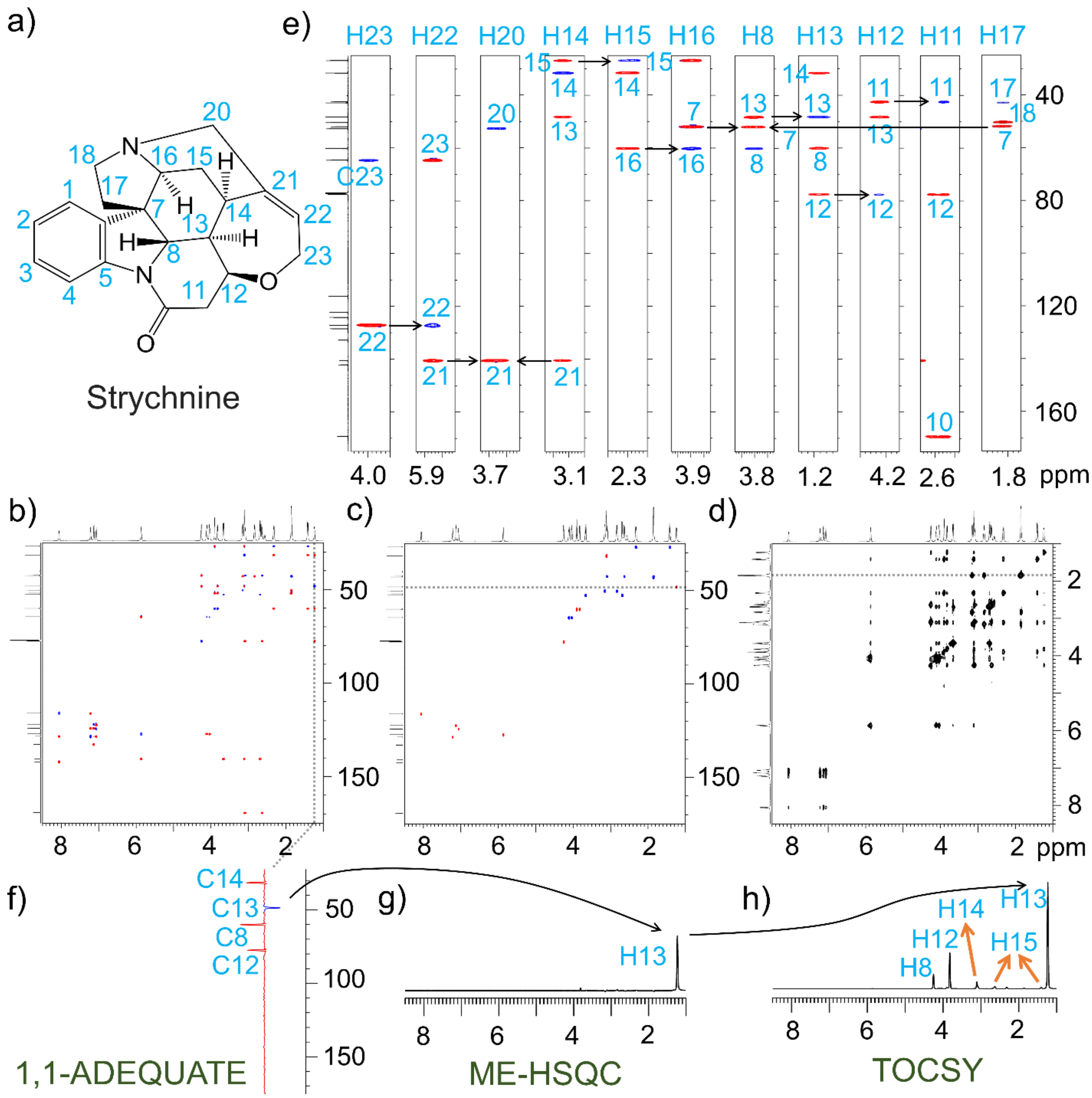


Figure S1: 1,1-ADEQUATE (b, e, f), ME-HSQC (c, g), and TOCSY (d, h) spectra obtained from a single NOAH-AST recorded on strychnine (a) molecule (~180 mM), using an 800 MHz magnetic field strength.

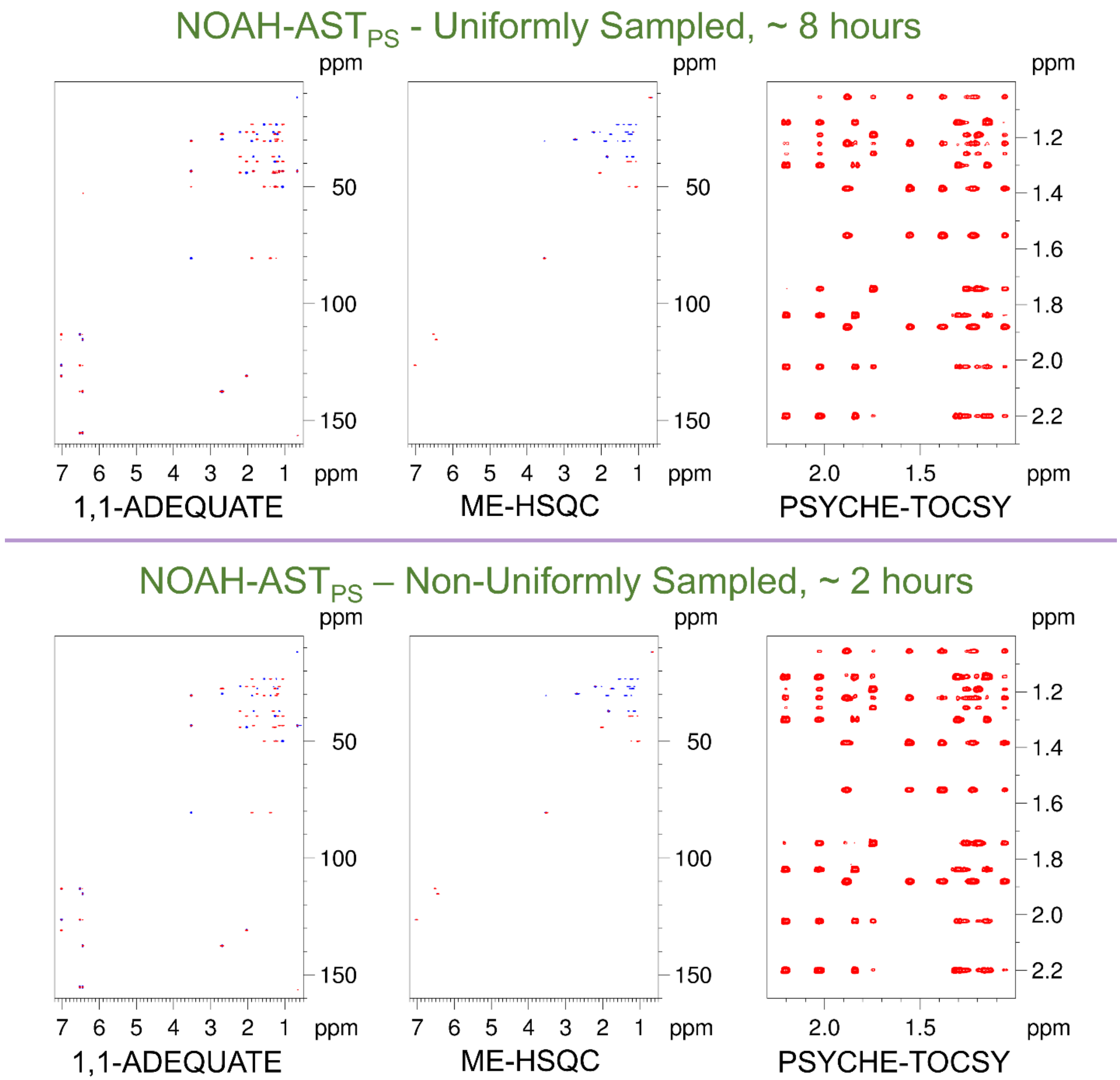


Figure S2: 1,1-ADEQUATE, ME-HSQC, and PSYCHE-TOCSY spectra obtained from a single NOAH-AST$_{PS}$ recorded on estradiol molecule in uniformly sampled (upper, ~ 7 hours 15 min), and NUS modes (lower, ~ 1 hour 50 min) using an 800 MHz magnetic field strength.

