Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Clean-G-SERF an NMR experiment for the Complete eradication of axial peaks and undesired couplings from the complex Spectrum

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Experimental Parameters

Table.1 Experimental parameters used for acquiring the G-SERF and Clean-G-SERF spectra of investigated molecules and molecular mixtures

Molecule/ Molecular mixtures Figure Number[X]	Experiment	Selective excitation pulse/Duration / Excitation Band width	Selective Refocusing pulse/Duration/ Excitation Band width	Interscan delay (Sec)	Time Domain Points	Used Gradient strengths (%)[Y]	Scans NS/DS	Total experimental time
1	***G-SERF***	*EBurp/45ms/ 100.3Hz*	Gaussian/10ms /88.2Hz	3	84	G2=0.8 G3=50 G4=40	4/4	27 mins and 4 secs.
	Clean-G-SERF	*Identical*	Identical	3	84	G1=15 G2=0.8 G3=40 G4=50	4/4	25 mins and 59 secs.
2	***G-SERF***	*EBurp/40ms/ 112.8Hz*	Gaussian/8ms/ 110.2Hz	3	64	G2=0.8 G3=50 G4=40	4/4	19 mins and 18 secs.
	Clean-G-SERF	*Identical*	Identical	3	64	G1=15 G2=0.8 G3=40 G4=50	4/4	19 mins and 51 secs.
3	***G-SERF***	*EBurp/50 ms/ 90.3 Hz*	Gaussian/10ms /88.2Hz	3	128	G2=0.8 G3=50 G4=40	4/4	42 mins and 54 secs.
	Clean-G-SERF	*Identical*	Identical	3	64	G1=15 G2=0.8 G3=40 G4=50	4/4	20 mins and 59 secs.
4	***G-SERF***	*EBurp/40ms/ 112.8Hz*	Gaussian/8ms/ 88.2Hz	3	84	G2=0.8 G3=50 G4=40	4/4	28 mins and 59 secs.
	Clean-G-SERF	*Identical*	Identical	3	84	G1=15 G2=0.8 G3=40 G4=50	4/4	27 mins and 15 secs.

X= the molecule and the mixture of molecules corresponding to figure numbers given in the main manuscript, Y= The percentage of the gradients used in every experiment are of maximum available gradient strength that is 53.5 G/cm. The length of the gradients used for all the experiment was set for 1 milliseconds.

Sensitivity of G-SERF vs Clean-G-SERF

To compare the sensitivity of the present experiment with G-SERF experiment we have carried out both the experiments with the identical common parameters and the obtained integral values from the G-SERF [pulse sequence used is reported in; N. Giraud, L. B|guin, J. Courtieu, D. Merlet, *Angew. Chem. Int. Ed.,* **2010**, *49*, 3481-3484; *Angew. Chem.* **2010]** and Clean-G-SERF are given in the Tables 1 and 2 respectively.

Table 2. Integral values of peaks of the coupled partners of selectively excited proton of strychnine molecule using G-SERF experiment [acquired with NS=8, DS=16 and 64 TD points in the indirect dimension]. One peak of the doublet is integrated and the integral 4 represent the integral value of noise region.

Object	Integral [abs]	Integral [rel]	Type	Peaks	v(F2) [ppm]	v(F1) [ppm]
Integral 1	11031000000.00	1.0000	Manual	0	1.4865	-0.0143
Integral 2	7547800000.00	0.6842	Manual	0	3.1692	-0.0062
Integral 3	7891200000.00	0.7154	Manual	0	3.9638	-0.0052
Integral 4	273850000.00	0.0248	Manual	0	3.4083	-0.0277

Table 3. Integral values of peaks of the coupled partners of selectively excited proton obtained for strychnine molecule using Clean-G-SERF experiment [acquired with NS=8, DS=16 and 64 TD points in the indirect dimension]. One peak of the doublet is integrated and the integral 4 represent the integral value of noise region.

