

Supplementary information to manuscript

PRESERVE: adding variable flip-angle excitation to TROSY NMR spectroscopy

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1. Bruker pulse sequence code: HN water-flip-back PRESERVE-TROSY

```

;HN_WFB_PRESERVE_TROSY
;BB 2024
;
;
; $CLASS=IBS
; $DIM=2D
; $TYPE=
; $SUBTYPE=
; $COMMENT=

prosol relations=<IBS>

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

define list<gradient> EA3 = { 1.0000 0.8750 }
define list<gradient> EA5 = { 0.6667 1.0000 }
define list<gradient> EA7 = { 1.0000 0.6595 }

/*****
/* Predefined shapes for 1H pulses *****/
/*****

/* water pulse (p48, pl48) */
"p48=1m"
"plw48=plw1*(pow((p1/p48),2))"

"p16=1000u"
"p17=300u"

/
*****/
/* 13C Adiabatic pulse */
/
*****/

"p8=200u"
"spoff13=0.0" /* BIP offset */
"spw13=plw2*(pow((p3*8/p8),2))" /* BIP power level */

/
*****/
/* calculation of shaped 15N pulse parameters */
/*
/
*****/
"p50 =500u" /* BIP pulse length */
"spoff50=0.0" /* BIP offset */

"spw50=plw3*(pow((p21*8/p50),2))" /* BIP power level */

"p51=4.875/(40*bf3/1000000)" /* REBURP pulse length */
"spw51=plw3*(pow((p21*1.97/p51)/0.0798,2))" /* REBURP power level */
/*
"spoff51=0.0" /* REBURP offset */
"spoa151=0.5"

"p52 =p21*22" /* UREV2 pulse length */
"spoff52=0.0" /* UREV2 offset */
"spw52=plw3" /* UREV2 power level */
"spoa152=0.5"

/
*****/
/* DELAYS */
/*
/
*****/
"d11=30m"

;"d25=2.6m"
"d26=2.7m"
"d27=2.5m" /* set slightly shorter than d26 for relaxation
compensation */

"DELTA1=d25-p21-p17-d16"
"DELTA2=d27-p17-d16-p21"
"DELTA3=d26-p17-d16-p21"
"DELTA4=d26-p21-p17-d16"

# ifdef LABEL_CN
"DELTA=p8+d0*2"
# else
"DELTA=d0*2"
# endif /*LABEL_CN*/

/
*****/
/* time increments in 15N dimension */
/*
/
*****/
"d0=0"
"in0=inf1/2"

"acqt0=0"
baseopt_echo

1 d11 ze
2 d11

```

```

3 5u pl1:f1 pl2:f2 pl3:f3
  (p50:sp50 ph8):f3
  d1 pl3:f3
  50u UNBLKGRAD
/*****
/* H-N transfer (PRESERVE) */
/*****
(ralign (p1 ph10) (p21 ph13):f3 )
p17:gp1
d16
DELTA1
(center (p1*2 ph1) (p21*2 ph1):f3 )
DELTA1 pl3:f3
p17:gp1
d16

(lalign (p1 ph11) (p21 ph14):f3 )

DELTA4
p17:gp2
d16

(center (p1*2 ph1) (p21*2 ph1):f3 )
p17:gp2
d16
DELTA4

(p1 ph12)

3u pl48:f1
(p48 ph15)
3u pl1:f1

/*****
/* 15N labeling */
/*****
d0
# ifdef LABEL_CN
  (p8:sp13 ph1):f2
# else
# endif /*LABEL_CN*/

d0
(p50:sp50 ph1):f3
DELTA

p16:gp3*EA3
d16

/*****
/* TROSY-type H-N back transfer */
/*****
3u pl48:f1

(p48 ph1)
3u pl1:f1
(p1 ph6)
p17:gp4
d16
DELTA2 pl1:f1
(center (p1*2 ph2) (p50:sp50 ph2):f3 )
DELTA2 pl3:f3
p17:gp4
d16
3u pl1:f1
(p1 ph1)
/*****

p16:gp5*EA5
d16

/*****
(p21 ph9):f3
p17:gp6
d16
DELTA3
(center (p1*2 ph2) (p51:sp51 ph2):f3 )
DELTA3 pl3:f3
p17:gp6
d16
(p21 ph7):f3
/*****

p16:gp7*EA7
d16 BLKGRAD
/*****
/* Signal detection & looping */
/*****
go=2 ph31
d11 mc #0 to 2
  F1EA(calgrad(EA3) & calgrad(EA5) & calgrad(EA7) & calph(ph6,
+180) & calph(ph7, +180) & calph(ph12, +180) & calph(ph13, +180),
caldel(d0, +in0) & calph(ph7, +180) & calph(ph9, +180) & calph(ph31,
+180))
exit

ph1=0
ph2=3
ph3=2
ph4=3
ph5=0
ph6=1
ph7=1 1 3 3
ph8=0
ph9=0 0 2 2
ph10=1 3
ph11=0 2
ph12=0 2
ph13=0 2
ph14=0 2
ph15=3 1
ph31=0 2 2 0