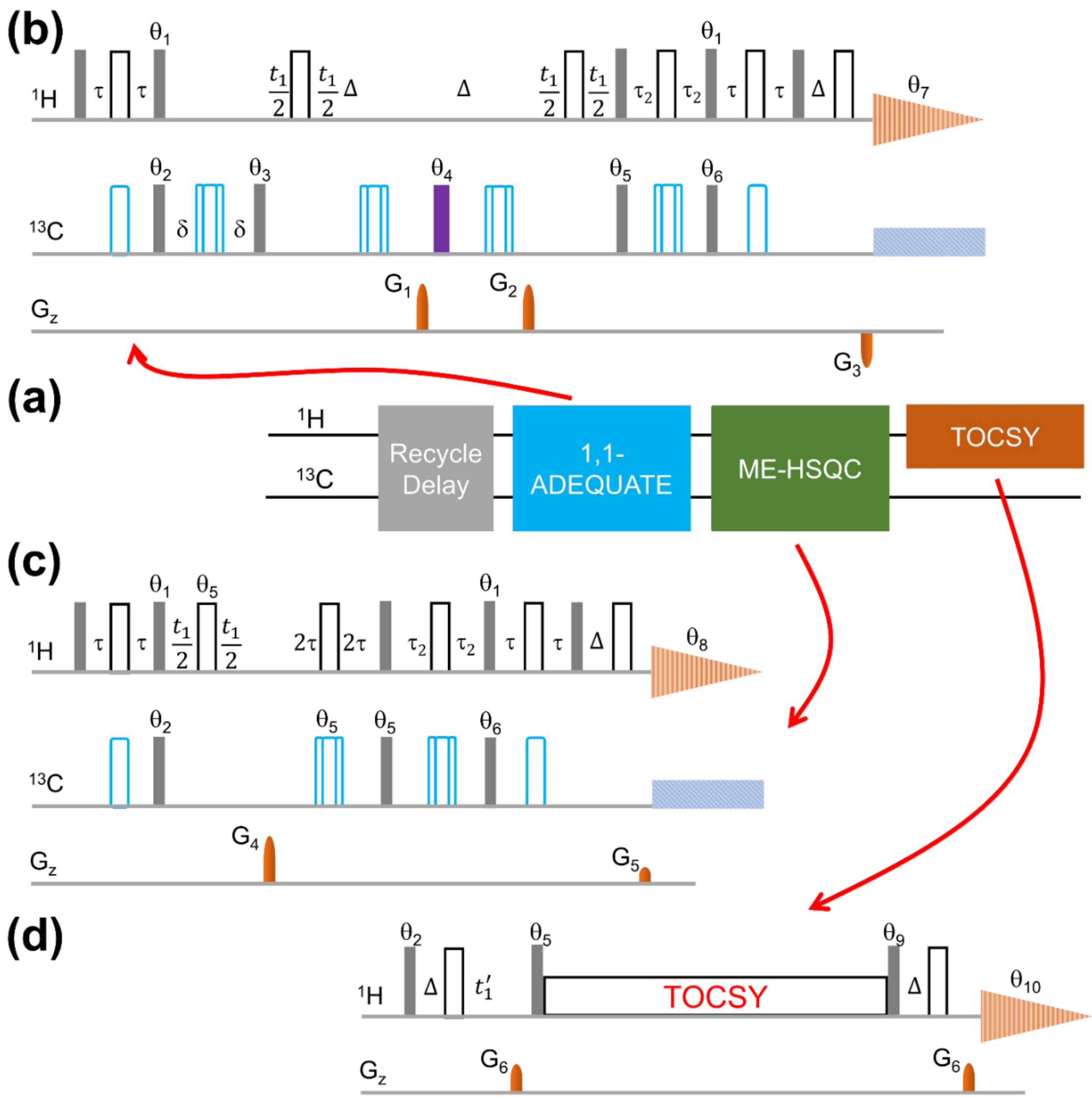


Figure S3: Schematic of NOAH-AST pulse sequence (a). The 1,1-ADEQUATE, ME-HSQC, and TOCSY pulse modules are shown in (b), (c), and (d), respectively. On both the frequency channels filled and open rectangles, respectively represent the 90°, and 180° pulses. All the 180° pulses (open blue bars) on ^{13}C channel are the adiabatic pulses (0.5 ms), whereas composite pulses (2 ms) are depicted with blue bars in 1:2:1 ratio. Phases of pulses: θ1=y; θ2=x, -x; θ3=x, x, x, x, -x, -x, -x, -x; θ4=x, x, x, x, x, x, x, x, -x, -x, -x, -x, -x, -x, -x, -x; θ5=x, x, -x, -x; θ6=y, y, -y, -y; θ7= x, -x, -x, x, -x, x, x, -x, -x, x, x, -x, x, -x, -x, x; θ8= -x, x, x, -x; θ9= -x, -x, x, x; θ10= x, -x; remaining all the pulses are applied along the x-axis. Delays: $\tau=1/(4*{}^1J_{CH})$; $\delta=1/(4*{}^1J_{CC})$; Δ=1.2 ms; $\tau_2=1/(8*{}^1J_{CH})$; $t_1' = \left({SW_{13C}}/{SW_{1_H}}\right) t_1$ (where SW presents the spectral-width). Gradients (1 ms duration at a maximum 53.5 G/cm): G1= +78.5%; G2= +77.6%; G3= -59%; G4= +80.0%; G5= +20.1%; G6= +30.0%.

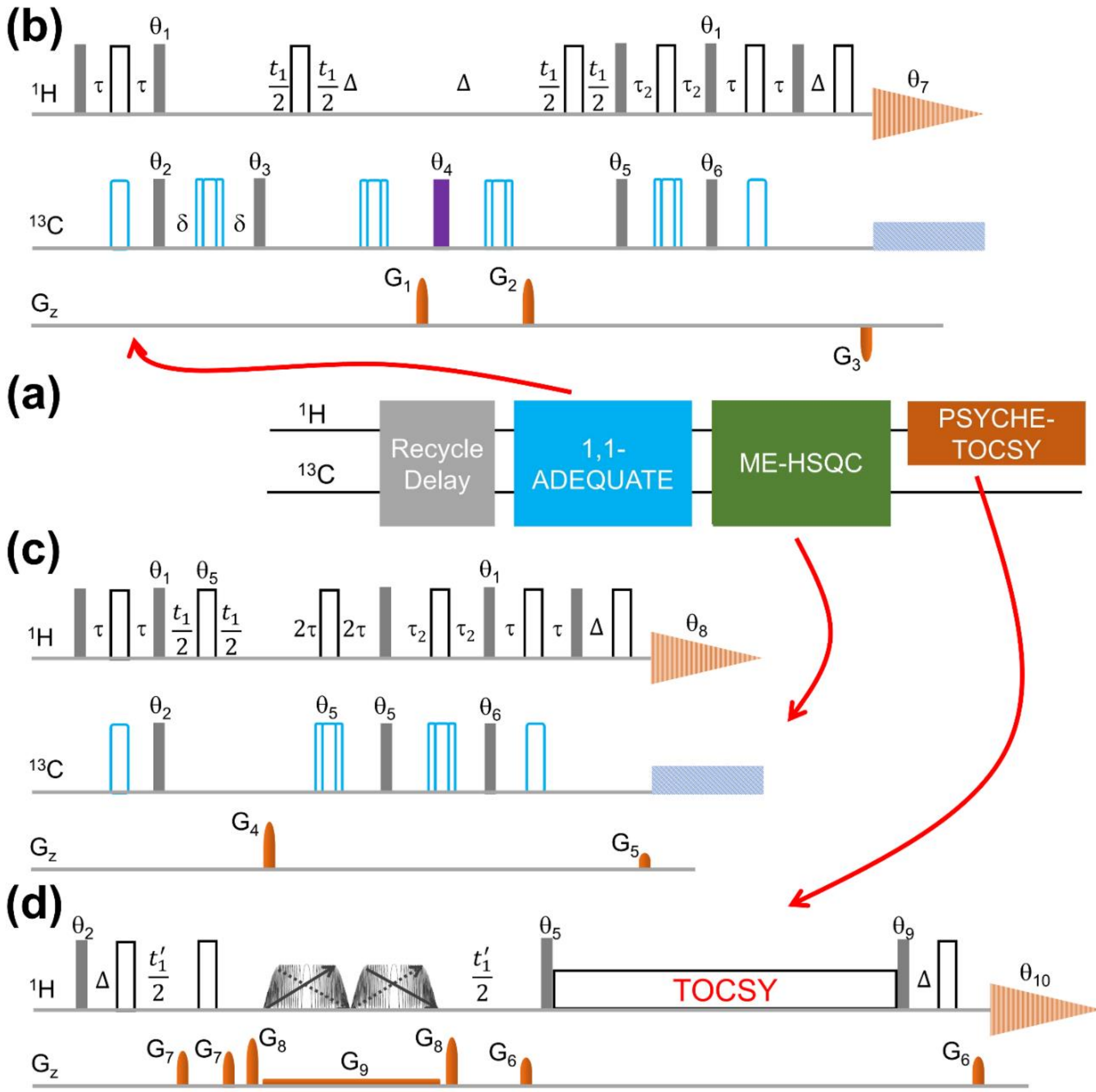
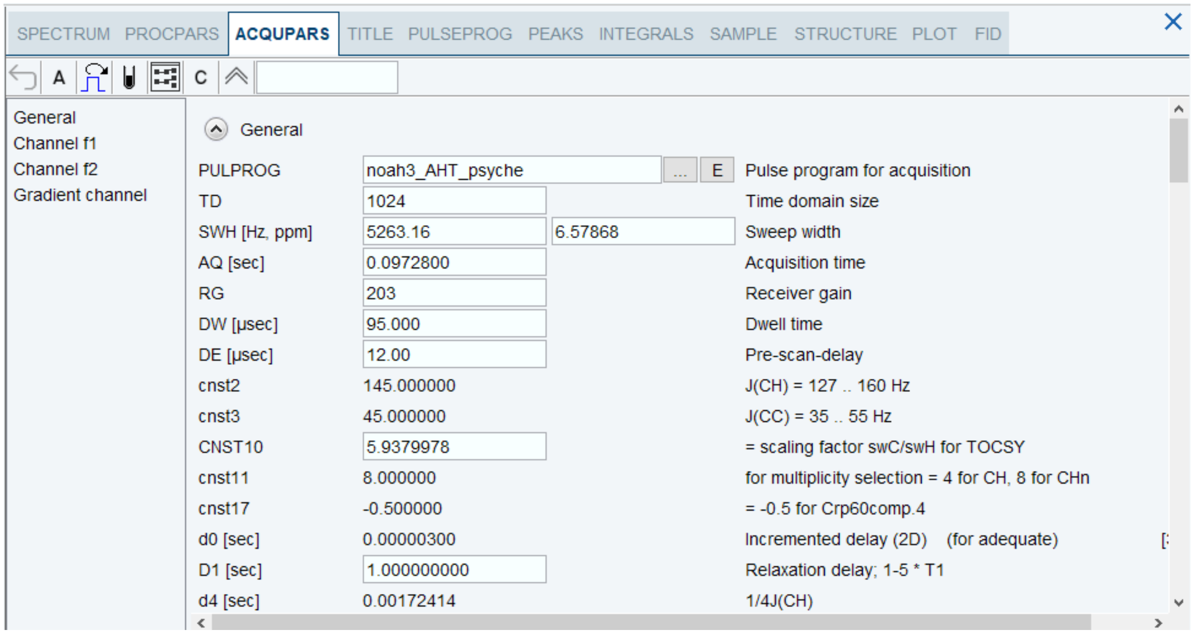
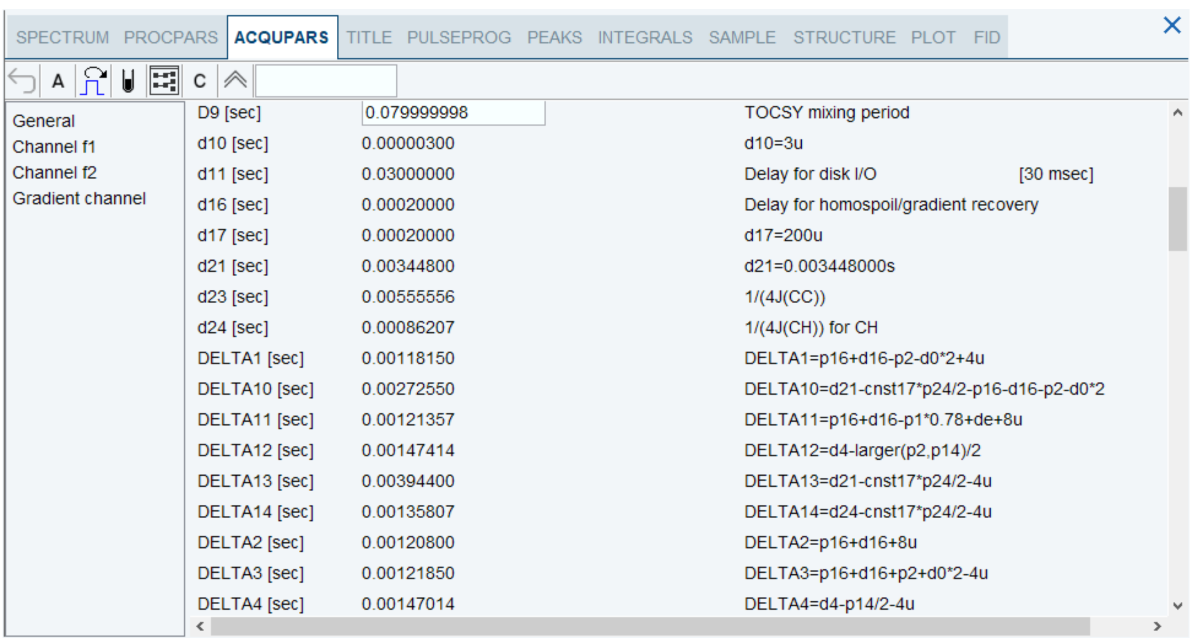
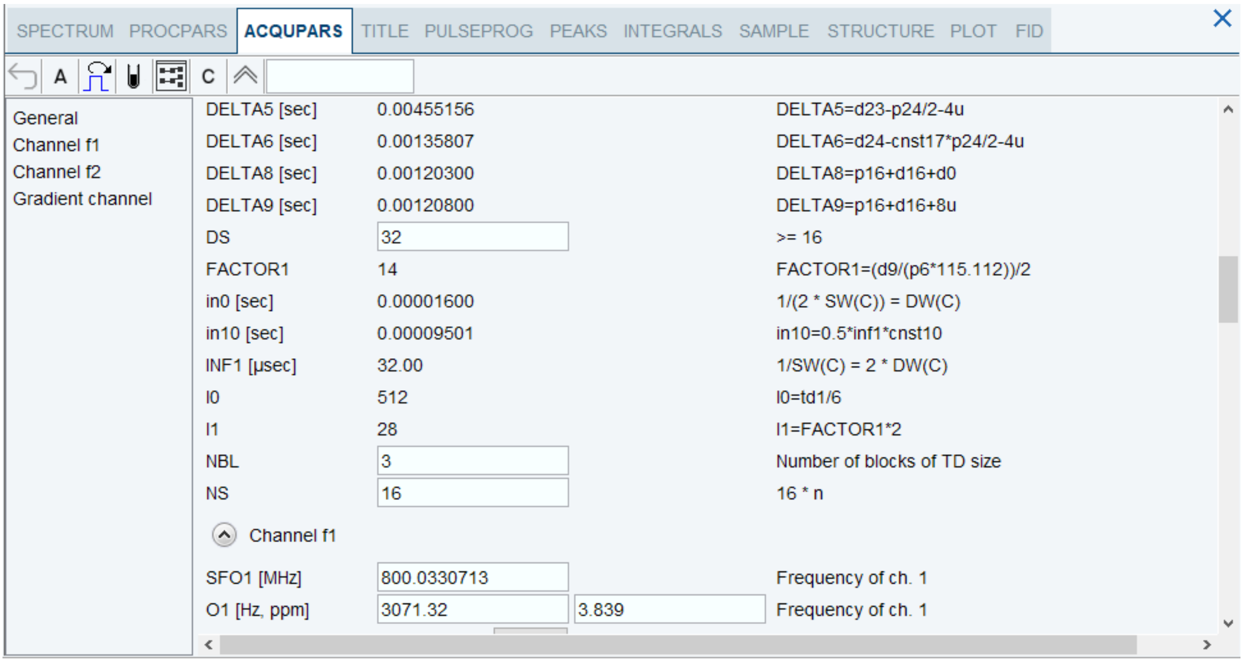


