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Supporting Information.

Sensitivity Enhancement in Slice-Selective NMR Experiments through Polarization Sharing

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Contents

All the experiments were carried out on a 800 MHz Bruker NMR spectrometer facilitated with cryoprobe. The maximum gradient strength of gradient coil is 53.5 Gcm^{-1}.

(A) ASAP-Sel1d and Sel1d

The ASAP-Sel1d and Sel1d are recorded on Propylene carbonate (5mg in 500 ul of $CDCl_3$).

The ASAP-Sel1d pulse sequence, without initial block consisting of DIPSI-2 and flanked by two gradients constitute normal Sel1d pulse sequence. In both ASAP-Sel1d and Sel1d a 90^0 Gaussian-shaped pulse with pulse length of 20 ms (band width of 100Hz) is used for selective excitation. In ASAP-Sel1D, DIPSI-2 block of an optimized duration of 40 ms (at 1.14 watt power) flanked by gradients G1 of 33% and G2 of 44% of maximum gradient strength is used for polarization transfer. An acquisition time of 1sec is used in all experiments. The inter scan delay of 2 sec, 75 ms and 35 ms are respectively used in two Sel1d experiments and ASAP-Sel1d experiment.

(B) Pure-shift ASAP-ZS and pure-shift ZS experiment.

The pure-shift ASAP-ZS pulse sequence without initial block consisting of DIPSI-2, flanked by two gradients and last two pulses (hard 180^0 and soft 180^0 pulses) constitute pure-shift ZS pulse sequence.

The ASAP-ZS and ZS experiments are recorded on sample mixture of propylene carbonate, γ-valerolactone, 1-indanol and *L*-menthol in $CDCl_3$ (each of them taken as 5 mg or 5 ul in 500 ul of $CDCl_3$)

The first pure-shift ZS experiment is recorded in 5.24 min with 4 scans at each data point, dummy scans of 2 and inter scan delay of 2 sec. The second pure-shift ZS experiment is recorded in 5.24 min with 16 scans at each data point, dummy scans of 4 and inter scan delay of 135 ms.

The ASAP-ZS experiment is recorded in 5.28 min with number of scans of 16 at each data point, dummy scans of 4 and inter scan delay of 35 ms. In ASAP-ZS the polarization transfer is achieved by initial DIPSI-2 block with duration of 40 ms (at 1.14 watt power) flanked by gradients G1 of 33% and G2 of 44% of maximum gradient strength. The other experimental parameters remained constant in both cases.

In all the experiments, selective 90^0 EBurp-shaped pulse and 180^0 ReBurp-shaped pulse with pulse length of 60 ms (band width of 100Hz) are used. Slice selection is achieved by using GS of 1% of maximum gradient strength. The coherence selection is achieved by G3 of 26 and -G3 of -26% of maximum gradient strength. Acquisition time of 0.213 sec and 0.16 s with data points

of 2048 X 32, corresponding to spectral width of 4795 Hz and 100 Hz along F_2 and F_1 dimensions respectively are used.

The ASAP-ZS and ZS experiments are recorded on 50mM cyclosporin-A sample in C_6D_6

The first pure-shift ZS experiment is recorded in 5. 26 min with 4 scans at each data point, dummy scans of 2 and inter scan delay of 2 sec. The secound pure-shift ZS experiment is recorded in 5. 33 min with 16 scans at each data point, dummy scans of 4 and inter scan delay of 135 ms.

The ASAP-ZS experiment is recorded in 5.13 min with number of scans of 16 at each data point, dummy scans of 4 and inter scan delay of 35 ms. In ASAP-ZS the polarization transfer is achieved by initial DIPSI-2 block with duration of 40 ms (at 1.14 watt power) flanked by gradients G1 of 33% and G2 of 44% of maximum gradient strength. The other experimental parameters remained constant in both cases.

In both experiments, selective 90^0 EBurp-shaped pulse and 180^0 ReBurp-shaped pulse with pulse length of 60 ms (band width of 100Hz) are used. Slice selection is achieved by using GS of 0.7% of maximum gradient strength. The coherence selection is achieved by G3 of 26 and -G3 of -26% of maximum gradient strength. Acquisition time of 0.319 sec and 0.16 s with data points of 2048 X 32, corresponding to spectral width of 3201 Hz and 100 Hz along F_2 and F_1 dimensions respectively are used in both experiments.

(C) ASAP-G-SERF and G-SERF experiment.

ASAP-G-SERF and G-SERF experiment on *L*-menthol and Strychnine.