```

2 Bruker pulse sequence code: HN SOFAST-TROSY (PC9, REBURP)

```

;HN_SOFAST_TROSY_PC9_UREV2
;BB 2024
;
;
;CLASS=IBS
;SDIM=2D
;STYPE=
;SSUBTYPE=
;SCOMMENT=

prosol relations=<IBS>

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

define list<gradient> EA3 = { 1.0000 0.8750 }
define list<gradient> EA5 = { 0.6667 1.0000 }
define list<gradient> EA7 = { 1.0000 0.6595 }

/*****
/* Predefined shapes for 1H pulses
/* cnst1: center of excitation band
/* cnst2: excitation band width
*****/

/* PC9 (p41, sp25) */
"p41=7.2/(cnst2*bf1/1000000)" /* PC9 pulse length */
"spw25=plw1*(pow((p1*1.01/p41)/0.125,2))" /* PC9 power level */
"spoff25=bf1*(cnst1/1000000)-o1" /* PC9 offset */
"spoa125=0.5"

/* REBURP (p42, sp26) */

"p42=4.875/(cnst2*bf1/1000000)" /* REBURP pulse length */
"spw26=plw1*(pow((p1*1.97/p42)/0.0798,2))" /* REBURP power level */
"spoff26=bf1*(cnst1/1000000)-o1" /* REBURP offset */
"spoa126=0.5"

/* EBURP & EBURP_TR (p43, sp28, sp29) */

"p43=4.6/(cnst2*bf1/1000000)" /* EBURP pulse length */
"spw28=plw1*(pow((p1*1.04/p43)/0.06103,2))" /* EBURP power level */
"spw29=plw1*(pow((p1*1.04/p43)/0.06103,2))" /* EBURP power level */
"spoff28=bf1*(cnst1/1000000)-o1" /* EBURP offset */
"spoa128=0"
"spoff29=bf1*(cnst1/1000000)-o1" /* EBURP_REV offset */

"spoa129=1.0"
"p16=1000u"
"p17=300u"

/
*****
/* 13C Adiabatic pulse
*/
/
*****
"p8=200u"
"spoff13=0.0" /* BIP offset */
"spw13=plw2*(pow((p3*8/p8),2))" /* BIP power level */

/
*****
/* calculation of shaped 15N pulse parameters
*/
/
*****
"p50 =500u" /* BIP pulse length */
"spoff50=0.0" /* BIP offset */
"spw50=plw3*(pow((p21*8/p50),2))" /* BIP power level */

"p51=4.875/(50*bf3/1000000)" /* REBURP pulse length */
"spw51=plw3*(pow((p21*1.97/p51)/0.0798,2))" /* REBURP power level */
"spoff51=0.0" /* REBURP offset */
"spoa151=0.5"

"p52 =p21*22" /* UREV2 pulse length */
"spoff52=0.0" /* UREV2 offset */
"spw52=plw3" /* UREV2 power level */
"spoa152=0.5"

/
*****
/* DELAYS
*/
/
*****
"d11=30m"
;"d25=2.6m"
"d26=2.7m"
"d27=2.5m" /* set slightly shorter than d26 for relaxation
compensation */
"d28=(p41*0.5-p51)*0.5"
"d29=(p41*1.5-p51)*0.5"

