

;decodes.tw  
;avance-version  
;diffusion edited preparation period w/LED sequence  
;homonuclear Hartman-Hahn transfer using MLEV17 sequence  
; for mixing  
;using two power levels for excitation and spinlock  
;phase sensitive using TPPI  
;A. Bax & D.G. Davis, J. Magn. Reson. 65, 355-360 (1985)

;using gradient during SL for pure absorption phase  
;see for ref. Titman et al.; JMR Ser. A 105, 167-183 (1993).

;TOCSY portion written by Dr. Katalin Kover

;DECODES expt. by Williamson R. T., Gerwick W. H. submitted to Org. Lett.

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

```
"p5=p6*.667"  
"p7=p6*2"  
;"d0=3u"  
"d12=20u"  
"d2=d6-p16-d16-p1-p1-d13"  
"d13=4u"
```

```
1 ze  
  d12 p1:f1  
2 d1  
  50u UNBLKGRAD  
  p1 ph1  
  d13  
  GRADIENT(cnst21)  
  d16  
  p1 ph1  
  d2  
  p1 ph1  
  d13  
  GRADIENT(cnst22)  
  d16  
  p1 ph1  
  d26  
  p1 ph1  
  d0
```

```
p16:f1:ngrad:c34 ph26  
d16  
p2 ph26  
d16 p110:f1
```

```
4 (p6 ph22 p7 ph23 p6 ph22)  
  (p6 ph24 p7 ph25 p6 ph24)  
  (p6 ph24 p7 ph25 p6 ph24)  
  (p6 ph22 p7 ph23 p6 ph22)  
  (p6 ph24 p7 ph25 p6 ph24)  
  (p6 ph24 p7 ph25 p6 ph24)
```

```

(p6 ph22 p7 ph23 p6 ph22)
(p6 ph22 p7 ph23 p6 ph22)
(p6 ph24 p7 ph25 p6 ph24)
(p6 ph22 p7 ph23 p6 ph22)
(p6 ph22 p7 ph23 p6 ph22)
(p6 ph24 p7 ph25 p6 ph24)
(p6 ph22 p7 ph23 p6 ph22)
(p6 ph22 p7 ph23 p6 ph22)
(p6 ph24 p7 ph25 p6 ph24)
(p6 ph24 p7 ph25 p6 ph24)
(p5 ph23)
lo to 4 times l1

```

```

p16:f1:ngrad:c34 ph26
d16 p11:f1
p2 ph26
d15 ;d15+4u=d16=200u
4u BLKGRAD

```

```

go=2 ph31
d11 wr #0 if #0 id0 ip1 zd
lo to 2 times td1
exit

```

```
ph1=0 2 2 0 1 3 3 1
```

```

ph22=3 1 3 1 0 2 0 2
ph23=0 2 0 2 1 3 1 3
ph24=1 3 1 3 2 0 2 0
ph25=2 0 2 0 3 1 3 1
ph26=0 2 0 2 1 3 1 3
ph31=0 2 2 0 1 3 3 1

