DIM=2D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

prosol relations=<triple>

#include <Avance.incl>
#include <Grad.incl>
#include <Delay.incl>

; Ensure the -DNOPOL is set if ZGOPTS is empty
#ifndef POL1
#ifndef POL2
#define NOPOL
#endif
#endif

; Unset other flags if using one of polarization schemes
#ifdef POL2
#undef POL1
#undef NOPOL
#endif

#ifdef POL1
#undef POL2
#undef NOPOL
#endif



"cnst21=o1/bf1" ; acquisition frequency should be set the same as O1P
"p11=p1*2"      ; 1H 180degree pulse at hard power
"p21=p2*2"      ; 13C 180degree pulse at hard power
"d11=10u"       ; hardware delay
"d16=250u"      ; gradient recovery delay
```

```
"d28=p21"       ; compensation for 13C 180
"d29=p1*4+8u"   ; compensation for 1H composite pulse
"TAU=3.91m"     ; 1/(2JCH), JCH=128 Hz
"TAU2=0.75m"    ; sin(2piJCH*TAU2) = 3^(-1/2)
"in0=inf1"      ; t1 increment
"d0=in0/2"      ; initial t1 delay (1/2 dwell)
"l0=td1/4"      ; number of t1 complex points
"l1=0"          ; initialize loop counter

"DELTA1=TAU/4"
"DELTA2=(TAU/4)-p16-d16-d11"
"DELTA7=TAU*cnst2/2"
"DELTA8=(TAU*cnst2/2)-p16-d16-d11"

#   ifdef POL1
"DELTA3=TAU/2-1*TAU2-larger(p1,p2)-p1*0.6366-p17-d16"
"DELTA4=TAU/2+1*TAU2-larger(p1,p2)"
"DELTA5=TAU/2+1*TAU2-larger(p1,p2)-p17-d16-4u"
"DELTA6=TAU/2-1*TAU2-d16-p16-d11-4u-larger(p1,p2)"
#   endif

#   ifdef POL2
"DELTA3=TAU-p1*0.6366"
"DELTA4=TAU-p16-d16-d11"
"DELTA5=TAU/2+TAU2-p1-p17-d16"
"DELTA6=TAU/2-TAU2-p1-p17-d16-4u"
#   endif

#   ifdef NOPOL
"DELTA3=TAU-d11-p1*0.6366"
"DELTA4=TAU-p16-d16-d11"
#   endif



1 ze
  d11 BLKGRAD
2 30m
3 d11 do:f2 fq=cnst20(bf ppm):f1
  d11 pl9:f1
  d1 cw:f1 ph0 pl2:f2
  4u do:f1
  d11 pl1:f1 fq=cnst21(bf ppm):f1
```

```
  d11 UNBLKGRAD

#ifdef NOPOL
  ;***purge***
  (p2 ph0):f2
  4u
  p15:gp1
  d16
  ;***evolve AP to MQ***
  (p1 ph1):f1
  d11 BLKGRAD
  DELTA3
  if "l1 % 4 == 0" goto 4
  if "l1 % 4 == 1" goto 5
  if "l1 % 4 == 2" goto 6
  if "l1 % 4 == 3" goto 7
#endif

#ifdef POL1
  p15:gp1
  d16
  ;***transfer polarization from 13C to 1H***
  (p2 ph7):f2
  TAU2
  TAU2
  (p1 ph1):f1
  ;***evolve AP to MQ***
  DELTA3
  p17:gp6
  d16
  (center (p11 ph20):f1 (p21 ph7):f2 )
  4u
  p17:gp6
  d16
  DELTA5
  if "l1 % 4 == 0" goto 6
  if "l1 % 4 == 1" goto 7
  if "l1 % 4 == 2" goto 4
  if "l1 % 4 == 3" goto 5
#endif

#ifdef POL2
```

```
  p15:gp1
  d16
  ;***transfer polarization from 13C to 1H***
  (p2 ph7):f2
  DELTA5
  p17:gp6
  d16
  (p11 ph20):f1
  4u
  p17:gp7
  d16
  DELTA6
  (ralign (p1 ph1):f1 (p21 ph2):f2 )
  ;***evolve AP to MQ***
  DELTA3
  if "l1 % 4 == 0" goto 4
  if "l1 % 4 == 1" goto 5
  if "l1 % 4 == 2" goto 6
  if "l1 % 4 == 3" goto 7
#endif