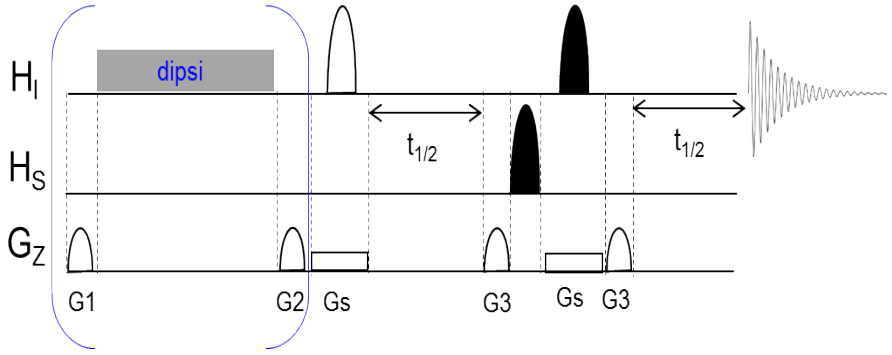

Fig. S1: The pulse sequence of ASAP-G-SERF. Without the initial blue block consisting of DIPSI-2 block flanked by two gradients G1 and G2 constitute normal G-SERF pulse sequence.

Experimental details of ASAP-G-SERF and G-SERF spectra of *L*-menthol.

First G-SERF is recorded in 11 min 33 sec with number of scans 4, dummy scans 2 and inter scan relaxation delay of 2 s. The second G-SERF is recorded in 11 min 43 sec with number of scans 16, dummy scans4 and inter scan relaxation delay of 75 ms.

ASAP-G-SERF is recorded in 11 min 45 sec with number of scans 8, dummy scans 4 and inter scan delay of 35 ms. In ASAP-G-SERF the polarization transfer is achieved by initial DIPSI-2 block with duration of 40 ms (at 1.14 watt power),which is flanked by gradients G1 of 33% and G2 of 44% of maximum gradient strength prior to G-SERF pulse sequence.

The other experimental parameters are maintained identical in both cases. Selective 90^0 EBurp-shaped pulse and 180^0 ReBurp-shaped pulse with pulse length of 60 ms (band width of 100Hz) are used. Slice selection is achieved by using GS of 0.7% of maximum gradient strength. The coherence selection is achieved by G3 of 26 of maximum gradient strength. The acquisition time of 0.319 sec and 0.8 sec with data points of 2048 X 64, corresponding to spectral width of 3201 Hz and 40 Hz along F_2 and F_1 dimensions respectively are used.

Experimental details and spectra of ASAP-G-SERF and G-SERF of Strychnine (5 mg in 500 ul).