```

```

;grdprog 4sine
;cnst21=cnst22=variable
;cnst23=cnst24=20

```

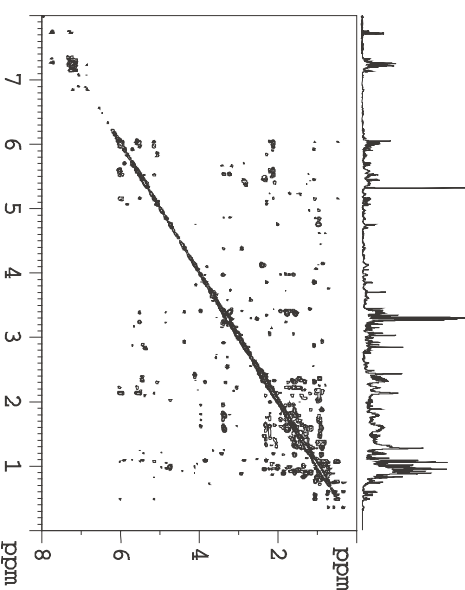
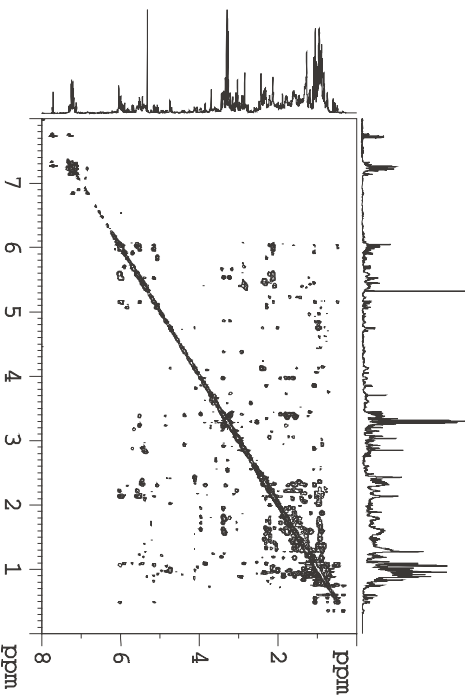
```

;p11 : f1 channel - power level for pulse (default)
;p110: f1 channel - power level for TOCSY-spinlock
;p1 : f1 channel - 90 degree high power pulse
;p5 : f1 channel - 60 degree low power pulse
;p6 : f1 channel - 90 degree low power pulse
;p7 : f1 channel - 180 degree low power pulse
;p17: f1 channel - trim pulse [2.5 msec]
;d0 : incremented delay (2D) [3 usec]
;d1 : relaxation delay; 1-5 * T1
;d12: delay for power switching [20 usec]
;L1: loop for MLEV cycle: (((p6*64) + p5) * l1) + (p17*2) = mixing time
;in0: 1/(2 * SW) = DW
;nd0: 2
;NS: 8 * n
;DS: 16
;td1: number of experiments
;MC2: TPPI
;d6 : encode delay (2D)
;d26: delay for eddy current decay

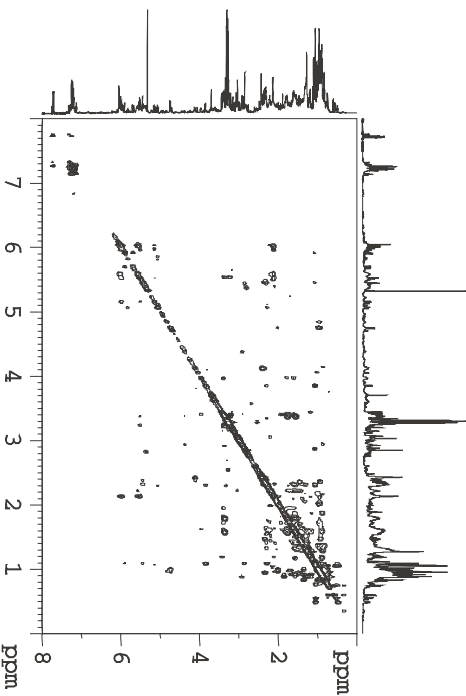
```

# DECODES spectra of crude symplostatin 1

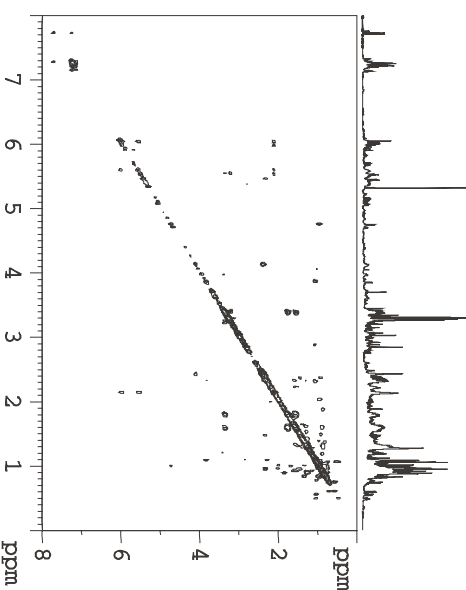
15% max (100 msec diffusion) 25% max (100 msec diffusion)