    ;***create MQ magnetization***
 4  (p2 ph2):f2
    4u
    (p21 ph20):f2
    ;***Relaxation delay (T/2)***
    DELTA7
    ;***J-filter***
    4u
    DELTA1
    d29
    (p21 ph20):f2
    ;***t1***
    d0
    (p1 ph10 4u p11 ph11 4u p1 ph10):f1
    ;***Relaxation delay (T/2)***
    DELTA7
    ;***J-filter***
    DELTA2
    d11 UNBLKGRAD
    p16:gp3 ; DQ encode gradient
    d16
```

```
   ;***create AP magnetization***
   (p2 ph5):f2
   d29
   8u
goto 8

5  d29
   ;***create MQ magnetization***
   (p2 ph7):f2
   4u
   ;***Relaxation delay (T/2)***
   DELTA7
   (p21 ph20):f2
   ;***J-filter***
   4u
   DELTA1
   ;***t1***
   d0
   (p1 ph10 4u p11 ph11 4u p1 ph10):f1
   ;***Relaxation delay (T/2)***
   DELTA7
   (p21 ph20):f2
   d29
   ;***J-filter***
   DELTA2
   d11 UNBLKGRAD
   p16:gp2 ; ZQ encode gradient
   d16
   ;***create AP magnetization***
   (p2 ph6):f2
   8u
goto 8

6  d29
   ;***create MQ magnetization***
   (p2 ph2):f2
   4u
   (p21 ph20):f2
   ;***J-filter***
   DELTA1
   4u
   ;***Relaxation delay (T/2)***
```

```
   DELTA7
   (p1 ph10 4u p11 ph11 4u p1 ph10):f1
   ;***t1***
   d0
   (p21 ph20):f2
   ;***J-filter***
   DELTA1
   d29
   ;***Relaxation delay (T/2)***
   DELTA8
   d11 UNBLKGRAD
   p16:gp3 ; DQ encode gradient
   d16
   ;***create AP magnetization***
   (p2 ph5):f2
   8u
goto 8

7  d29
   ;***create MQ magnetization***
   (p2 ph2):f2
   ;***J-filter***
   4u
   DELTA1
   (p21 ph20):f2
   4u
   ;***Relaxation delay (T/2)***
   DELTA7
   (p1 ph10 4u p11 ph11 4u p1 ph10):f1
   ;***t1***
   d0
   ;***J-filter***
   DELTA1
   (p21 ph20):f2
   d29
   ;***Relaxation delay (T/2)***
   DELTA8
   d11 UNBLKGRAD
   p16:gp3 ; DQ encode gradient
   d16
   ;***create AP magnetization***
   (p2 ph5):f2
```

```
    8u
 goto 8


#ifdef POL1
 8  DELTA4
    (center (p11 ph10):f1 (p21 ph20):f2 )
    4u
    p16:gp5 ; SQ decode gradient
    d16 pl12:f2
    d11 BLKGRAD
    DELTA6
#else
 8  4u
    p16:gp4 ; SQ decode gradient
    d16 pl12:f2
    d11 BLKGRAD
    DELTA4
#endif


    ;***detect***
    go=2 ph30 cpd2:f2
    10u do:f2
    30m wr #0 if #0 zd
    30m iu1
    lo to 2 times 4
    30m id0
    lo to 3 times l0
exit

ph0=0
ph1=0 0
ph2=0 2
ph5=0 0
ph6=2 2
ph7=2 0
ph10=0 0
ph11=1 1
ph20=0 0

#ifdef POL2
```

```
ph30=2 0
#else
ph30=0 2
#endif

;*** VARIABLES SET BY USER ***
;d1 = recycle delay
;td1 = 4 * number of complex points (e.g. for 250 t1 points, td1=1000)
;o1p = set offset to just outside of methyl region [2.0 ppm]

;p1 = 1H hard 90 @ pl1
;p2 = 13C hard 90 at pl2
;p11 = 1H hard 180 @ pl1
;p21 = 13C hard 180 @ pl2
;p15 = pulse for gz1 [1ms]
;p16 = pulse for gz2-gz5 [500us]
;p17 = pulse for gz6-gz7 [500us]