Figure S4: Schematic of NOAH-AST$_{PS}$ pulse sequence (a). The 1,1-ADEQUATE, ME-HSQC, and PSYCHE-TOCSY pulse modules are shown in (b), (c), and (d), respectively. On both the frequency channels filled and open rectangles, respectively represent the 90°, and 180° pulses. All the 180° pulses (open blue bars) on ^{13}C channel are the adiabatic pulses (0.5 ms), whereas composite pulses (2 ms) are depicted with blue bars in 1:2:1 ratio. Trapezoids with arrows represent the PSYCHE pulse (30 ms). Phases of pulses: θ1=y; θ2=x, -x; θ3=x, x, x, x, -x, -x, -x, -x; θ4=x, x, x, x, x, x, x, x, -x, -x, -x, -x, -x, -x, -x, -x; θ5=x, x, -x, -x; θ6=y, y, -y, -y; θ7= x, -x, -x, x, -x, x, x, -x, -x, x, x, -x, x, -x, -x, x; θ8= -x, x, x, -x; θ9= -x, -x, x, x; θ10= x, -x; remaining all the pulses are applied along the x-axis. Delays: $\tau=1/(4{*}^{1}J_{CH})$; $\delta=1/(4{*}^{1}J_{CC})$; Δ=1.2 ms; $\tau_2=1/(8{*}^{1}J_{CH})$; $t_1' = \left({SW_{13_C}}/{SW_{1_H}} \right) t_1$ (where SW presents the spectral-width). Gradients (1 ms duration at a maximum 53.5 G/cm, except G9): G1= +78.5%; G2= +77.6%; G3= -59%; G4= +80.0%; G5= +20.1%; G6= +30.0%; G7= +49.0%; G8= +77.0%; G9= +1.0-3.0% (30 ms).

Screenshots of acquisition parameters used to record NOAH-AST$_{PS}$ experiments on estradiol sample.







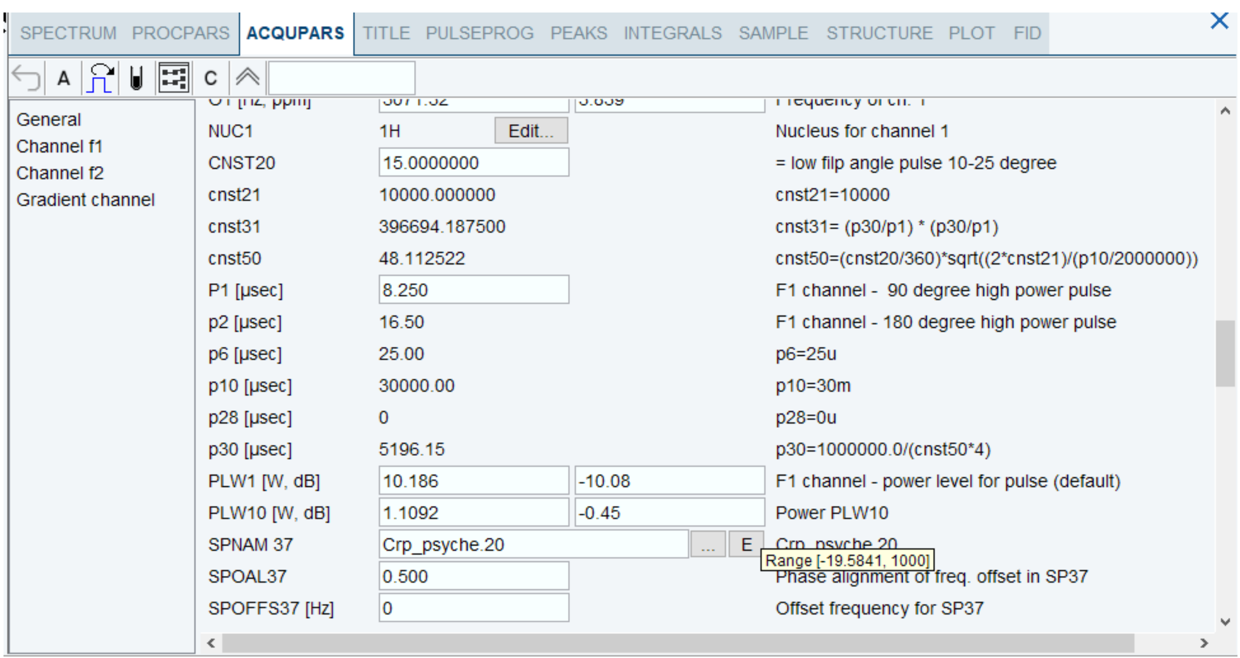
SPECTRUM PROCPARS ACQUPARS TITLE PULSEPROG PEAKS INTEGRALS SAMPLE STRUCTURE PLOT FID

General
Channel f1
Channel f2
Gradient channel

DELTA5 [sec]	0.00455156		DELTA5=d23-p24/2-4u
DELTA6 [sec]	0.00135807		DELTA6=d24-cnst17*p24/2-4u
DELTA8 [sec]	0.00120300		DELTA8=p16+d16+d0
DELTA9 [sec]	0.00120800		DELTA9=p16+d16+8u
DS	32		>= 16
FACTOR1	14		FACTOR1=(d9/(p6*115.112))/2
in0 [sec]	0.00001600		1/(2 * SW(C)) = DW(C)
in10 [sec]	0.00009501		in10=0.5*inf1*cnst10
INF1 [µsec]	32.00		1/SW(C) = 2 * DW(C)
l0	512		l0=td1/6
l1	28		l1=FACTOR1*2
NBL	3		Number of blocks of TD size
NS	16		16 * n