35% max (100 msec diffusion)



45% max (100 msec diffusion)



72 G/cm<sup>2</sup> max grad strength

```

;decodehet.tw

;avance-version
;2D H-1/X correlation via double inept transfer
; using sensitivity improvement
;phase sensitive using Echo/Antiecho gradient selection
;with decoupling during acquisition
;using trim pulses in inept transfer
;A.G. Palmer III, J. Cavanagh, P.E. Wright & M. Rance, J. Magn.
; Reson. 93, 151-170 (1991)
;L.E. Kay, P. Keifer & T. Saarinen, J. Am. Chem. Soc. 114,
; 10663-5 (1992)
;J. Schleucher, M. Schwendinger, M. Sattler, P. Schmidt, O. Schedletzky,
; S.J. Glaser, O.W. Sorensen & C. Griesinger, J. Biomol. NMR 4,
; 301-306 (1994)

```

```

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

```

```

"p2=p1*2"
"p4=p3*2"
"d0=3u"
"d4=1s/(cnst2*4)"
"d11=30m"
"d13=3u"

```

```
"d2=d6-p16-d16-p1-p1-d13"
```

```
"d20=p16+d16+50u+p2+d0*2"
"d21=d13+p16+d16+4u"

```

```
"d31=p3-p1"
```

```
"I3=(td1/2)"
"ds=ns*2*cnst0"

```

```

1 ze
  d11 p112:f2
2 d1 do:f2
  6m
3 d11
4 50u UNBLKGRAD
  p1 ph11
  d13
  GRADIENT(cnst21)
  d16
  p1 ph11
  d2
  p1 ph11
  d13
  GRADIENT(cnst22)
  d16
  p1 ph11

```

```

d26
p1 ph11
d4 pl2:f2
(d31 p2 ph1) (p4 ph1):f2
d4
p28 ph1
d13
(p1 ph2) (p3 ph3):f2
d0
p2 ph6
d0
50u ;UNBLKGRAD
GRADIENT(cnst23)
d16
(p4 ph4):f2
d20
(p1 ph1) (p3 ph4):f2
d24
(d31 p2 ph1) (p4 ph1):f2
d24
(p1 ph2) (p3 ph5):f2
d4
(d31 p2 ph1) (p4 ph1):f2
d4
(p1 ph1)
d21
(p2 ph1)
d13
GRADIENT(cnst24)
d16 pl12:f2
4u BLKGRAD
go=2 ph31 cpd2:f2
d1 do:f2 wr #0 if #0 zd
3m ip5
3m ip5
lo to 3 times 2
d11 id0
lo to 4 times l3
exit

```

```

ph1=0
ph2=1
ph3=0 2
ph4=0 0 2 2
ph5=1 1 3 3
ph6=0 0 2 2
ph11=0; 2 2 0 1 3 3 1
ph31=0 2 2 0

```

```

;p1 : f1 channel - power level for pulse (default)
;p2 : f2 channel - power level for pulse (default)
;p12: f2 channel - power level for CPD/BB decoupling
;p1 : f1 channel - 90 degree high power pulse
;p2 : f1 channel - 180 degree high power pulse