;pl0 = 120 dB
;pl1 = 1H hard power
;pl2 = 13C hard power
;pl12 = 13C broadband decoupling power
;p15 = pulse for gpz1 [1ms]
;p16 = pulse for gpz2-gpz5 [500us]
;p17 = pulse for gpz6-gpz7 [500us]

;cnst2 = number of 1/(2JCH) intervals for relaxation delay (T)
;cnst20 = water offset [4.7ppm]

;gpz1 7.5 G/cm (15%)
;gpz2 30 G/cm (60%)
;gpz3 18 G/cm (36%)
;gpz4 -22.5 G/cm (-45%)
;gpz5 22.5 G/cm (45%)
;gpz6 5 G/cm (10%)
;gpz7 -5 G/cm (-10%)

;gpnam1: SINE.100
;gpnam2: SINE.50
;gpnam3: SINE.50
;gpnam4: SINE.50
;gpnam5: SINE.50
```

```
;gpnam6: SINE.50
;gpnam7: SINE.50

; F1 frequency discrimination has been coded for echo/antiecho, thus
; FnMODE: undefined

; preprocessor flags, use ONLY ONE of the following:
; NOPOL : to purge 13C polarization, this is the default if nothing is set
;         option -DNOPOL (eda: ZGOPTNS)
; POL1  : to use 13C polarization enhancement scheme in Figure 1B
;         option -DPOL1 (eda: ZGOPTNS)
; POL2  : to use 13C polarization enhancement scheme in Figure 1C
;         option -DPOL2 (eda: ZGOPTNS)

; Data processing: For each consecutive block of four data rows,
;                  add the first to the second and the third to the fourth,
;                  then process using Rance-Kay (Echo-Antiecho) for frequency
discrimination
```

```
##TITLE= Parameter file, TOPSPIN        Version 2.1
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##NPOINTS= 682  $$ modification sequence number
##ORIGIN= Bruker BioSpin GmbH
##OWNER= mgill
$$ 2011-05-05 15:55:39.604 -0400  mgill@bh009902.nysbc.org
$$ /opt/topspin/data/mgill/nmr/RNaseH.D2O_methylTROSY_MQRELAX/111/acqus
$$ process /opt/topspin/prog/mod/shimcntl
##$ACQT0= 1000000
##$AMP= (0..31)
100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100
100 100 100 100 100 100 100 100 100 100 100 100 100 100
##$ANAVPT= -1
##$AQSEQ= 0
##$AQ_mod= 3
##$AUNM= <au_getlinv>
##$AUTOPOS= <>
##$BF1= 700.13
##$BF2= 176.047829
##$BF3= 70.943557
##$BF4= 700.13
##$BF5= 600.13
##$BF6= 600.12
##$BF7= 600.12
##$BF8= 600.12
##$BYTORDA= 1
##$CFDGTYP= 2
##$CFRGTYP= 5
##$CHEMSTR= <none>
##$CNST= (0..63)
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 -0.5 1 1 4.703 2 30 20 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##$CPDPRG= <garp>
##$CPDPRG1= <>
##$CPDPRG2= <waltz16>
##$CPDPRG3= <garp>
##$CPDPRG4= <mlev>
##$CPDPRG5= <mlev>
##$CPDPRG6= <mlev>
##$CPDPRG7= <mlev>
##$CPDPRG8= <mlev>
```

```
##$CPDPRGB= <>
##$CPDPRGT= <>
##$D= (0..63)
0.0001142929 1.2 0.00345 0.0023 0.001725 0 0 0.484 0 0.07 0 1e-05 2e-05
3e-06 0 0.012 0.00025 0 0 0 0 0 0 0 0.00086207 0 0 0 2.9e-05 5.776e-05
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$DATE= 1304620685
##$DBL= (0..7)
120 120 120 120 120 120 120 120
##$DBP= (0..7)
150 150 150 150 150 150 150 150
##$DBP07= 0
##$DBPNAM0= <>
##$DBPNAM1= <>
##$DBPNAM2= <>
##$DBPNAM3= <>
##$DBPNAM4= <>
##$DBPNAM5= <>
##$DBPNAM6= <>
##$DBPNAM7= <>
##$DBPOAL= (0..7)
0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
##$DBPOFFS= (0..7)
0 0 0 0 0 0 0 0
##$DE= 6
##$DECBNUC= <off>
##$DECIM= 16
##$DECNUC= <off>
##$DECSTAT= 4
##$DIGMOD= 1
##$DIGTYP= 8
##$DL= (0..7)
120 120 120 120 120 120 120 120
##$DP= (0..7)
150 150 150 150 150 150 150 150
##$DP07= 0
##$DPNAME0= <>
##$DPNAME1= <>
##$DPNAME2= <>
##$DPNAME3= <>
##$DPNAME4= <>
##$DPNAME5= <>
```