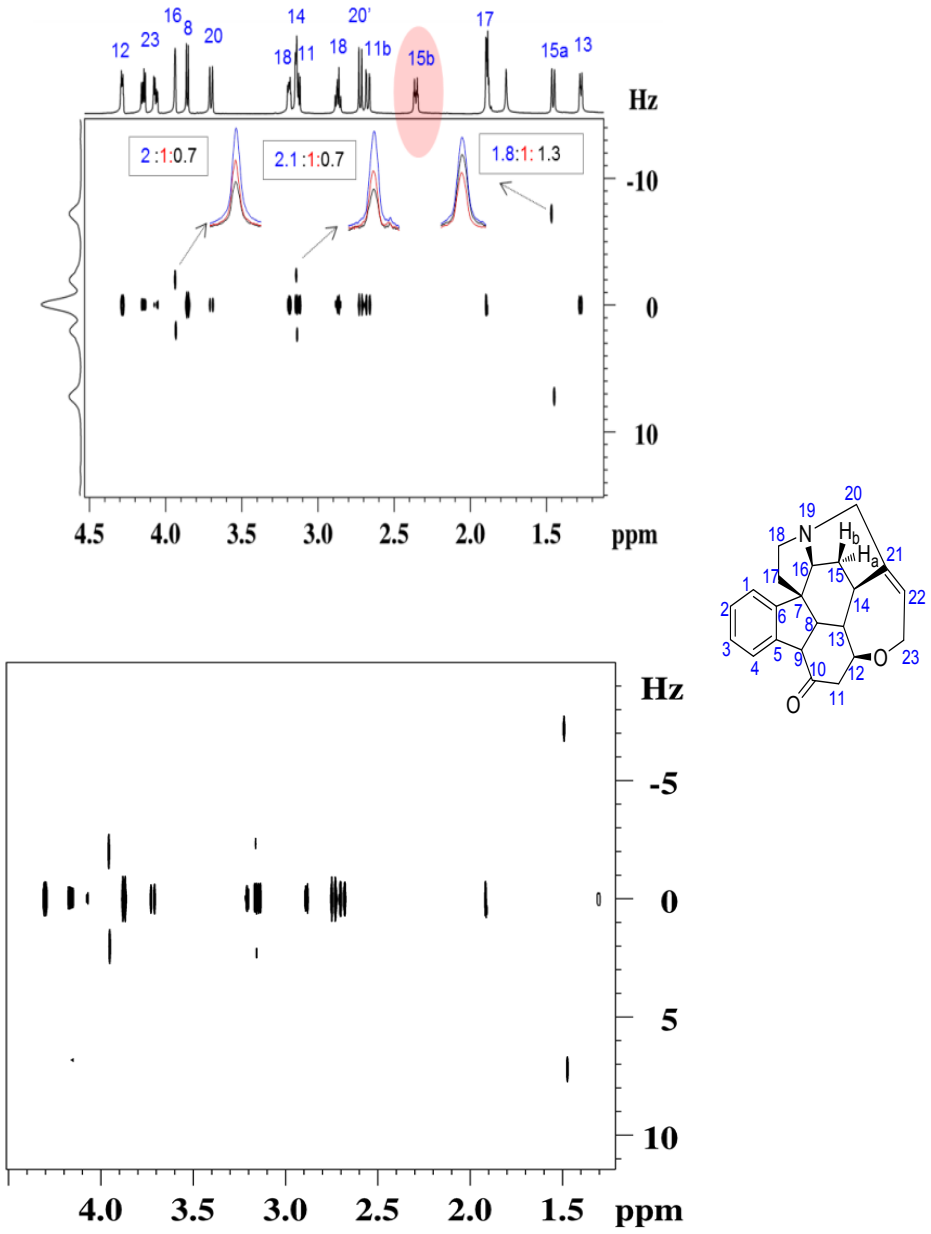

Fig. S2: Chemical structure, ASAP-G-SERF (above) and G-SERF (below) 2D ^{1}H spectrum of strychnine. The intensities of cross peaks from ASAP-G-SERF (blue) are compared with that of

G-SERF with 95 ms (black) and 2 s (red) inter-scan delay, shows nearly 2-fold sensitivity enhancement per unit time in ASAP-G-SERF spectrum (blue).

The first G-SERF is recorded in 15 min 39 sec with number of scans 4, dummy scans 2 and inter scan relaxation delay of 1.9 s. The second G-SERF is recorded in 15 min 45 sec with number of scans 8, dummy scans 4 and inter scan relaxation delay of 95 ms.

ASAP-G-SERF is recorded in 14 min 56 sec with number of scans 8, dummy scans 4 and inter scan delay of 50 ms. In ASAP-G-SERF the polarization transfer is achieved by initial DIPSI-2 block with duration of 40 ms (at 1.14 watt power), which is flanked by gradients G1 of 33% and G2 of 44% of maximum gradient strength prior to G-SERF pulse sequence.

The other experimental parameters are maintained identical in both cases. Selective 90^0 EBurp-shaped pulse and 180^0 ReBurp-shaped pulse with pulse length of 60 ms (band width of 100Hz) are used. Slice selection is achieved by using GS of 0.7 % of maximum gradient strength. The coherence selection is achieved by G3 of 26% of maximum gradient strength. The acquisition time of 0.51 sec and1.06 sec with data points of 4096 X 64, corresponding to spectral width of 4000 Hz and 30Hz along F_2 and F_1 dimensions respectively are used.

Pulse Program Codes

1. ASAP-ZS pulse program code for Bruker NMR spectrometer

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


"in0=inf1/2"
"p2=p1*2"
"d0=3u"
"FACTOR1=(d9/(p6*115.112))/2+0.5"
"l1=FACTOR1*2"

1 ze
2 d1
  50u UNBLKGRAD
  p16:gp1
  d16
  d20 pl10:f1

                                    ;begin DIPSI2
3 p6*3.556 ph23
  p6*4.556 ph25
  p6*3.222 ph23
  p6*3.167 ph25
  p6*0.333 ph23
  p6*2.722 ph25
  p6*4.167 ph23
  p6*2.944 ph25
  p6*4.111 ph23

  p6*3.556 ph25
  p6*4.556 ph23
  p6*3.222 ph25
  p6*3.167 ph23
  p6*0.333 ph25
  p6*2.722 ph23
  p6*4.167 ph25
  p6*2.944 ph23
  p6*4.111 ph25

  p6*3.556 ph25
  p6*4.556 ph23
  p6*3.222 ph25
```

```
p6*3.167 ph23
p6*0.333 ph25
p6*2.722 ph23
p6*4.167 ph25
p6*2.944 ph23
p6*4.111 ph25