Channel f1

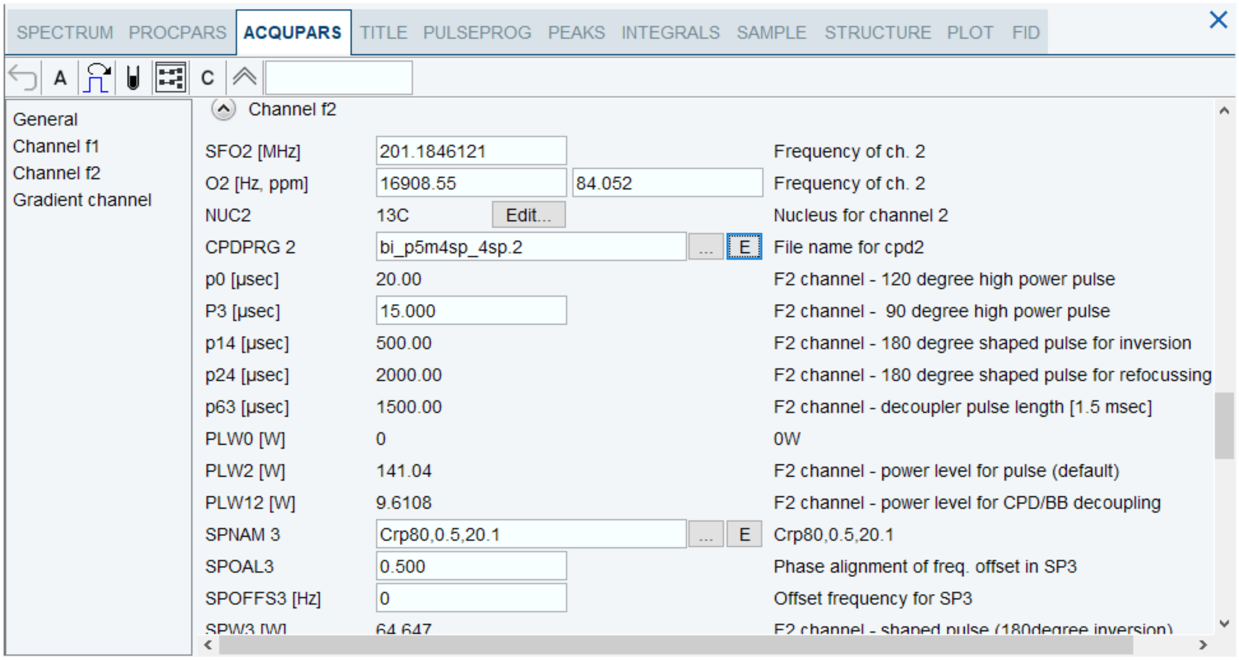
SFO1 [MHz]	800.0330713		Frequency of ch. 1
O1 [Hz, ppm]	3071.32	3.839	Frequency of ch. 1



SPECTRUM PROCPARS ACQUPARS TITLE PULSEPROG PEAKS INTEGRALS SAMPLE STRUCTURE PLOT FID

General
Channel f1
Channel f2
Gradient channel

NUC1	1H	Edit...	Nucleus for channel 1
CNST20	15.0000000		= low filp angle pulse 10-25 degree
cnst21	10000.000000		cnst21=10000
cnst31	396694.187500		cnst31= (p30/p1) * (p30/p1)
cnst50	48.112522		cnst50=(cnst20/360)*sqrt((2*cnst21)/(p10/2000000))
P1 [µsec]	8.250		F1 channel - 90 degree high power pulse
p2 [µsec]	16.50		F1 channel - 180 degree high power pulse
p6 [µsec]	25.00		p6=25u
p10 [µsec]	30000.00		p10=30m
p28 [µsec]	0		p28=0u
p30 [µsec]	5196.15		p30=1000000.0/(cnst50*4)
PLW1 [W, dB]	10.186	-10.08	F1 channel - power level for pulse (default)
PLW10 [W, dB]	1.1092	-0.45	Power PLW10
SPNAM 37	Crp_psyche.20	... E	Crp_psyche.20
SPOAL37	0.500	Range [-19.5841, 1000]	Phase alignment of freq. offset in SP37
SPOFFS37 [Hz]	0		Offset frequency for SP37

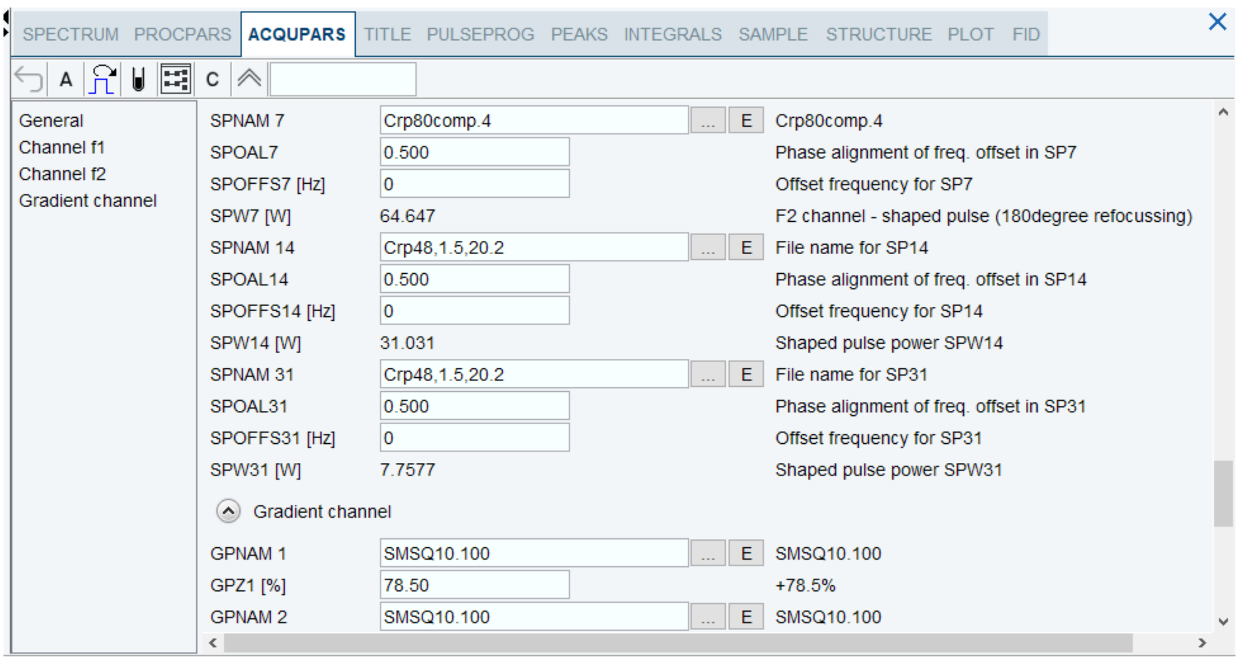


SPECTRUM PROCPARS ACQUPARS TITLE PULSEPROG PEAKS INTEGRALS SAMPLE STRUCTURE PLOT FID

General
Channel f1
Channel f2
Gradient channel

Channel f2

SFO2 [MHz]	201.1846121		Frequency of ch. 2
O2 [Hz, ppm]	16908.55	84.052	Frequency of ch. 2
NUC2	13C	Edit...	Nucleus for channel 2
CPDPRG 2	bi_p5m4sp_4sp.2	... E	File name for cpd2
p0 [µsec]	20.00		F2 channel - 120 degree high power pulse
P3 [µsec]	15.000		F2 channel - 90 degree high power pulse
p14 [µsec]	500.00		F2 channel - 180 degree shaped pulse for inversion
p24 [µsec]	2000.00		F2 channel - 180 degree shaped pulse for refocussing
p63 [µsec]	1500.00		F2 channel - decoupler pulse length [1.5 msec]
PLW0 [W]	0		0W
PLW2 [W]	141.04		F2 channel - power level for pulse (default)
PLW12 [W]	9.6108		F2 channel - power level for CPD/BB decoupling
SPNAM 3	Crp80,0.5,20.1	... E	Crp80,0.5,20.1
SPOAL3	0.500		Phase alignment of freq. offset in SP3
SPOFFS3 [Hz]	0		Offset frequency for SP3
SPW3 [W]	64.647		F2 channel - shaped pulse (180degree inversion)



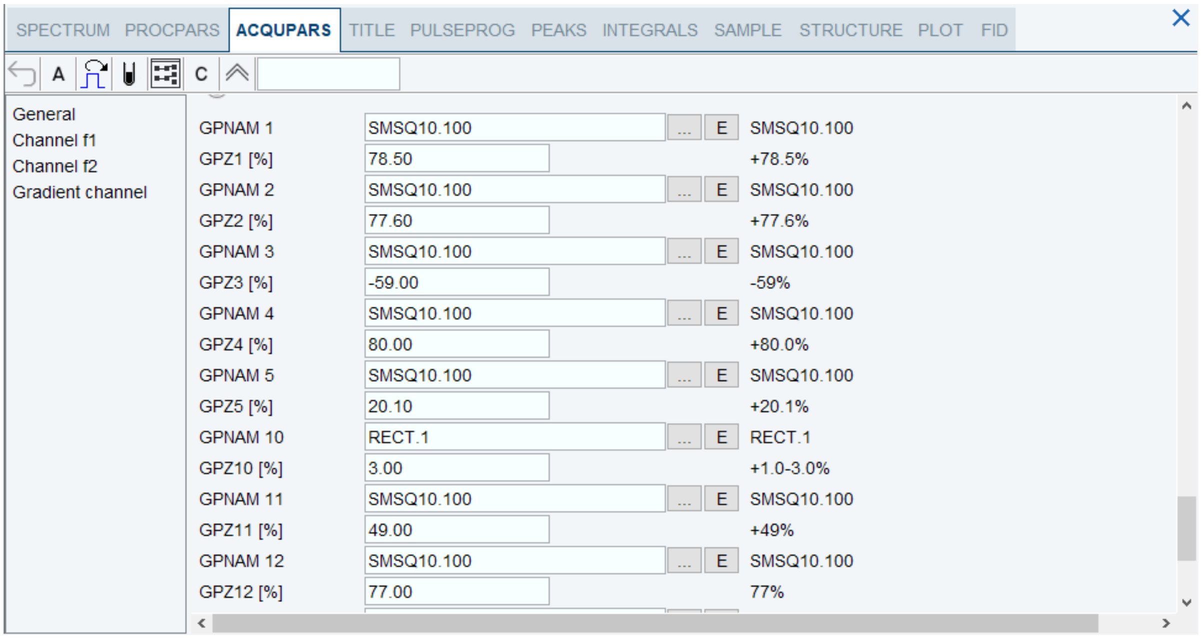
SPECTRUM PROCPARS ACQUPARS TITLE PULSEPROG PEAKS INTEGRALS SAMPLE STRUCTURE PLOT FID