```

```

"DELTA1=d25-p41*0.5-p42*0.5"
"DELTA2=d27-p17-d16-p42*0.5-p41*0.5"
"DELTA3=d26-p17-d16-p42*0.5"
"DELTA4=d26-p41*0.5-p42*0.5"
"DELTA5=p41*0.51"

/
*****
/* time increments in 15N dimension */
/
*****
"d0=3u"
"in0=inf1/2"

# ifdef LABEL_CN
"DELTA=p41*0.51-(d0*2+p8)"
# else
"DELTA=p41*0.51-(d0*2)"
# endif /*LABEL_CN*/

"acqt0=0"
baseopt_echo

1 d11 ze
2 d11
3 5u p11:f1 p12:f2 p13:f3
(p50:sp50 ph8):f3
d1 p13:f3
50u UNBLKGRAD
/*****
/* H-N transfer (PRESERVE) */
/*****

(center (p41:sp25 ph10) (p21 ph13):f3 ) /* PC9 */

DELTA1
(center (p42:sp26 ph1) (p52:sp52 ph1):f3 )

DELTA1 p13:f3

(center (p41:sp25 ph11) (p21 ph14):f3 ) /* PC9 */

DELTA4
(center (p42:sp26 ph1) (p52:sp52 ph1):f3 )
DELTA4

(p41:sp25 ph12) /* PC9 */

/*****
/* 15N labeling */
/*****

(p50:sp50 ph1):f3
d0

# ifdef LABEL_CN
(p8:sp13 ph1):f2
# else
# endif /*LABEL_CN*/

d0
DELTA

p16:gp3*EA3
d16

/*****
/* TROSY-type H-N back transfer */
/*****
(lalign (p41:sp25 ph6) (p50:sp50 ph2):f3 )
p17:gp4
d16
DELTA2
(center (p42:sp26 ph2) (p50:sp50 ph2):f3 )
DELTA2 p13:f3
p17:gp4
d16
(ralign (p41:sp25 ph1) (p50:sp50 ph2):f3 )
/*****

p16:gp5*EA5
d16 p13:f3

/*****
(p21 ph9):f3
p17:gp6
d16
DELTA3
(center (p42:sp26 ph2) (p52:sp52 ph2):f3 )
DELTA3 p13:f3
p17:gp6
d16
(p21 ph7):f3
/*****
DELTA5

p16:gp7*EA7
d16 BLKGRAD

/*****
/* Signal detection & looping */
/*****
go=2 ph31
d11 mc #0 to 2
F1EA(calgrad(EA3) & calgrad(EA5) & calgrad(EA7) & calph(ph6,
+180) & calph(ph7, +180) & calph(ph12, +180) & calph(ph13, +180),
caldel(d0, +in0) & calph(ph7, +180) & calph(ph9, +180) & calph(ph31,

```

```
+180))
exit
```

```
ph1=0
ph2=1
ph4=3
ph6=3
ph7=1 1 3 3
ph8=0
ph9=0 0 2 2
ph10=1 3
ph11=0 2
ph12=0 2
ph13=0 2
ph14=0 2
ph31=0 2 2 0
```

```
;p10 : 0W
;p11 : f1 channel - power level for pulse (default)
;p13 : f3 channel - power level for pulse (default)
;p16: gradient pulse [1 msec]
;p17: gradient pulse
;p21: f3 channel - 90 degree high power pulse
;d0 : incremented delay (F1) [3 usec]
;d1 : relaxation delay
;d11: delay for disk I/O [30 msec]
;d16: delay for gradient recovery
;d25: 1/(4J(NH))*lambda - for variable flip angle excitation
;d26: 1/(4J(NH))
;d27: 1/(4J(NH))
;cnst1: H(N) excitation frequency (in ppm)
;cnst2: H(N) excitation band width (in ppm)
;inf1: 1/SW(N) = 2 * DW(N)
;in0: 1/(2 * SW(N)) = DW(N)
;nd0: 2
;ns: 2 * n
;ds: >= 16
;td1: number of experiments in F1
;FnMODE: echo-antiecho in F1
```