```
##$DPNAME6= <>
##$DPNAME7= <>
##$DPOAL= (0..7)
0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
##$DPOFFS= (0..7)
0 0 0 0 0 0 0 0
##$DQDMODE= 0
##$DR= 18
##$DS= 8
##$DSLIST= <SSSSSSSSSSSSSSS>
##$DSPFIRM= 0
##$DSPFVS= 12
##$DTYPA= 0
##$EXP= <>
##$F1LIST= <111111111111111>
##$F2LIST= <222222222222222>
##$F3LIST= <333333333333333>
##$FCUCHAN= (0..9)
0 2 1 3 0 0 0 0 0 0
##$FL1= 90
##$FL2= 90
##$FL3= 90
##$FL4= 90
##$FOV= 20
##$FQ1LIST= <freqlist>
##$FQ2LIST= <freqlist>
##$FQ3LIST= <freqlist>
##$FQ4LIST= <freqlist>
##$FQ5LIST= <freqlist>
##$FQ6LIST= <freqlist>
##$FQ7LIST= <freqlist>
##$FQ8LIST= <freqlist>
##$FRQLO3= 1894531.25
##$FRQLO3N= 0
##$FS= (0..7)
83 83 83 83 83 83 83 83
##$FTLPGN= 0
##$FW= 125000
##$FnMODE= 0
##$FnTYPE= 0
##$GP031= 0
##$GPNAM0= <SINE.100>
```

```
##$GPNAM1= <SINE.100>
##$GPNAM10= <SINE.100>
##$GPNAM11= <SINE.100>
##$GPNAM12= <SINE.100>
##$GPNAM13= <SINE.100>
##$GPNAM14= <SINE.100>
##$GPNAM15= <SINE.100>
##$GPNAM16= <SINE.100>
##$GPNAM17= <SINE.100>
##$GPNAM18= <SINE.100>
##$GPNAM19= <SINE.100>
##$GPNAM2= <SINE.50>
##$GPNAM20= <SINE.100>
##$GPNAM21= <SINE.100>
##$GPNAM22= <SINE.100>
##$GPNAM23= <SINE.100>
##$GPNAM24= <SINE.100>
##$GPNAM25= <SINE.100>
##$GPNAM26= <SINE.100>
##$GPNAM27= <SINE.100>
##$GPNAM28= <SINE.100>
##$GPNAM29= <SINE.100>
##$GPNAM3= <SINE.50>
##$GPNAM30= <SINE.100>
##$GPNAM31= <SINE.100>
##$GPNAM4= <SINE.50>
##$GPNAM5= <SINE.50>
##$GPNAM6= <SINE.50>
##$GPNAM7= <SINE.50>
##$GPNAM8= <SINE.100>
##$GPNAM9= <SINE.100>
##$GPX= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$GPY= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$GPZ= (0..31)
0 15 60 36 -45 45 10 -10 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0
##$GRDPROG= <grad_out>
##$GRPDLY= -1
##$HDDUTY= 20
##$HDRATE= 20
```