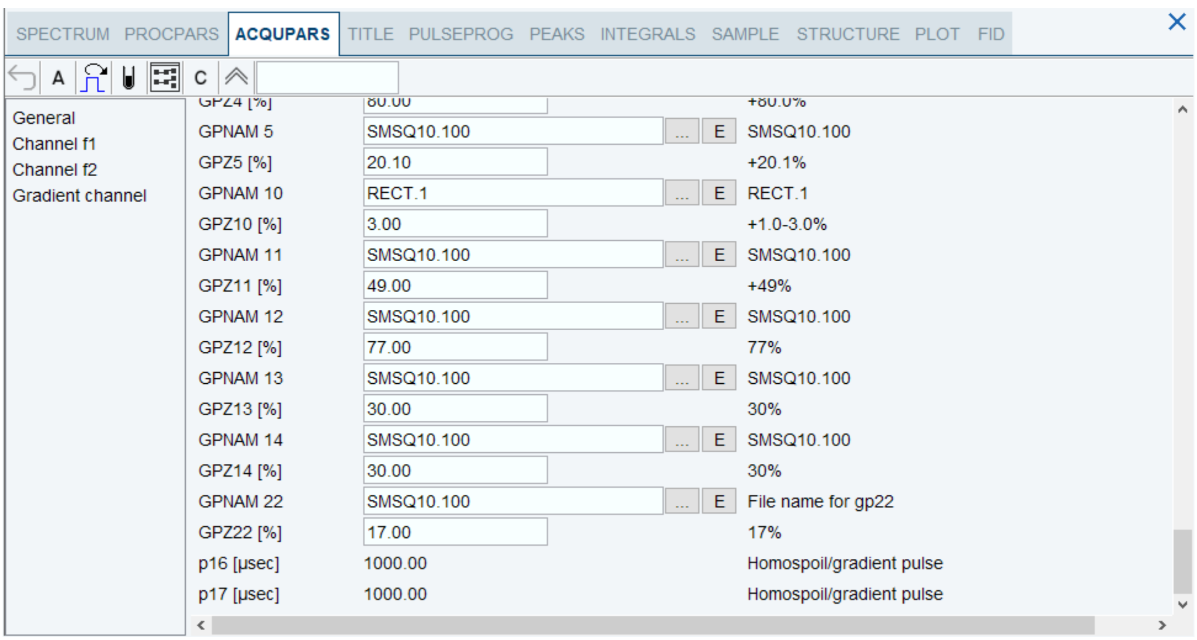
General
Channel f1
Channel f2
Gradient channel

SPNAM 7	Crp80comp.4	... E	Crp80comp.4
SPOAL7	0.500		Phase alignment of freq. offset in SP7
SPOFFS7 [Hz]	0		Offset frequency for SP7
SPW7 [W]	64.647		F2 channel - shaped pulse (180degree refocussing)
SPNAM 14	Crp48,1.5,20.2	... E	File name for SP14
SPOAL14	0.500		Phase alignment of freq. offset in SP14
SPOFFS14 [Hz]	0		Offset frequency for SP14
SPW14 [W]	31.031		Shaped pulse power SPW14
SPNAM 31	Crp48,1.5,20.2	... E	File name for SP31
SPOAL31	0.500		Phase alignment of freq. offset in SP31
SPOFFS31 [Hz]	0		Offset frequency for SP31
SPW31 [W]	7.7577		Shaped pulse power SPW31

Gradient channel

GPNAM 1	SMSQ10.100	... E	SMSQ10.100
GPZ1 [%]	78.50		+78.5%
GPNAM 2	SMSQ10.100	... E	SMSQ10.100


SPECTRUM PROCPARS ACQUPARS TITLE PULSEPROG PEAKS INTEGRALS SAMPLE STRUCTURE PLOT FID
A
C
General
Channel f1
Channel f2
Gradient channel
GPNAM 1 SMSQ10.100 ... E SMSQ10.100
GPZ1 [%] 78.50 +78.5%
GPNAM 2 SMSQ10.100 ... E SMSQ10.100
GPZ2 [%] 77.60 +77.6%
GPNAM 3 SMSQ10.100 ... E SMSQ10.100
GPZ3 [%] -59.00 -59%
GPNAM 4 SMSQ10.100 ... E SMSQ10.100
GPZ4 [%] 80.00 +80.0%
GPNAM 5 SMSQ10.100 ... E SMSQ10.100
GPZ5 [%] 20.10 +20.1%
GPNAM 10 RECT.1 ... E RECT.1
GPZ10 [%] 3.00 +1.0-3.0%
GPNAM 11 SMSQ10.100 ... E SMSQ10.100
GPZ11 [%] 49.00 +49%
GPNAM 12 SMSQ10.100 ... E SMSQ10.100
GPZ12 [%] 77.00 77%


SPECTRUM PROCPARS ACQUPARS TITLE PULSEPROG PEAKS INTEGRALS SAMPLE STRUCTURE PLOT FID
A
C
General
Channel f1
Channel f2
Gradient channel
GPNAM 5 SMSQ10.100 ... E SMSQ10.100
GPZ5 [%] 20.10 +20.1%
GPNAM 10 RECT.1 ... E RECT.1
GPZ10 [%] 3.00 +1.0-3.0%
GPNAM 11 SMSQ10.100 ... E SMSQ10.100
GPZ11 [%] 49.00 +49%
GPNAM 12 SMSQ10.100 ... E SMSQ10.100
GPZ12 [%] 77.00 77%
GPNAM 13 SMSQ10.100 ... E SMSQ10.100
GPZ13 [%] 30.00 30%
GPNAM 14 SMSQ10.100 ... E SMSQ10.100
GPZ14 [%] 30.00 30%
GPNAM 22 SMSQ10.100 ... E File name for gp22
GPZ22 [%] 17.00 17%
p16 [μsec] 1000.00 Homospoil/gradient pulse
p17 [μsec] 1000.00 Homospoil/gradient pulse

Experimental parameters used to record NOAH-AST spectra on artemisinin molecule

20 mg of compound dissolved in 0.5 ml of DMSO-D_6: ~ 140 mM

Number of scans: 32

Recycle delay: 1s

TOCSY mixing time: 80 ms

SW_{13C}/ SW_{1H} : 7.74

Total experimental time: 7 hr 11 min

Parameter	**F2**	**F1**
Size of FID	1024	1536 (for three blocks)
Spectral width (Hz)	4425	34250
Acquisition time (s)	0.116	0.0224
FID resolution (Hz)	8.64	44.6
Transmitter Frequency offset (ppm)	3.509	93.555

Experimental parameters used to record NOAH-AST spectra on strychnine molecule

30 mg of compound dissolved in 0.5 ml of $CDCl_3$: ~ 180 mM

Number of scans: 16

Recycle delay: 1s

TOCSY mixing time: 80 ms

SW_{13C}/ SW_{1H} : 4.21

Total experimental time: 1 hr 45 min

Parameter	**F2**	**F1**
Size of FID	2048	768 (for three blocks)
Spectral width (Hz)	11904	31185
Acquisition time (s)	0.086	0.0123
FID resolution (Hz)	11.6	81.2
Transmitter Frequency offset (ppm)	4.178	100.0

Experimental parameters used to record NOAH-AST spectra on estradiol molecule

50 mg of compound dissolved in 0.5 ml of DMSO-D_6: ~ 370 mM

Number of scans: 16

Recycle delay: 1s

TOCSY mixing time: 80 ms

SW_{13C}/ SW_{1H} : 5.94

Total experimental time: ~ 7 hours 4 min

Parameter	**F2**	**F1**
Size of FID	1024	3072 (for three blocks)
Spectral width (Hz)	5263	31252
Acquisition time (s)	0.097	0.049
FID resolution (Hz)	10.28	20.35
Transmitter Frequency offset (ppm)	3.839	84.05

Experimental parameters used to record NOAH-AST$_{PS}$ spectra on estradiol molecule

Number of scans: 16

Recycle delay: 1s

TOCSY mixing time: 80 ms

SW_{13C}/ SW_{1H} : 5.94

PSYCHE pulse duration and β-angle: 30 ms/ 15^{o}

Total experimental time: ~ 7 hours 15 min

Parameter	**F2**	**F1**
Size of FID	1024	3072 (for three blocks)
Spectral width (Hz)	5263	31252
Acquisition time (s)	0.097	0.049
FID resolution (Hz)	10.28	20.35
Transmitter Frequency offset (ppm)	3.839	84.05

Experimental parameters used to record NUS-NOAH-AST$_{PS}$ spectra on estradiol molecule

Number of scans: 16

Recycle delay: 1s

TOCSY mixing time: 80 ms

SW_{13C}/ SW_{1H} : 5.94

PSYCHE pulse duration and β-angle: 30 ms/ 15°

Total experimental time: ~ 1 hour 50 min

Parameter	**F2**	**F1**
Size of FID	1024	768 (25%, for three blocks)
Spectral width (Hz)	5263	31252
Acquisition time (s)	0.097	0.049
FID resolution (Hz)	10.28	20.35
Transmitter Frequency offset (ppm)	3.839	84.05

NUS sampling setting-up is performed with the python script “noah_nus.py”

Experimental parameters used to record NOAH-AST spectra on mixture of D-glucose and D-xylose

10 mg of D-Glucose and 0.5 mg of D-Xylose are dissolved in 0.5 ml of D_2O: ~ 110 mM + 6 mM

Number of scans: 16

Recycle delay: 1s

TOCSY mixing time: 80 ms

SW_{13C}/ SW_{1H} : 2.52

Total experimental time: ~ 1 hour 40 min

Parameter	**F2**	**F1**
Size of FID	1024	768 (for three blocks)
Spectral width (Hz)	6250	10000
Acquisition time (s)	0.082	0.038
FID resolution (Hz)	12.2	26.04
Transmitter Frequency offset (ppm)	4.7	80.3

Data processing

Individual spectra from NOAH-AST and NOAH-AST$_{PS}$ experiments have been separated out by using a topspin 4.0.5 inbuilt AU macro “splitx_au”. In this regard, the user parameters have been used as follows,

USERP1 → noah_hsqc

USERP2 → noah_hsqc

USERP3 → noah_noesy

The following noah-ast.py and noah-ast_psyche.py scripts have to be copied into the folder

“C:\Bruker\Topspin4.0.X\exp\stan\nmr\py\user”

Otherwise the following scripts can be obtained from the author.