3 Bruker pulse sequence code: HN SOFAST-TROSY (EBURP2, REBURP)

```

;HN_SOFAST_TROSY_EBURP_UREV2
;BB 2024
;
;CLASS=IBS
;$DIM=2D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

prosol relations=<IBS>

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

define list<gradient> EA3 = { 1.0000 0.8750 }
define list<gradient> EA5 = { 0.6667 1.0000 }
define list<gradient> EA7 = { 1.0000 0.6595 }

/*****
/* Predefined shapes for 1H pulses *****/
/* cnst1: center of excitation band *****/
/* cnst2: excitation band width *****/
/*****

/* PC9 (p41, sp25) */
"p41=7.2/(cnst2*bf1/1000000)" /* PC9 pulse length */
"spw25=plw1*(pow((p1*1.01/p41)/0.125,2))" /* PC9 power level */
"spoff25=bf1*(cnst1/1000000)-o1" /* PC9 offset */
"spoa125=0.5"

/* REBURP (p42, sp26) */

"p42=4.875/(cnst2*bf1/1000000)" /* REBURP pulse length */
"spw26=plw1*(pow((p1*1.97/p42)/0.0798,2))" /* REBURP power level */
"spoff26=bf1*(cnst1/1000000)-o1" /* REBURP offset */
"spoa126=0.5"

/* EBURP2 EBURP2_TR (p43, sp28, sp29) */

"p43=4.6/(cnst2*bf1/1000000)"
"spw28=plw1*(pow((p1*1.04/p43)/0.06103,2))"
"spw29=plw1*(pow((p1*1.04/p43)/0.06103,2))"
"spoff28=bf1*(cnst1/1000000)-o1"
"spoa128=0"
"spoff29=bf1*(cnst1/1000000)-o1"
"spoa129=1.0"

"p16=1000u"

"p17=300u"
/
/*****
/* 13C Adiabatic pulse *****/
/*
/*
/*****
"p8=200u" /* BIP pulse length */
"spoff13=0.0" /* BIP offset */
"spw13=plw2*(pow((p3*8/p8),2))" /* BIP power level */

/
/*****
/* calculation of shaped 15N pulse parameters *****/
/*
/*****
"p50=500u" /* BIP pulse length */
"spoff50=0.0" /* BIP offset */
"spw50=plw3*(pow((p21*8/p50),2))" /* BIP power level */
"spoa150=0.5"

"p51=4.875/(50*bf3/1000000)" /* REBURP pulse length */
"spw51=plw3*(pow((p21*1.97/p51)/0.0798,2))" /* REBURP power level */
"spoff51=0.0" /* REBURP offset */
"spoa151=0.5"

"p52=p21*22" /* UREV2 pulse length */
"spoff52=0.0" /* UREV2 offset */
"spw52=plw3" /* UREV2 power level */
"spoa152=0.5"

/
/*****
/* DELAYS *****/
/*
/*****
"d11=30m"
;"d25=2.6m"
"d28=2.6m"
"d26=2.7m"
"d27=2.5m" /* set slightly shorter than d26 for relaxation
compensation */

"DELTA1=d25-p42*0.5"
"DELTA4=d28-p42*0.5-p43*0.5-p17-d16"

"DELTA2=d27-p17-d16-p42*0.5-p43*0.5"