```
##$HGAIN= (0..3)
0 0 0 0
##$HL1= 400
##$HL2= 90
##$HL3= 90
##$HL4= 90
##$HOLDER= 0
##$HPMOD= (0..7)
0 0 0 0 0 0 0 0
##$HPPRGN= 0
##$IN= (0..63)
0.0002286 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
0.001 0.001 0.001 0.001
##$INF= (0..7)
0 228.585849160409 0 0 0 0 0 0
##$INP= (0..63)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$INSTRUM= <spect>
##$L= (0..31)
378 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##$LFILTER= 200
##$LGAIN= -15
##$LINPSTP= 10
##$LOCKED= yes
##$LOCKFLD= 3588
##$LOCKGN= 116.099998474121
##$LOCKPOW= -30
##$LOCKPPM= 4.69999980926514
##$LOCNUC= <2H>
##$LOCPHAS= 209.8
##$LOCSHFT= no
##$LOCSW= 0
##$LTIME= 0.136000007390976
##$MASR= 4200
##$MASRLST= <masrlst>
##$NBL= 1
##$NC= -2
```

```
##$NLOGCH= 4
##$NS= 2
##$NUC1= <1H>
##$NUC2= <13C>
##$NUC3= <15N>
##$NUC4= <off>
##$NUC5= <off>
##$NUC6= <off>
##$NUC7= <off>
##$NUC8= <off>
##$NUCLEI= 0
##$NUCLEUS= <off>
##$O1= 1400.26
##$O2= 3515.67514513
##$O3= 8371.339726
##$O4= 0
##$O5= 0
##$O6= -99990000
##$O7= -99990000
##$O8= -99990000
##$OBSCHAN= (0..9)
0 0 0 0 0 0 0 0 0 0
##$OVERFLW= 0
##$P= (0..63)
12.13 12.44 14.5 14 28 17.16 26 52 500 25 50 24.88 2000 277 220 1000 500
500 10000 600 2500 29 76 480 680 60 55 12.13 1000 2000 120 658 0 0 0 0
0 0 0 2571 1000 2571 1714 1645 171 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1000 155
0 1500
##$PACOIL= (0..15)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$PAPS= 2
##$PARMODE= 1
##$PCPD= (0..9)
100 55 65 190 100 100 100 100 100 100
##$PHCOR= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$PHLIST= <>
##$PHP= 1
##$PH_ref= 0
##$PL= (0..63)
120 -4.5 -1 -2 120 120 120 120 120 51.31 2.122251 15.76098 12.03 120 120
4.03624 11.98 120 -4.5 8.630037 120 43.22 120 1.97 120 120 120 16.94 10.02846
```

```
120 12.33571 4.864093 120 120 120 120 120 120 120 120 120 120 120 120 120
120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120
120
##$PLSTEP= 0.1
##$PLSTRT= -6
##$POWMOD= 0
##$PQPHASE= 0
##$PQSCALE= 0
##$PR= 3
##$PRECHAN= (0..15)
-1 3 0 4 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
##$PRGAIN= 0
##$PROBHD= <5 mm CPTXI 1H-13C/15N/2H Z-GRD Z44906/0010
>
##$PROSOL= no
##$PULPROG= <gsHZQC_HEDQ>
##$PW= 0
##$PYNM= <acqu.py>
##$QNP= 1
##$RD= 0
##$RECCHAN= (0..15)
-1 2 0 0 0 0 0 0 0 -1 -1 -1 -1 -1 -1 -1
##$RECPH= 0
##$RECPRE= (0..15)
-1 0 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
##$RECPRFX= (0..15)
-1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RECSEL= (0..15)
0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RG= 1024
##$RO= 0
##$ROUTWD1= (0..23)
0 1512 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0
##$ROUTWD2= (0..23)
1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RPUUSED= (0..8)
0 0 0 0 0 0 0 0 0
##$RSEL= (0..9)
0 1 2 3 0 0 0 0 0 0
##$S= (0..7)
83 83 83 83 83 83 83 83
##$SEOUT= 0
```