NOAH-AST.py script

save the following script as noah-ast.py

MSG("Initial step: 1D 1H and 13C experiments have to be recorded" "\nThen create a new data set with the command \a'new'" "\nThe present macro 'AST' takes care all the required parameters")

ct = XCMD("RPAR HMBCGP all")

MSG("DRAG 1D 1H data set into the present window" "\nClick on Copy Parameters Option" "\nClick on OK")

ct = XCMD("copypars.py")

MSG("DRAG 1D 13C data set into the present window" "\nClick on Copy Parameters Option" "\nClick on OK")

ct = XCMD("copypars.py")

PPTEXT = """

;$CLASS=HighRes

;$DIM=2D

;$TYPE=

;$SUBTYPE=

;$COMMENT=

```
#include <Avance.incl>

#include <Delay.incl>

#include <Grad.incl>



"p2=p1*2"

"d0=3u"

"d10=3u"

"d11=30m"

"d16=200u"

"d17=200u"

"p28=0u"

"p14=500u"

"p24=2000u"

"p63=1500u"

"p16=1000u"

"p17=1000u"

"p6=25u"


"cnst2=145"

"cnst3=45"

"cnst11=8"

"cnst17=-0.5"
```

"p0=p3*1.333"

"d4=1s/(cnst2*4)"

"d23=1s/(cnst3*4)"

"d24=1s/(cnst2*cnst11)"

"in0=inf1/2"

"DELTA1=p16+d16-p2-d0*2+4u"

"DELTA2=p16+d16+8u"

"DELTA3=p16+d16+p2+d0*2-4u"

"DELTA4=d4-p14/2-4u"

"DELTA5=d23-p24/2-4u"

"DELTA6=d24-cnst17*p24/2-4u"

"p4=p3*2"

"d21=0.003448000s"

"DELTA10=d21-cnst17*p24/2-p16-d16-p2-d0*2"

"DELTA11=p16+d16-p1*0.78+de+8u"

"DELTA12=d4-larger(p2,p14)/2"

"DELTA13=d21-cnst17*p24/2-4u"

"DELTA14=d24-cnst17*p24/2-4u"

```
"l0=td1/6"

"FACTOR1=(d9/(p6*115.112))/2"

"l1=FACTOR1*2"



"in10=0.5*inf1*cnst10"

"p11=20m"


"DELTA8=p16+d16+d0"

"DELTA9=p16+d16+8u"


"acqt0=0"

baseopt_echo


1 ze

  d11 pl12:f2

2 d11

3 4m do:f2

4 50u UNBLKGRAD

d1 st0

 4u pl2:f2

4u pl1:f1


4u pl2:f2

(p3 ph1):f2
```

```
p16:gp22
d16

13 (p1 ph1)
4u
DELTA4 pl0:f2
(center (p2 ph1) (p14:sp3 ph1):f2 )
4u
DELTA4 pl2:f2
(p1 ph2) (p3 ph4):f2
4u
DELTA5 pl0:f2
(p24:sp7 ph8):f2
4u
DELTA5 pl2:f2
(p3 ph9):f2
d0
(p2 ph1)
d0
DELTA1 pl0:f2
(p24:sp7 ph11):f2
4u
p16:gp1
```

```
d16 pl2:f2

(p0 ph10):f2

4u

DELTA3 pl0:f2

(p24:sp7 ph11):f2

p16:gp2

d16 pl2:f2

d0

(p2 ph1)

d0

(center (p1 ph1) (p3 ph5):f2 )

4u

DELTA6 pl0:f2

(center (p2 ph1) (p24:sp7 ph1):f2 )

4u

DELTA6 pl2:f2

(center (p1 ph2) (p3 ph6):f2 )

4u

DELTA4 pl0:f2

(center (p2 ph1) (p14:sp3 ph1):f2 )

4u

DELTA4

(p1 ph1)

DELTA2

(p2 ph1)
```

```
  4u
  p16:gp3*EA
  d16 pl12:f2
  4u BLKGRAD

 goscnp ph30 cpd2:f2
4u do:f2

2m st
 50u UNBLKGRAD
4u pl2:f2
4u pl1:f1
(p3 ph1):f2

 p16:gp22
  d16

23 (p1 ph21)
  DELTA12 pl0:f2
  4u
  (center (p2 ph21) (p14:sp3 ph26):f2 )
  4u
  DELTA12 pl2:f2 UNBLKGRAD
  p28 ph21
  4u
```

```
(p1 ph22) (p3 ph23):f2

d0

(p2 ph27)

d0

p16:gp4*EA

d16

DELTA10 pl0:f2

(center (p2 ph21) (p24:sp7 ph24):f2 )

4u

DELTA13 pl2:f2

(center (p1 ph21) (p3 ph24):f2 )

4u

DELTA14 pl0:f2

(center (p2 ph21) (p24:sp7 ph21):f2 )

4u

DELTA14 pl2:f2

(center (p1 ph22) (p3 ph25):f2 )

DELTA12 pl0:f2

(center (p2 ph21) (p14:sp3 ph21):f2 )

DELTA12

(p1 ph21)

DELTA11

(p2 ph21)

4u

p16:gp5
```

```
  d16 pl12:f2
  4u BLKGRAD
goscnp ph31 cpd2:f2
4u do:f2

2m st
4u pl2:f2
(p3 ph1):f2
  50u UNBLKGRAD
  p16:gp22
  d16

4u pl1:f1

  p1 ph12
  DELTA8
  p2 ph8

d10
d10

  p16:gp13*EA
  d16
  p1 ph14
  10u pl10:f1
```

```
;begin DIPSI2
14 p6*3.556 ph13
  p6*4.556 ph15
  p6*3.222 ph13
  p6*3.167 ph15
  p6*0.333 ph13
  p6*2.722 ph15
  p6*4.167 ph13
  p6*2.944 ph15
  p6*4.111 ph13

  p6*3.556 ph15
  p6*4.556 ph13
  p6*3.222 ph15
  p6*3.167 ph13
  p6*0.333 ph15
  p6*2.722 ph13
  p6*4.167 ph15
  p6*2.944 ph13
  p6*4.111 ph15

  p6*3.556 ph15
  p6*4.556 ph13
  p6*3.222 ph15
  p6*3.167 ph13
```

```
p6*0.333 ph15
p6*2.722 ph13
p6*4.167 ph15
p6*2.944 ph13
p6*4.111 ph15

p6*3.556 ph13
p6*4.556 ph15
p6*3.222 ph13
p6*3.167 ph15
p6*0.333 ph13
p6*2.722 ph15
p6*4.167 ph13
p6*2.944 ph15
p6*4.111 ph13
lo to 14 times l1
                                        ;end DIPSI2
50u pl1:f1
p1 ph16
DELTA9
p2 ph8
4u
p16:gp14
d16
4u BLKGRAD
```

go=2 ph18

d11 wr #0 if #0 zd igrad EA

1m ip6*2

1m ip12*2

1m ip14*2

1m ip23*2

1m ip25*2

1m ip26*2

1m ip31*2

1m ip18*2

lo to 3 times 2

1m rp6

1m rp12

1m rp14

1m rp23

1m rp25

1m rp26

1m rp31

1m rp18

1m id0

1m id10

lo to 4 times l0

exit

ph1=0

ph2=1

ph4=0 2

ph5=0 0 2 2

ph6=1 1 3 3

ph7=0

ph8=0

ph9=0 0 0 0 2 2 2 2

ph10=0 0 0 0 0 0 0 0 2 2 2 2 2 2 2 2

ph11=0

ph30=0 2 2 0 2 0 0 2 2 0 0 2 0 2 2 0

ph21=0

ph22=1

ph23=0 2

ph24=0 0 2 2

ph25=1 1 3 3

ph26=0

ph27=0 0 2 2

ph31=2 0 0 2

ph12=0 2

ph14=0 0 2 2

ph13=3

ph15=1

ph16=2 2 0 0

ph19=0

ph18=0 2

;pl0 : 0W

;pl1 : f1 channel - power level for pulse (default)

;pl2 : f2 channel - power level for pulse (default)

;pl12: f2 channel - power level for CPD/BB decoupling

;sp3: f2 channel - shaped pulse (180degree inversion)

;spnam3: Crp80,0.5,20.1

;spnam1: Crp80,20,20.10

;sp7: f2 channel - shaped pulse (180degree refocussing)

;spnam7: Crp80comp.4

;p0 : f2 channel - 120 degree high power pulse

;p1 : f1 channel - 90 degree high power pulse

;p2 : f1 channel - 180 degree high power pulse

;p3 : f2 channel - 90 degree high power pulse

;p14: f2 channel - 180 degree shaped pulse for inversion

;   = 500usec for Crp60,0.5,20.1

;p16: homospoil/gradient pulse

;   = 1msec

```
;p17: homospoil/gradient pulse
;                                = 1msec
;p20: PSYCHE gradient pulse
;                                = 30msec
;p24: f2 channel - 180 degree shaped pulse for refocussing
;    = 2msec for Crp60comp.4
;d0 : incremented delay (2D)    (for adequate)          [3 usec]
;d20 : incremented delay (2D)    (for HSQC)
;d0 : incremented delay (2D)      (for TOCSY)
;d1 : relaxation delay; 1-5 * T1
;d4 : 1/4J(CH)
;d11: delay for disk I/O                    [30 msec]
;d16: delay for homospoil/gradient recovery
;d23: 1/(4J(CC))
;d9: TOCSY mixing period
;d19: ASAP-TOCSY mixing period (for HSQC ~ 40 msec)
;d24: 1/(4J(CH)) for CH
;    1/(8J(CH)) for all multiplicities
;cnst2 : J(CH) = 127 .. 160 Hz
;cnst3 : J(CC) = 35 .. 55 Hz
;cnst11: for multiplicity selection = 4 for CH, 8 for CHn
;cnst17: = -0.5 for Crp60comp.4
;cnst20: = low filp angle pulse 10-25 degree
;inf1: 1/SW(C) = 2 * DW(C)
;in0: 1/(2 * SW(C)) = DW(C)
```

;nd0: 2

;in20: = in0

;ns: 16 * n

;ds: >= 16

;td1: number of experiments

;FnMODE: echo-antiecho

;cpd2:[bi_p5m4sp_4sp.2] decoupling according to sequence defined by cpdprg2

;pcpd2: f2 channel - 90 degree pulse for decoupling sequence

;cnst10: = scaling factor swC/swH for TOCSY

;p63: f2 channel - decoupler pulse length [1.5 msec]

;   = 1500usec for bi_p5m4sp_4sp.2.