Object	Integral [abs]	Integral [rel]	Type	Peaks	v(F2) [ppm]	v(F1) [ppm]
Integral 1	19065000000.00	1.0000	Manual	0	1.4877	-0.0144
Integral 2	12031000000.00	0.6311	Manual	0	3.1646	-0.0056
Integral 3	10525000000.00	0.5521	Manual	0	3.9569	-0.0054
Integral 4	540690000.00	0.0348	Manual	0	3.5077	2.7543

Pulse Programs

Pulse program code for optimization of constant delay delta (Δ) in Bruker NMR spectrometer

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

#   ifdef CALC_SPOFFS
"spoff1=bf1*(cnst21/1000000)-o1"
#   else
#   endif /*CALC_SPOFFS*/

"in0=inf1/2"
"p2=p1*2"
"d0=3u"

1 ze
2 30m
  d1
  4u pl0:f1
  p11:sp1:f1 ph1:r
  4u
  d14 pl1:f1
  50u UNBLKGRAD
  p16:gp1
  d16
  p0 ph2
  d13
  p16:gp1
  d16
  4u BLKGRAD
  go=2 ph31
  30m mc #0 to 2 F0(zd)
exit

ph1=0 2
ph2=0 0 2 2
ph31=0 2

;pl0 : 0W
;pl1 : f1 channel - power level for pulse (default)
;sp1: f1 channel - shaped pulse
;p1 : f1 channel -  90 degree high power pulse
```

;p11: f1 channel - 90 degree shaped pulse
;d1 : relaxation delay; 1-5 * T1
;d14: delay for evolution after shaped pulse:
;for 90 deg pulse (p11)/2 + d14 ~ 1/(2J)
;cnst21: chemical shift for selective pulse (offset, in ppm)
;ns: 2 * n, total number of scans: NS * TD0
;ds: 2
;use gradient ratio: gp 1
; 15
;for z-only gradients:
;gpz1: 15%
;use gradient files:
(topspin 2.1)
;gpnam1: SINE.100
;gpnam3: SINE.100
;gpnam4: SINE.100

(Topspin3.x)
;gpnam1: SMSQ10.100
;gpnam1: SMSQ10.100
;gpnam1: SMSQ10.100

;phcor 1 : phase difference between power levels sp1 and pl1

;choose p11 according to desired selectivity
;the flip-angle is determined by the amplitude
;set O1 on resonance on the multiplet to be excited or use spoffs

Clean-G-SERF pulse program code for Bruker spectrometer

```
;pp: Clean-G-SERF
;class: 2D
;Topspin2.1 & Topspin3.x

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


"d13=4u"
"d4=1s/(cnst2*2)"
"in0=inf1/2"
"d0=3u"


1 ze
2 d1 pl0:f1
3 (p11:sp1 ph1)                          ; 90 (selective)
  d4
  50u UNBLKGRAD
  p16:gp1
  d16 pl1:f1
  p1 ph2
  p16:gp1
  d16
  p16:gp3
  d16
  200u gron2                             ; slice selective gradient on
  (p12:sp2 ph2):f1                       ; 180 (selective)
  100u groff                             ;slice selective gradient off
  100u
  p16:gp3
  d16
  d0
  p16:gp4
  d16
  (p12:sp2 ph2):f1                    ; 180 (selective)

  200u gron2                          ; slice selective gradient on
  (p12:sp2 ph2):f1                    ; 180 (selective)
  100u groff                          ;slice selective gradient off
```

```
 100u
 d16
 d0
 (p12:sp2 ph2):f1                    ; 180 (selective)
 p16:gp4
 4u BLKGRAD
 go=2 ph31
 d1 mc #0 to 2 F1QF(id0)
exit

ph1=0 2
ph2=0 0 2 2
ph31=0 2


;pl1 : f1 channel - power level for pulse (default)
;p0 : f1 channel -  20 to 90 degree high power pulse
;p1 : f1 channel -  90 degree high power pulse
;p11: 90 degree shape pulse
;p12: 180 degree shape pulse
;sp1: 90 degree shape pulse power label
;sp2: 180 degree shape pulse power label
;p16: homospoil/gradient pulse
;d0 : incremented delay (2D)                [3 usec]
;d1 : relaxation delay; 1-5 * T1
;d13: short delay                           [4 usec]
;d16: delay for homospoil/gradient recovery
;inf1: 1/SW = 2 * DW
;in0: 1/(1 * SW) = 2 * DW
;nd0: 1
;NS: 2 * n
;DS: 16
;td1: number of experiments
;FnMODE: QF
;use gradient ratio:    gp 1
;                    10-15
;for z-only gradients:
;gpz1: 10-15%
;use gradient files:
(topspin 2.1)
;gpnam1: SINE.100
;gpnam3: SINE.100
;gpnam4: SINE.100
```

(Topspin3.x)
;gpnam1: SMSQ10.100
;gpnam1: SMSQ10.100
;gpnam1: SMSQ10.100