```
##$SFO1= 700.13140026
##$SFO2= 176.051344675145
##$SFO3= 70.951928339726
##$SFO4= 700.13
##$SFO5= 600.13
##$SFO6= 500.13
##$SFO7= 500.13
##$SFO8= 500.13
##$SOLVENT= <H2O+D2O>
##$SP= (0..31)
1 29.22361 -0.3434496 0.5123932 -0.3434496 0.5123932 -0.3434496 0.5123932
-0.3434496 10.31412 4.43178 35.24422 4.43178 2.987138 4.536158 10.02846
10.31412 10.31412 8.948763 33.82278 17.62942 150 150 21.46449 14.3981 23.96326
10.52356 23.96326 13.85691 13.85691 0.4209064 10.55676
##$SP07= 0
##$SPECTR= 0
##$SPNAM0= <gauss>
##$SPNAM1= <Sinc1.1000>
##$SPNAM10= <Q5.1000>
##$SPNAM11= <Sinc1.1000>
##$SPNAM12= <Q5tr.1000>
##$SPNAM13= <Crp80,0.5,20.1>
##$SPNAM14= <Crp42,1.5,20.2>
##$SPNAM15= <Q3.1000>
##$SPNAM16= <Q3.1000>
##$SPNAM17= <Q3.1000>
##$SPNAM18= <Crp60_xfilt.2>
##$SPNAM19= <Squa100.1000>
##$SPNAM2= <Q5.1000>
##$SPNAM20= <Squa100.1000>
##$SPNAM21= <gauss>
##$SPNAM22= <gauss>
##$SPNAM23= <Pc9_4_120.1000>
##$SPNAM24= <Rsnob.1000>
##$SPNAM25= <Pc9_4_90.1000>
##$SPNAM26= <Reburp.1000>
##$SPNAM27= <Pc9_4_90.1000>
##$SPNAM28= <Eburp2.1000>
##$SPNAM29= <Eburp2tr.1000>
##$SPNAM3= <Q3.1000>
##$SPNAM30= <Bip720,50,20.1>
##$SPNAM31= <Crp42,1.5,20.2>
```

```
##$SPNAM4= <Q5.1000>
##$SPNAM5= <Q3.1000>
##$SPNAM6= <Q5tr.1000>
##$SPNAM7= <Q3.1000>
##$SPNAM8= <Q5tr.1000>
##$SPNAM9= <Q3.1000>
##$SPOAL= (0..31)
0.5 0.5 1 0.5 1 0.5 0 0.5 0 0.5 1 0.5 0 0.5 0.5 0.5 0.5 0.5 0.5 0.5
0.5 0.5 1 0.5 1 0.5 0 1 0 0.5 0.5
##$SPOFFS= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$SUBNAM0= <"">
##$SUBNAM1= <"">
##$SUBNAM2= <"">
##$SUBNAM3= <"">
##$SUBNAM4= <"">
##$SUBNAM5= <"">
##$SUBNAM6= <"">
##$SUBNAM7= <"">
##$SUBNAM8= <"">
##$SUBNAM9= <"">
##$SW= 13.9482745615658
##$SWIBOX= (0..15)
0 1 2 3 0 0 6 0 0 0 0 0 0 0 0 0
##$SW_h= 9765.625
##$SWfinal= 0
##$TD= 4096
##$TD0= 1
##$TE= 285.7
##$TE2= 300
##$TE3= 300
##$TEG= 300
##$TL= (0..7)
120 120 120 120 120 120 120 120
##$TP= (0..7)
150 150 150 150 150 150 150 150
##$TP07= 0
##$TPNAME0= <>
##$TPNAME1= <>
##$TPNAME2= <>
##$TPNAME3= <>
##$TPNAME4= <>
```

```
##$TPNAME5= <>
##$TPNAME6= <>
##$TPNAME7= <>
##$TPOAL= (0..7)
0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5
##$TPOFFS= (0..7)
0 0 0 0 0 0 0 0
##$TUNHIN= 0
##$TUNHOUT= 0
##$TUNXOUT= 0
##$USERA1= <user>
##$USERA2= <user>
##$USERA3= <user>
##$USERA4= <user>
##$USERA5= <user>
##$V9= 5
##$VALIST= <valist>
##$VCLIST= <CCCCCCCCCCCCCCC>
##$VD= 0
##$VDLIST= <DDDDDDDDDDDDDDD>
##$VPLIST= <PPPPPPPPPPPPPPP>
##$VTLIST= <TTTTTTTTTTTTTTT>
##$WBST= 1024
##$WBSW= 4
##$XGAIN= (0..3)
0 0 0 0
##$XL= 0
##$YL= 0
##$YMAX_a= 4199
##$YMIN_a= -4384
##$ZGOPTNS= <>
##$ZL1= 120
##$ZL2= 120
##$ZL3= 120
##$ZL4= 120
##END=
```