;for z-only gradients:

;gpz1: +78.5%

;gpz2: +77.6%

;gpz3: -59%

;gpz4: +80.0%

;gpz5: +20.1%

;gpz10: +1.0%

;gpz11: +49%

;gpz12: 77%

;gpz13: 30%

;gpz14: 30%

;gpz22: 17%

```
;use gradient files:
;gpnam1: SMSQ10.100
;gpnam2: SMSQ10.100
;gpnam3: SMSQ10.100
;gpnam4: SMSQ10.100
;gpnam5: SMSQ10.100
;gpnam10: RECT.1
;gpnam11: SMSQ10.100
;gpnam12: SMSQ10.100
;gpnam13: SMSQ10.100
;gpnam14: SMSQ10.100
;gpnam21: SMSQ10.100


;cnst17: Factor to compensate for coupling evolution during a pulse
;       (usually +1). A positive factor indicates that coupling
;       evolution continues during the pulse, whereas a negative
;       factor is necessary if the coupling is (partially) refocussed.
"""
import math
pp = DEF_PULSPROG(PPTEXT)

ppName = "noah3_AST"
PUTPAR("PULPROG", ppName)
```

```
pp.SAVE_AS(ppName)

PUTPAR("1 FnMODE", "Echo-Antiecho")
PUTPAR("GPNAM 1", "SMSQ10.100")
PUTPAR("GPZ 1", "78.5")
PUTPAR("GPNAM 2", "SMSQ10.100")
PUTPAR("GPZ 2", "77.6")
PUTPAR("GPNAM 3", "SMSQ10.100")
PUTPAR("GPZ 3", "-59.0")
PUTPAR("GPNAM 4", "SMSQ10.100")
PUTPAR("GPZ 4", "80.0")
PUTPAR("GPNAM 5", "SMSQ10.100")
PUTPAR("GPZ 5", "20.1")
PUTPAR("GPNAM 13", "SMSQ10.100")
PUTPAR("GPZ 13", "30.0")
PUTPAR("GPNAM 14", "SMSQ10.100")
PUTPAR("GPZ 14", "30.0")
PUTPAR("GPNAM 22", "SMSQ10.100")
PUTPAR("GPZ 22", "17.0")

PUTPAR("SPNAM 3", "Crp80,0.5,20.1")
PUTPAR("SPNAM 1", "Crp80,20,20.10")
PUTPAR("SPNAM 7", "Crp80comp.4")

PUTPAR("CPDPRG 2", "bi_p5m4sp_4sp.2")
```

```
PUTPAR("NBL", "3")

PUTPAR("NS", "32")

PUTPAR("DS", "32")

PUTPAR("TD", "1024")

PUTPAR("1 TD", "512")

PUTPAR("D 1", "1")

PUTPAR("D 9", "0.08")


ct = XCMD("SWH")

ct.join()

ct = XCMD("O1")

ct.join()

ct = XCMD("D1")

ct.join()

ct = XCMD("NS")

ct.join()

ct = XCMD("DS")

ct.join()

ct = XCMD("TD")

ct.join()

aqdirect = GETPAR ("AQ")

MSG(str(aqdirect)+ "= Proton Acquisition time"+ "\nShould be <= 50 ms")

td1 = GETPAR("1 TD")

MSG(str(td1)+ "\nNumber of indirect increments" "\nBy default it takes 512 increments \nIn the AST
experiments it shows 1536 for the three pulse blocks")

ct = XCMD("D9")
```

```
ct.join()


td11 = int (td1)
td111 = 3*td11
PUTPAR("1 TD", str(td111))

a = GETPAR("SWH")
aa = 1.0 / float (a)
b = GETPAR("1 SWH")
bb = float (b)
c = aa * bb
PUTPAR("CNST 10", str(c))

p = GETPAR("P 1")
pf = str (p)
pk = GETPAR("PLdB 1")
pkf = str (pk)

XCMD ("2 WDW QSINE")
XCMD ("1 WDW QSINE")
XCMD ("1 SSB 2")
XCMD ("2 SSB 2")
XCMD ("2 PH_mod pk")
XCMD ("1 PH_mod pk")
```

XCMD ("1 MC2 echo-antiecho")

XCMD ("1 USERP1 noah_hsqc")

XCMD ("1 USERP2 noah_hsqc")

XCMD ("1 USERP3 noah_noesy")

MSG("Perform with the known P1 and PLdB1" "\ngetprosol 1H P1 PLdB1")

Noah_ast_psyche.py script

save the following script as noah-ast_psyche.py

```
MSG("Initial step: 1D 1H and 13C experiments have to be recorded" "\nThen create a new data set with the command \a'new'" "\nThe present macro 'AST' takes care all the required parameters")

ct = XCMD("RPAR HMBCGP all")

MSG("DRAG 1D 1H data set into the present window" "\nClick on Copy Parameters Option" "\nClick on OK")

ct = XCMD("copypars.py")

MSG("DRAG 1D 13C data set into the present window" "\nClick on Copy Parameters Option" "\nClick on OK")

ct = XCMD("copypars.py")

PPTEXT = """

;$CLASS=HighRes

;$DIM=2D

;$TYPE=

;$SUBTYPE=

;$COMMENT=
```

```
#include <Avance.incl>

#include <Delay.incl>

#include <Grad.incl>



"p2=p1*2"

"d0=3u"

"d10=3u"

"d11=30m"

"d16=200u"

"d17=200u"

"p28=0u"

"p14=500u"

"p24=2000u"

"p63=1500u"

"p16=1000u"

"p17=1000u"

"p6=25u"


"cnst2=145"

"cnst3=45"

"cnst11=8"

"cnst17=-0.5"

"p0=p3*1.333"
```

"d4=1s/(cnst2*4)"

"d23=1s/(cnst3*4)"

"d24=1s/(cnst2*cnst11)"

"in0=inf1/2"

"DELTA1=p16+d16-p2-d0*2+4u"

"DELTA2=p16+d16+8u"

"DELTA3=p16+d16+p2+d0*2-4u"

"DELTA4=d4-p14/2-4u"

"DELTA5=d23-p24/2-4u"

"DELTA6=d24-cnst17*p24/2-4u"

"p4=p3*2"

"d21=0.003448000s"

"DELTA10=d21-cnst17*p24/2-p16-d16-p2-d0*2"

"DELTA11=p16+d16-p1*0.78+de+8u"

"DELTA12=d4-larger(p2,p14)/2"

"DELTA13=d21-cnst17*p24/2-4u"

"DELTA14=d24-cnst17*p24/2-4u"

"l0=td1/6"

```
"FACTOR1=(d9/(p6*115.112))/2"

"l1=FACTOR1*2"



"in10=0.5*inf1*cnst10"

"p11=20m"


"cnst21=10000"

"cnst50=(cnst20/360)*sqrt((2*cnst21)/(p10/2000000))"

"p30=1000000.0/(cnst50*4)"

"cnst31= (p30/p1) * (p30/p1)"

"spw37=plw1/cnst31"


"p10=30m"


"DELTA8=p16+d16+d0"

"DELTA9=p16+d16+8u"


"acqt0=0"

baseopt_echo


1 ze

  d11 pl12:f2

2 d11

3 4m do:f2
```

```
4 50u UNBLKGRAD
d1 st0
 4u pl2:f2
4u pl1:f1

4u pl2:f2
(p3 ph1):f2

 p16:gp22
  d16


13 (p1 ph1)
  4u
  DELTA4 pl0:f2
  (center (p2 ph1) (p14:sp3 ph1):f2 )
  4u
  DELTA4 pl2:f2
  (p1 ph2) (p3 ph4):f2
  4u
  DELTA5 pl0:f2
  (p24:sp7 ph8):f2
  4u
  DELTA5 pl2:f2
  (p3 ph9):f2
```

```
d0
(p2 ph1)
d0
DELTA1 pl0:f2 UNBLKGRAD
(p24:sp7 ph11):f2
4u
p16:gp1
d16 pl2:f2
(p0 ph10):f2
4u
DELTA3 pl0:f2
(p24:sp7 ph11):f2
p16:gp2
d16 pl2:f2
d0
(p2 ph1)
d0
(center (p1 ph1) (p3 ph5):f2 )
4u
DELTA6 pl0:f2
(center (p2 ph1) (p24:sp7 ph1):f2 )
4u
DELTA6 pl2:f2
(center (p1 ph2) (p3 ph6):f2 )
4u
```

```
  DELTA4 pl0:f2
  (center (p2 ph1) (p14:sp3 ph1):f2 )
  4u
  DELTA4
  (p1 ph1)
  DELTA2
  (p2 ph1)
  4u
  p16:gp3*EA
  d16 pl12:f2
  4u BLKGRAD

 goscnp ph30 cpd2:f2
4u do:f2

2m st
 50u UNBLKGRAD
4u pl2:f2
4u pl1:f1
(p3 ph1):f2

 p16:gp22
  d16

23 (p1 ph21)
```

```
DELTA12 pl0:f2

4u

(center (p2 ph21) (p14:sp3 ph26):f2 )

4u

DELTA12 pl2:f2 UNBLKGRAD

p28 ph21

4u

(p1 ph22) (p3 ph23):f2

d0

(p2 ph27)

d0

p16:gp4*EA

d16

DELTA10 pl0:f2

(center (p2 ph21) (p24:sp7 ph24):f2 )

4u

DELTA13 pl2:f2

(center (p1 ph21) (p3 ph24):f2 )

4u

DELTA14 pl0:f2

(center (p2 ph21) (p24:sp7 ph21):f2 )

4u

DELTA14 pl2:f2

(center (p1 ph22) (p3 ph25):f2 )

DELTA12 pl0:f2
```

```
  (center (p2 ph21) (p14:sp3 ph21):f2 )
  DELTA12
  (p1 ph21)
  DELTA11
  (p2 ph21)
  4u
  p16:gp5
  d16 pl12:f2
  4u BLKGRAD
goscnp ph31 cpd2:f2
4u do:f2

2m st
4u pl2:f2
(p3 ph1):f2
  50u UNBLKGRAD
  p16:gp22
  d16

4u pl1:f1

  p1 ph12
  DELTA8
  p2 ph8
```

```
d10

50u UNBLKGRAD

p16:gp11

d16

p2 ph8

50u

p16:gp11

d16

p17:gp12

d17

10u pl0:f1

d16

(center (p10:gp10) (p10:sp37 ph8):f1 )

d16

10u pl1:f1

p17:gp12

d17

d10


  p16:gp13*EA

  d16

  p1 ph14

  10u pl10:f1

                                                        ;begin DIPSI2

14 p6*3.556 ph13
```