p6*3.556 ph23
p6*4.556 ph25
p6*3.222 ph23
p6*3.167 ph25
p6*0.333 ph23
p6*2.722 ph25
p6*4.167 ph23
p6*2.944 ph25
p6*4.111 ph23
 lo to 3 times l1
       ;end DIPSI2

d21
p16:gp2
d16
4u pl0:f1
300u gron2            ; Slice selection gradient On
(p11:sp1 ph1):f1      ; 90 (selective)
100u groff            ; Slice selection gradient Off
200u
d0
4u
p17:gp3
d16 pl1:f1
(p2 ph2):f1
4u pl0:f1
300u gron2            ; Slice selection gradient On
(p12:sp2 ph2):f1      ; 180 (selective)
100u groff            ; Slice selection gradient Off
200u
4u
p17:gp4
d16
d0
4u
p17:gp3
d16 pl1:f1
(p2 ph2):f1
4u pl0:f1
```

```
  300u gron2            ; Slice selection gradient On
  (p12:sp2 ph2):f1      ; 180 (selective)
  100u groff            ; Slice selection gradient Off
  200u
  4u
  p17:gp4
  d16
  50u BLKGRAD
  go=2 ph31
  30m mc #0 to 2 F1QF(id0)
exit


ph1 = 0 0
ph2 = 1 3
ph23 =3
ph25 =1
ph31 =0 0



;pl1 : High power
;p11: 90 degree shape pulse
;p12: 180 degree shape pulse
;sp1: 90 degree shape pulse power label
;sp2: 180 degree shape pulse power label
;p1 : f1 channel -  90 degree high power pulse
;d0 : incremented delay (2D)                    [3 usec]
;d1 : relaxation delay; 1-5 * T1
;in0: 1/(1 * SW) = 2 * DW
;nd0: 2
;NS: 2 * n
;DS: 8
;td1: number of t1 increments
;MC2: QF
```

2. ASAP-G_SERF pulse program code for Bruker NMR spectrometer

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


"in0=inf1/2"
"p2=p1*2"
"d0=3u"
"FACTOR1=(d9/(p6*115.112))/2+0.5"
"l1=FACTOR1*2"

1 ze
2 d1
  50u UNBLKGRAD
  p16:gp1
  d16
  d20 pl10:f1

                                    ;begin DIPSI2
3 p6*3.556 ph23
  p6*4.556 ph25
  p6*3.222 ph23
  p6*3.167 ph25
  p6*0.333 ph23
  p6*2.722 ph25
  p6*4.167 ph23
  p6*2.944 ph25
  p6*4.111 ph23

  p6*3.556 ph25
  p6*4.556 ph23
  p6*3.222 ph25
  p6*3.167 ph23
  p6*0.333 ph25
  p6*2.722 ph23
  p6*4.167 ph25
  p6*2.944 ph23
  p6*4.111 ph25

  p6*3.556 ph25
  p6*4.556 ph23
  p6*3.222 ph25
  p6*3.167 ph23
```

```
  p6*0.333 ph25
  p6*2.722 ph23
  p6*4.167 ph25
  p6*2.944 ph23
  p6*4.111 ph25

  p6*3.556 ph23
  p6*4.556 ph25
  p6*3.222 ph23
  p6*3.167 ph25
  p6*0.333 ph23
  p6*2.722 ph25
  p6*4.167 ph23
  p6*2.944 ph25
  p6*4.111 ph23
   lo to 3 times l1
         ;end DIPSI2

  d21
  p16:gp2
  d16
  4u pl0:f1
  300u gron2            ; Slice selection gradient On
  (p11:sp1 ph1):f1      ; 90 (selective)
  100u groff            ; Slice selection gradient Off
  200u
  d0
  4u
  p17:gp3
  d16
  (p14:sp4 ph2):f1
  4u
  300u gron2            ; Slice selection gradient On
  (p12:sp2 ph2):f1      ; 180 (selective)
  100u groff            ; Slice selection gradient Off
  200u
  4u
  p17:gp3
  d16
  d0
  50u BLKGRAD
  go=2 ph31
  30m mc #0 to 2 F1QF(id0)
exit
```

```
ph1 = 0 0
ph2 = 1 3
ph23 =3
ph25 =1
ph31 =0 0



;pl1 : High power
;p11: 90 degree shape pulse
;p12: 180 degree shape pulse
;sp1: 90 degree shape pulse power label
;sp2: 180 degree shape pulse power label
;p1 : f1 channel -  90 degree high power pulse
;d0 : incremented delay (2D)                    [3 usec]
;d1 : relaxation delay; 1-5 * T1
;in0: 1/(1 * SW) = 2 * DW
;nd0: 2
;NS: 2 * n
;DS: 8
;td1: number of t1 increments
;MC2: QF
```