```

```

"DELTA3=d26-p17-d16-p42*0.5"

/
*****
/* time incremennts in 15N dimension
*/
/
*****
"d0=0"
"in0=inf1/2"

# ifdef LABEL_CN
"DELTA=d0*2+p8"
# else
"DELTA=d0*2"
# endif /*LABEL_CN*/

"acqt0=0"
baseopt_echo

1 d11 ze
2 d11
3 5u p1:f1 p2:f2 p3:f3
   (p50:sp50 ph1):f3
   d1 p13:f3
   50u UNBLKGRAD
/*****
/* H-N transfer (PRESERVE)
*/
/*****

( ralign (p43:sp28 ph10) (p21 ph13):f3 )

DELTA1
(center (p42:sp26 ph1) (p52:sp52 ph1):f3 )

DELTA1 p13:f3

( lalign (p43:sp29 ph11) (p21 ph14):f3 )

p17:gp1
d16

DELTA4
(center (p42:sp26 ph1) (p52:sp52 ph1):f3 )
p17:gp1
d16
DELTA4

(p43:sp28 ph12)

/*****

/* 15N labeling
*/
/*****
d0

# ifdef LABEL_CN
(p8:sp13 ph1):f2
# else
# endif /*LABEL_CN*/

d0
(p50:sp50 ph1):f3
DELTA

p16:gp3*EA3
d16

/*****
/* TR0SY-type H-N back transfer
*/
/*****
(p43:sp29 ph6) /* EBURP_REV */
p17:gp4
d16
DELTA2
(center (p42:sp26 ph2) (p50:sp50 ph2):f3 )
DELTA2 p13:f3
p17:gp4
d16
(p43:sp28 ph1) /* EBURP */
/*****

p16:gp5*EA5
d16

/*****
(p21 ph8):f3
p17:gp6
d16
DELTA3
(center (p42:sp26 ph2) (p52:sp52 ph2):f3 )
DELTA3 p13:f3
p17:gp6
d16
(p21 ph7):f3
/*****

p16:gp7*EA7
d16 BLKGRAD
/*****
/* Signal detection & looping
*/
/*****
go=2 ph31
d11 mc #0 to 2
F1EA(calgrad(EA3) & calgrad(EA5) & calgrad(EA7) & calph(ph6,
+180) & calph(ph7, +180) & calph(ph12, +180) & calph(ph13, +180),

```



```
caldel(d0, +in0) & calph(ph7, +180) & calph(ph8, +180) & calph(ph31,
+180) )
exit
```

```
ph1=0
ph2=1
ph4=3
ph6=1
ph7=1 1 3 3
ph8=0 0 2 2
ph10=1 3
ph11=0 2
ph12=0 2
ph13=0 2
ph14=0 2
ph31=0 2 2 0
```

```
;pl0 : 0W
;pl1 : f1 channel - power level for pulse (default)
;pl3 : f3 channel - power level for pulse (default)
;p16: gradient pulse [1 msec]
;p17: gradient pulse
;p21: f3 channel - 90 degree high power pulse
;p22: f3 channel - 180 degree high power pulse
;d0 : incremented delay (F1) [3 usec]
;d1 : relaxation delay
;d11: delay for disk I/O [30 msec]
;d16: delay for homospoil/gradient recovery
;d25: 1/(4J(NH))*lambda - for variable flip angle excitation
;d26: 1/(4J(NH))
;d27: 1/(4J(NH))
;cnst1: H(N) excitation frequency (in ppm)
;cnst2: H(N) excitation band width (in ppm)
;inf1: 1/SW(N) = 2 * DW(N)
;in0: 1/(2 * SW(N)) = DW(N)
;nd0: 2
;ns: 2 * n
;ds: >= 16
;td1: number of experiments in F1
;FnMODE: echo-antiecho in F1
```