p6*4.556 ph15

p6*3.222 ph13

p6*3.167 ph15

p6*0.333 ph13

p6*2.722 ph15

p6*4.167 ph13

p6*2.944 ph15

p6*4.111 ph13

p6*3.556 ph15

p6*4.556 ph13

p6*3.222 ph15

p6*3.167 ph13

p6*0.333 ph15

p6*2.722 ph13

p6*4.167 ph15

p6*2.944 ph13

p6*4.111 ph15

p6*3.556 ph15

p6*4.556 ph13

p6*3.222 ph15

p6*3.167 ph13

p6*0.333 ph15

p6*2.722 ph13

```
p6*4.167 ph15
p6*2.944 ph13
p6*4.111 ph15

p6*3.556 ph13
p6*4.556 ph15
p6*3.222 ph13
p6*3.167 ph15
p6*0.333 ph13
p6*2.722 ph15
p6*4.167 ph13
p6*2.944 ph15
p6*4.111 ph13
lo to 14 times l1
                                        ;end DIPSI2
50u pl1:f1
p1 ph16
DELTA9
p2 ph8
4u
p16:gp14
d16
4u BLKGRAD
go=2 ph18
```

```
d11 wr #0 if #0 zd igrad EA

1m ip6*2

1m ip12*2

1m ip14*2

1m ip23*2

1m ip25*2

1m ip26*2

1m ip31*2

1m ip18*2


lo to 3 times 2

1m rp6

1m rp12

1m rp14

1m rp23

1m rp25

1m rp26

1m rp31

1m rp18

1m id0

1m id10


lo to 4 times l0


exit
```

ph1=0

ph2=1

ph4=0 2

ph5=0 0 2 2

ph6=1 1 3 3

ph7=0

ph8=0

ph9=0 0 0 0 2 2 2 2

ph10=0 0 0 0 0 0 0 0 2 2 2 2 2 2 2 2

ph11=0

ph30=0 2 2 0 2 0 0 2 2 0 0 2 0 2 2 0

ph21=0

ph22=1

ph23=0 2

ph24=0 0 2 2

ph25=1 1 3 3

ph26=0

ph27=0 0 2 2

ph31=2 0 0 2

ph12=0 2

ph14=0 0 2 2

ph13=3

ph15=1

ph16=2 2 0 0

ph19=0

ph18=0 2

;pl0 : 0W

;pl1 : f1 channel - power level for pulse (default)

;pl2 : f2 channel - power level for pulse (default)

;pl12: f2 channel - power level for CPD/BB decoupling

;sp3: f2 channel - shaped pulse (180degree inversion)

;spnam3: Crp80,0.5,20.1

;spnam1: Crp60,20,20.10

;spnam37: Crp_psyche.20

;sp7: f2 channel - shaped pulse (180degree refocussing)

;spnam7: Crp80comp.4

;p0 : f2 channel - 120 degree high power pulse

;p1 : f1 channel - 90 degree high power pulse

;p2 : f1 channel - 180 degree high power pulse

;p3 : f2 channel - 90 degree high power pulse

;p14: f2 channel - 180 degree shaped pulse for inversion

;   = 500usec for Crp60,0.5,20.1

;p16: homospoil/gradient pulse

;   = 1msec

;p17: homospoil/gradient pulse

; = 1msec

;p20: PSYCHE gradient pulse

; = 30msec

;p24: f2 channel - 180 degree shaped pulse for refocussing

; = 2msec for Crp60comp.4

;d0 : incremented delay (2D) (for adequate) [3 usec]

;d20 : incremented delay (2D) (for HSQC)

;d0 : incremented delay (2D) (for TOCSY)

;d1 : relaxation delay; 1-5 * T1

;d4 : 1/4J(CH)

;d11: delay for disk I/O [30 msec]

;d16: delay for homospoil/gradient recovery

;d23: 1/(4J(CC))

;d9: TOCSY mixing period

;d19: ASAP-TOCSY mixing period (for HSQC ~ 40 msec)

;d24: 1/(4J(CH)) for CH

; 1/(8J(CH)) for all multiplicities

;cnst2 : J(CH) = 127 .. 160 Hz

;cnst3 : J(CC) = 35 .. 55 Hz

;cnst11: for multiplicity selection = 4 for CH, 8 for CHn

;cnst17: = -0.5 for Crp60comp.4

;cnst20: = low filp angle pulse 10-25 degree

;inf1: 1/SW(C) = 2 * DW(C)

;in0: 1/(2 * SW(C)) = DW(C)

;nd0: 2

;in20: = in0

;ns: 16 * n

;ds: >= 16

;td1: number of experiments

;FnMODE: echo-antiecho

;cpd2:[bi_p5m4sp_4sp.2] decoupling according to sequence defined by cpdprg2

;pcpd2: f2 channel - 90 degree pulse for decoupling sequence

;cnst10: = scaling factor swC/swH for TOCSY

;p63: f2 channel - decoupler pulse length [1.5 msec]

;   = 1500usec for bi_p5m4sp_4sp.2.

;for z-only gradients:

;gpz1: +78.5%

;gpz2: +77.6%

;gpz3: -59%

;gpz4: +80.0%

;gpz5: +20.1%

;gpz10: +1.0-3.0%

;gpz11: +49%

;gpz12: 77%

;gpz13: 30%

;gpz14: 30%

;gpz22: 17%

```
;use gradient files:
;gpnam1: SMSQ10.100
;gpnam2: SMSQ10.100
;gpnam3: SMSQ10.100
;gpnam4: SMSQ10.100
;gpnam5: SMSQ10.100
;gpnam10: RECT.1
;gpnam11: SMSQ10.100
;gpnam12: SMSQ10.100
;gpnam13: SMSQ10.100
;gpnam14: SMSQ10.100
;gpnam21: SMSQ10.100


;cnst17: Factor to compensate for coupling evolution during a pulse
;       (usually +1). A positive factor indicates that coupling
;       evolution continues during the pulse, whereas a negative
;       factor is necessary if the coupling is (partially) refocussed.
"""
import math
pp = DEF_PULSPROG(PPTEXT)

ppName = "noah3_AST_psyche"
PUTPAR("PULPROG", ppName)
pp.SAVE_AS(ppName)
```

```
PUTPAR("1 FnMODE", "Echo-Antiecho")
PUTPAR("GPNAM 1", "SMSQ10.100")
PUTPAR("GPZ 1", "78.5")
PUTPAR("GPNAM 2", "SMSQ10.100")
PUTPAR("GPZ 2", "77.6")
PUTPAR("GPNAM 3", "SMSQ10.100")
PUTPAR("GPZ 3", "-59.0")
PUTPAR("GPNAM 4", "SMSQ10.100")
PUTPAR("GPZ 4", "80.0")
PUTPAR("GPNAM 5", "SMSQ10.100")
PUTPAR("GPZ 5", "20.1")
PUTPAR("GPNAM 13", "SMSQ10.100")
PUTPAR("GPZ 13", "30.0")
PUTPAR("GPNAM 14", "SMSQ10.100")
PUTPAR("GPZ 14", "30.0")
PUTPAR("GPNAM 22", "SMSQ10.100")
PUTPAR("GPZ 22", "17.0")
PUTPAR("GPNAM 10", "RECT.1")
PUTPAR("GPZ 10", "3.0")
PUTPAR("GPNAM 11", "SMSQ10.100")
PUTPAR("GPZ 11", "49.0")
PUTPAR("GPNAM 12", "SMSQ10.100")
PUTPAR("GPZ 12", "77.0")
```

```
PUTPAR("SPNAM 3", "Crp80,0.5,20.1")

PUTPAR("SPNAM 1", "Crp80,20,20.10")

PUTPAR("SPNAM 37", "Crp_psyche.20")

PUTPAR("SPNAM 7", "Crp80comp.4")


PUTPAR("CPDPRG 2", "bi_p5m4sp_4sp.2")

PUTPAR("NBL", "3")

PUTPAR("NS", "32")

PUTPAR("DS", "32")

PUTPAR("TD", "1024")

PUTPAR("1 TD", "512")

PUTPAR("D 1", "1")

PUTPAR("D 9", "0.08")

PUTPAR("CNST 20", "15")


ct = XCMD("SWH")

ct.join()

ct = XCMD("O1")

ct.join()

ct = XCMD("D1")

ct.join()

ct = XCMD("NS")

ct.join()

ct = XCMD("DS")

ct.join()
```

```
ct = XCMD("TD")

ct.join()

aqdirect = GETPAR ("AQ")

MSG(str(aqdirect)+ "= Proton Acquisition time"+ "\nShould be <= 50 ms")

td1 = GETPAR("1 TD")

MSG(str(td1)+ "\nNumber of indirect increments" "\nBy default it takes 512 increments \nIn the AST experiments it shows 1536 for the three pulse blocks")

ct = XCMD("D9")

ct.join()



td11 = int (td1)

td111 = 3*td11

PUTPAR("1 TD", str(td111))


a = GETPAR("SWH")

aa = 1.0 / float (a)

b = GETPAR("1 SWH")

bb = float (b)

c = aa * bb

PUTPAR("CNST 10", str(c))


p = GETPAR("P 1")

pf = str (p)

pk = GETPAR("PLdB 1")

pkf = str (pk)
```

```
XCMD ("2 WDW QSINE")

XCMD ("1 WDW QSINE")

XCMD ("1 SSB 2")

XCMD ("2 SSB 2")

XCMD ("2 PH_mod pk")

XCMD ("1 PH_mod pk")

XCMD ("1 MC2 echo-antiecho")

XCMD ("USERP1 noah_hsqc")

XCMD ("USERP2 noah_hsqc")

XCMD ("USERP3 noah_noesy")


MSG("Perform with the known P1 and PLdB1" "\ngetprosol 1H P1 PLdB1")
```