```

```

;p3 : f2 channel - 90 degree high power pulse
;p4 : f2 channel - 180 degree high power pulse
;p16: homospoil/gradient pulse
;p28: f1 channel - trim pulse
;d0 : incremented delay (2D)           [3 usec]
;d1 : relaxation delay; 1-5 * T1
;d4 : 1/(4J)XH
;d11: delay for disk I/O               [30 msec]
;d13: short delay                       [3 usec]
;d16: delay for homospoil/gradient recovery
;d20: = p16+d16+50u+p2+d0*2
;d21: = d13+p16+d16+4u
;d24: 1/(4J)XH for XH
;    1/(8J)XH for all multiplicities
;cnst0: ds = ns * 2 * cnst0
;cnst2: = J(XH)
;l3: loop for phase sensitive 2D using E/A method : l3 = td1/2
;in0: 1/(2 * SW(X)) = DW(X)
;nd0: 2
;NS: 1 * n
;DS: >= 16, but 2 * ns * m
;td1: number of experiments
;MC2: echo-antiecho
;cpd2: decoupling according to sequence defined by cpdprg2
;pcpd2: f2 channel - 90 degree pulse for decoupling sequence

;d6 : encode delay (2D)
;d26: delay for eddy current decay

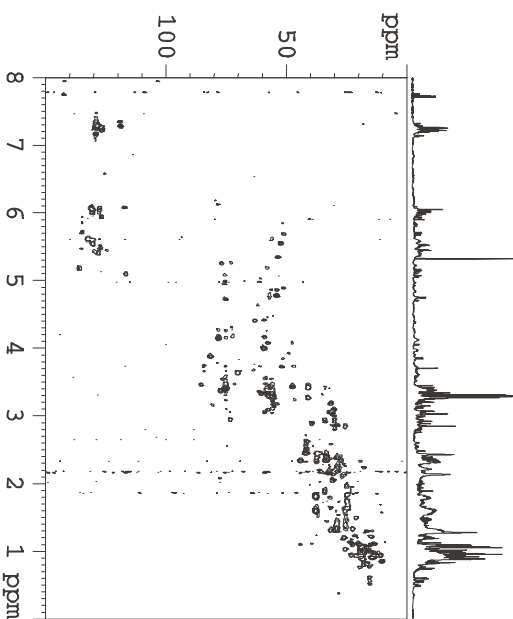
;use gradient program (GRDPROG) : 4sineea_4

;use gradient ratio: cnst21 : cnst22 : cnst23 : cnst24
;   var :   var :   80 :   20 for C-13
;   var :   var :   80 :    8 for N-15

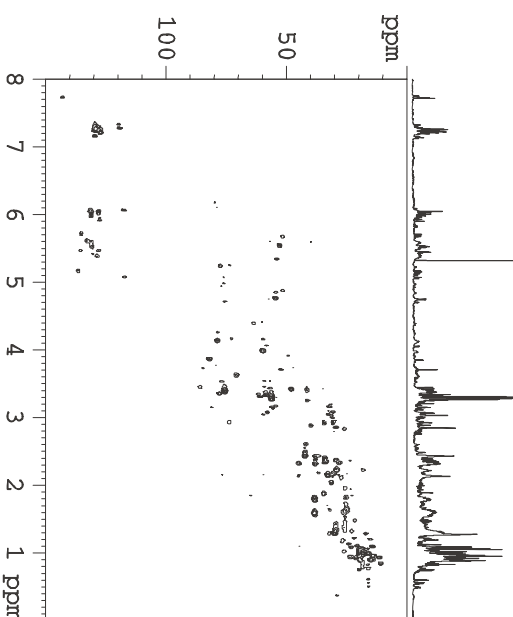
```

# HETDECODES spectra of crude symplostatin 1

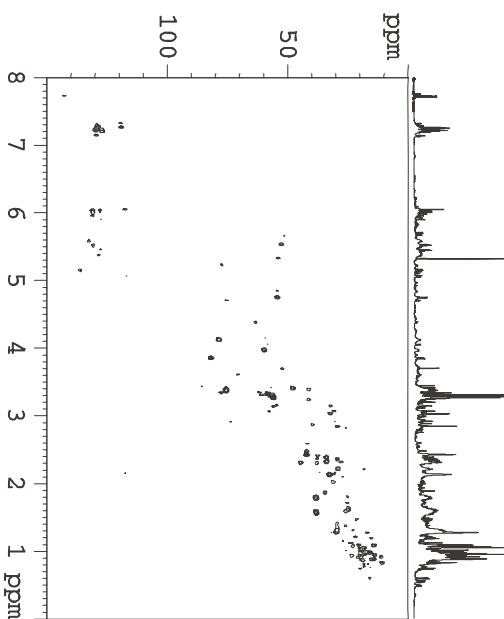
5% max (50 msec diffusion)



25% max (50 msec diffusion)



45% max (50 msec diffusion)



65% max (50 msec diffusion)