4 Bruker pulse sequence code: HC SOFAST-TROSY

```

;HC_SOFAST_C_TROSY_noCT
;BB 2024
;
;
; $CLASS=IBS
; $DIM=2D
; $TYPE=
; $SUBTYPE=
; $COMMENT=

prosol relations=<IBS>

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

define list<gradient> EA3 = { 1.0000 0.7500 }
define list<gradient> EA5 = { 0.5000 1.0000 }
define list<gradient> EA7 = { 0.9028 0.2972 }

/*****
/* Predefined shapes for 1H pulses *****/
/* cnst1: center of excitation band *****/
/* cnst2: excitation band width *****/
/*****

/* PC9 (p41, sp25) */
"p41=7.2/(cnst2*bf1/1000000)" /* PC9 pulse length */
"spw25=plw1*(pow((p1*1.01/p41)/0.125,2))" /* PC9 power level */
"spoff25=bf1*(cnst1/1000000)-o1" /* PC9 offset */
"spoa125=0.5"

/* REBURP (p42, sp26) */

"p42=4.875/(cnst2*bf1/1000000)" /* REBURP pulse length */
"spw26=plw1*(pow((p1*1.97/p42)/0.0798,2))" /* REBURP power level */
"spoff26=bf1*(cnst1/1000000)-o1" /* REBURP offset */
"spoa126=0.5"

/* EBURP & EBURP_TR (p43, sp28, sp29) */

"p43=4.6/(cnst2*bf1/1000000)" /* EBURP pulse length */
"spw28=plw1*(pow((p1*1.04/p43)/0.06103,2))" /* EBURP power level */
"spw29=plw1*(pow((p1*1.04/p43)/0.06103,2))" /* EBURP power level */
"spoff28=bf1*(cnst1/1000000)-o1" /* EBURP offset */
"spoa128=0"
"spoff29=bf1*(cnst1/1000000)-o1" /* EBURP_REV offset */
"spoa129=1.0"

"p16=1000u"
"p17=300u"

/
*****/
/* 13C pulse shapes */
*/
/
*****/
"p14=4.875/(50.0*bf2/1000000)" /* REBURP pulse length */
"spw3=plw2*(pow((p3*1.97/p14)/0.0798,2))" /* REBURP power level */
"spoa13=0.5"
"spoff3=0"

/
*****/
"p40 =p3*8" /* BIP pulse length */
"spoff40=0.0" /* BIP offset */
"spw40=plw2" /* BIP power level */
"spoa140=0.5"

/
*****/
/* calculation of shaped 15N pulse parameters */
*/
/
*****/
"p50 =500u" /* BIP pulse length */
"spoff50=0.0" /* BIP offset */
"spw50=plw3*(pow((p21*8/p50),2))" /* BIP power level */

"p51=4.875/(50*bf3/1000000)" /* REBURP pulse length */
"spw51=plw3*(pow((p21*1.97/p51)/0.0798,2))" /* REBURP power level */
"spoff51=0.0" /* REBURP offset */
"spoa151=0.5"

/
*****/
/* DELAYS */
*/
/
*****/
"d11=30m"

;d25=1.0m /* adjustable delay for flip angle */
"d26=1.4m"
"d27=1.2m" /* set slightly shorter than d26 for relaxation
compensation */
"d28=1.4m" /* 1/(2JCH) */

```

```

"DELTA1=d25-p42*0.5"
"DELTA2=d26-p42*0.5-p43*0.5"
"DELTA3=d27-p17-d16-p42*0.5"
"DELTA4=d28-p42*0.5-p43*0.5"

"DELTA=d0*2+p3*4/3.1416"

/
*****
/* time increments in 13C dimension (semi CT)
*/
/
*****
"d0=3u"
"in0=inf1"

"acqt0=0"
baseopt_echo

1 d11 ze
2 d11
3 5u p11:f1 p12:f2 p13:f3
d1
50u UNBLKGRAD
/*****
/* PRESERVE H-C transfer */
/*****
(ralign (p43:sp28 ph10) (p3 ph13):f2 )

DELTA1
(center (p42:sp26 ph1) (p14:sp3 ph1):f2 )

DELTA1 pl2:f2

(lalign (p43:sp29 ph11) (p3 ph14):f2 )

DELTA4

(center (p42:sp26 ph1) (p14:sp3 ph1):f2 )

DELTA4

(p43:sp28 ph12)

/*****
/* 13C labeling */
/*****
(p40:sp40 ph1):f2
d0

p16:gp3*EA3
d16 pl2:f2

/*****
/* TROSY-type H-C back transfer */
/*****
(p43:sp29 ph6) /* EBURP_REV */
DELTA2
(center (p42:sp26 ph2) (p40:sp40 ph2):f2 )
DELTA2 pl2:f2
(p43:sp28 ph1) /* EBURP */
/*****

p16:gp5*EA5
d16

/*****
(p3 ph8):f2
p17:gp6
d16
DELTA3
(center (p42:sp26 ph2) (p14:sp3 ph2):f2 )
DELTA3 pl2:f2
p17:gp6
d16
(p3 ph7):f2
/*****

p16:gp7*EA7
d16 BLKGRAD

/*****
/* Signal detection & looping */
/*****
go=2 ph31
d11 mc #0 to 2
F1EA(calgrad(EA3) & calgrad(EA5) & calgrad(EA7) & calph(ph6,
+180) & calph(ph7, +180) & calph(ph12, +180) & calph(ph13, +180),
caldel(d0, +in0) & caldel(d31, -in31) & calph(ph7, +180) &
calph(ph8, +180) & calph(ph31, +180))
exit

ph1=0
ph2=1
ph4=3
ph6=1
ph7=3 3 1 1
ph8=0 0 2 2
ph10=1 3
ph11=0 2
ph12=0 2
ph13=0 2
ph14=0 2
ph31=0 2 2 0

