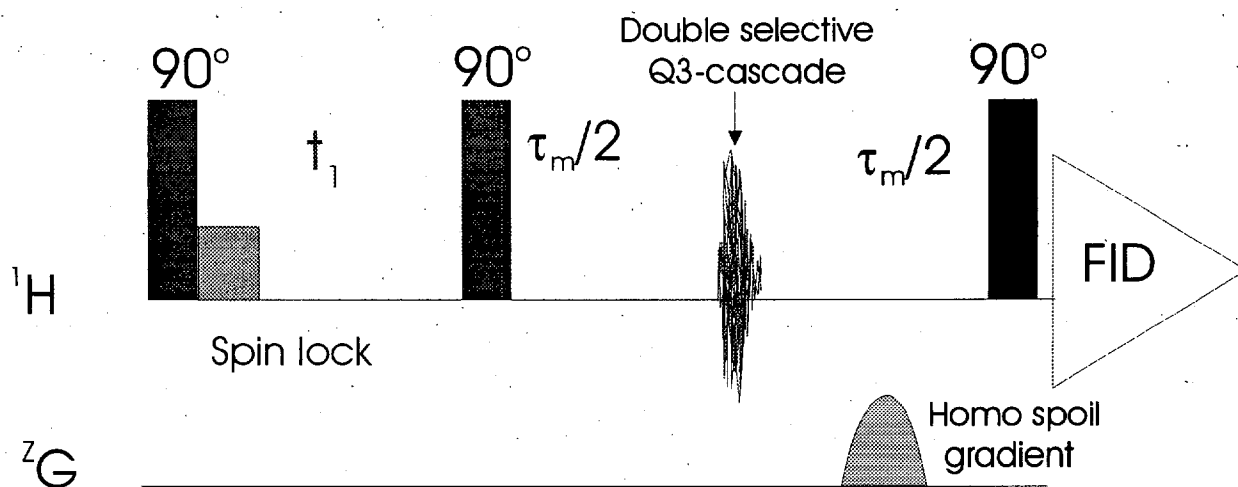


Supporting Information

NMR Experiments Reveal Distinct Antibody-Bound Conformations of a Synthetic Disaccharide Representing a General Structural Element of Bacterial Lipopolysaccharide Epitopes

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pulse sequence



Pulse program for Bruker DRX machines

```

QUIET2DNOESY.th
;avance-version
;2D homonuclear correlation via dipolar coupling
;dipolar coupling may be due to noe or chemical exchange.
;phase sensitive using TPPI
;with presaturation during relaxation delay
;with spin lock filter after first 90 deg pulse
;gradient pulse during mixing time (homo spoil)
;with double-selective Gaussian cascade (Q3) during the mixing time

;Vincent et al., JBiomolNMR 7 (1996) 169
;Vincent et al., AngewChem 106 (1994) 340
;Vincent et al., AngewChemIntEdEngl 33 (1994) 343
;Zwahlen et al., JACS 116 (1994) 362
;Vincent et al., PNAS 94 (1997) 4383-4388

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

;;"d0=3u"
;;"d11=30m"
;;"d12=20u"
;;"d13=3u"

1 ze
2 d11
3 d12 pl9:f1
  d1 cw:f1 ;cw (watersupression)
  d13 do:f1
  d12 pl1:f1
  p1 ph1 ;first 90 deg pulse
  d12 pl2:f1
  p2 ph4 ;spin lock pulse
  d0
  d12 pl1:f1
  p1 ph2 ;second 90 deg pulse
  d16 UNBLKGRAD
  d17
  d8 pl12:f1 ;first half of mixing time
  pl1:sp1:f1 ph8 ;double selective pulse (Q3)
  d8 pl1:f1 ;second half of mixing time
  p16:gp1 ;homo spoil gradient
  d16 BLKGRAD
  p1 ph3 ;third 90 deg pulse
  go=2 ph31
  d11 wr #0 if #0 id0 ip1 zd
  d11 ip4
  lo to 3 times td1
exit

ph1=0 2
ph2=0 0 0 0 0 0 0 0 2 2 2 2 2 2 2
ph3=0 0 2 2 1 1 3 3
ph4=1 3
ph8=0 2

```

```
ph31=0 2 2 0 1 3 3 1 2 0 0 2 3 1 1 3
```

```
;p11 : f1 channel - power level for pulse (default)
;p19 : f1 channel - power level for presaturation
;p12 : f1 channel - power for spin lock pulse
;p1 : f1 channel - 90 degree high power pulse
;p11 ; f1 channel- duration of 180-Q3
;sp1 : f1 channel - power and shape of 180 degree Q3 Gaussian cascade
;p2 : f1 channel - spin lock pulse [5-30 msec]
;p16: gradient pulse [1 msec]
;d16: recovery delay [100 usec]
;gpname: sine.100
;d0 : incremented delay (2D) [3 usec]
;d1 : relaxation delay; 1-5 * T1
;mixing time = (2*d8)+(2*d16)+d17+p16+p11
;d11: delay for disk I/O [30 msec]
;d12: delay for power switching [20 usec]
;d13: short delay [3 usec]
;d17 = p16 [1 msec]
;in0: 1/(2 * SW) = DW
;nd0: 2
;NS: 8 * n
;DS: 16
;td1: number of experiments
;MC2: TPPI

;create double selective pulse with MULE (modify shape for MULTiple
Excitation, ;(Bruker) and XSHAPE (Bruker)
;for calibration of the double selective pulse use the same pulse program
but ;delete d0, id0, id1 and td1
;calibrate the double selective pulse (180°) to maximum inversion (!!!!)
```