```

5 Bruker pulse sequence code: HC SOFAST-TROSY (semi-CT ¹³C editing)

```

;HC_SOFAST_C_TROSY
;BB 2024
;
;CLASS=IBS
;$DIM=2D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

prosol relations=<IBS>

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

define list<gradient> EA3 = { 1.0000 0.7500 }
define list<gradient> EA5 = { 0.5000 1.0000 }
define list<gradient> EA7 = { 0.9028 0.2972 }

/*****
/* Predefined shapes for 1H pulses *****/
/* cnst1: center of excitation band *****/
/* cnst2: excitation band width *****/
/*****

/* PC9 (p41, sp25) */
"p41=7.2/(cnst2*bf1/1000000)" /* PC9 pulse length */
"spw25=plw1*(pow((p1*1.01/p41)/0.125,2))" /* PC9 power level */
"spoff25=bf1*(cnst1/1000000)-o1" /* PC9 offset */
"spoa125=0.5"

/* REBURP (p42, sp26) */

"p42=4.875/(cnst2*bf1/1000000)" /* REBURP pulse length */
"spw26=plw1*(pow((p1*1.97/p42)/0.0798,2))" /* REBURP power level */
"spoff26=bf1*(cnst1/1000000)-o1" /* REBURP offset */
"spoa126=0.5"

/* EBURP & EBURP_TR (p43, sp28, sp29) */

"p43=4.6/(cnst2*bf1/1000000)" /* EBURP pulse length */
"spw28=plw1*(pow((p1*1.04/p43)/0.06103,2))" /* EBURP power level */
"spw29=plw1*(pow((p1*1.04/p43)/0.06103,2))" /* EBURP power level */
"spoff28=bf1*(cnst1/1000000)-o1" /* EBURP offset */
"spoa128=0"
"spoff29=bf1*(cnst1/1000000)-o1" /* EBURP_REV offset */
"spoa129=1.0"

"p16=1000u"
"p17=300u"

/
*****/
/* 13C pulse shapes */
*/
/
*****/
"p14=4.875/(50.0*bf2/1000000)" /* REBURP pulse length */
"spw3=plw2*(pow((p3*1.97/p14)/0.0798,2))" /* REBURP power level */
*/
"spoa13=0.5"
"spoff3=0"

/
*****/
"p40 =p3*8" /* BIP pulse length */
"spoff40=0.0" /* BIP offset */
"spw40=plw2" /* BIP power level */
"spoa140=0.5"

/
*****/
/* calculation of shaped 15N pulse parameters */
*/
/
*****/
"p50 =500u" /* BIP pulse length */
"spoff50=0.0" /* BIP offset */
"spw50=plw3*(pow((p21*8/p50),2))" /* BIP power level */

"p51=4.875/(50*bf3/1000000)" /* REBURP pulse length */
"spw51=plw3*(pow((p21*1.97/p51)/0.0798,2))" /* REBURP power level */
*/
"spoff51=0.0" /* REBURP offset */
"spoa151=0.5"

/
*****/
/* DELAYS */
*/
/
*****/
"d11=30m"

;"d25=1.0m" /* adjustable delay for flip angle */
"d26=1.4m"
"d27=1.2m" /* set slightly shorter than d26 for relaxation
compensation */
"d28=1.4m" /* 1/(2JCH) */

```

```

"DELTA1=d25-p42*0.5"
"DELTA2=d26-p42*0.5-p43*0.5"
"DELTA3=d27-p17-d16-p42*0.5"
"DELTA4=d28-p42*0.5-p43*0.5"

"DELTA=d0*2+p3*4/3.1416"

/
*****
/* time increments in 13C dimension (semi CT)
*/
/
"d0=3u"

"d22=1/(2*70)"
"d24=d22-d26*2-d16-p16-p3*2/3"
"d31=d24"

"d15=td1*inf1/4" /* t1(max)/2 */
"in30=(d15-d24)/(td1/2)"
"in31=d24/(td1/2)"
"in0=in30*2+in31"

"acqt0=0"
baseopt_echo

1 d11 ze
2 d11
3 5u pl1:f1 pl2:f2 pl3:f3
  d1
  50u UNBLKGRAD
/*****
/* PRESERVE H-C transfer */
/*****
(ralign (p43:sp28 ph10) (p3 ph13):f2 )

DELTA1
(center (p42:sp26 ph1) (p14:sp3 ph1):f2 )

DELTA1 pl2:f2

(lalign (p43:sp29 ph11) (p3 ph14):f2 )

DELTA4

(center (p42:sp26 ph1) (p14:sp3 ph1):f2 )

DELTA4

(p43:sp28 ph12)

/*****
/* 13C labeling */
/*****
d0
d24
(p40:sp40 ph1):f2
d31 /* d24 - t1/2 */

p16:gp3*EA3
d16 pl2:f2

/*****
/* TR0SY-type H-C back transfer */
/*****
(p43:sp29 ph6) /* EBURP_REV */
DELTA2
(center (p42:sp26 ph2) (p40:sp40 ph2):f2 )
DELTA2 pl2:f2
(p43:sp28 ph1) /* EBURP */
/*****

p16:gp5*EA5
d16

/*****
(p3 ph8):f2
p17:gp6
d16
DELTA3
(center (p42:sp26 ph2) (p14:sp3 ph2):f2 )
DELTA3 pl2:f2
p17:gp6
d16
(p3 ph7):f2
/*****

p16:gp7*EA7
d16 BLKGRAD

/*****
/* Signal detection & looping */
/*****
go=2 ph31
d11 mc #0 to 2
F1EA(calgrad(EA3) & calgrad(EA5) & calgrad(EA7) & calph(ph6,
+180) & calph(ph7, +180) & calph(ph12, +180) & calph(ph13, +180),
caldel(d0, +in0) & caldel(d31, -in31) & calph(ph7, +180) &
calph(ph8, +180) & calph(ph31, +180))
exit

ph1=0
ph2=1
ph4=3
ph6=1

```

```
ph7=3 3 1 1
ph8=0 0 2 2
ph10=1 3
ph11=0 2
ph12=0 2
ph13=0 2
ph14=0 2
ph31=0 2 2 0
```

```
;p10 : 0W
;p11 : f1 channel - power level for pulse (default)
;p13 : f3 channel - power level for pulse (default)
;sp13: f2 channel - shaped pulse 180 degree (Ca and C=0, adiabatic)
;p16: gradient pulse [1 msec]
;p17: gradient pulse
;p21: f3 channel - 90 degree high power pulse
;p22: f3 channel - 180 degree high power pulse
;p8 : f2 channel - 180 degree shaped pulse for inversion (adiabatic)
;d0 : incremented delay (F1) [3 usec]
;d1 : relaxation delay; 1-5 * T1
;d11: delay for disk I/O [30 msec]
;d16: delay for homospoil/gradient recovery
;d25: 1/(4J(NH))
;d26: 1/(4J(NH))
;d27: 1/(4J(NH))
;cnst1: H(N) excitation frequency (in ppm)
;cnst2: H(N) excitation band width (in ppm)
;inf1: 1/SW(N) = 2 * DW(N)
;in0: 1/(2 * Sw(N)) = DW(N)
;nd0: 2
;ns: 2 * n
;ds: >= 16
;td1: number of experiments in F1
;FnMODE: echo-antiecho in F1
```