Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Measurement of ^{1}H NMR Relaxation Times in Complex Organic Chemical Systems: Application of PSYCHE

Veera Mohana Rao Kakita,[a] Vaibhav Kumar Shukla,[a] Mandar Bopardikar,[b] Tannistha Bhattacharya,[c] and Ramakrishna V. Hosur[a,b*]

a UM-DAE Centre for Excellence in Basic Sciences,
University of Mumbai, Kalina Campus, Santacruz,
Mumbai 400 098, India
E-mail: hosur@tifr.res.in

b Department of Chemical Sciences,
Tata Institute of Fundamental Research (TIFR),
1-Homi Bhabha Road, Colaba,
Mumbai 400 005, India

c Department of Chemistry
National Institute of Technology, Jamshedpur 831014, India

Experimental details of Inrec and Inrec-PSYCHE recorded for estradiol

Spectral width: 7000 Hz (F2) and 50 Hz (F1)
Number of data points (F2): 8192
Number of decoupling chunks (F1): 32
Recycle delay: 10 s
Number of scans/ Dummy scans: 4/ 4

Inrec		**PSYCHE-Inrec**	
Delay τ	Experimental time	Delay τ	Experimental time
0.0 s	1 min 24 s	0.0 s	24 min 6 s
0.2 s	1 min 26 s	0.2 s	24 min 33 s
0.4 s	1 min 28 s	0.4 s	24 min 59 s
0.6 s	1 min 29 s	0.6 s	25 min 26 s
0.8 s	1 min 31 s	0.8 s	25 min 52 s
1.0 s	1 min 32 s	1.0 s	26 min 18 s
1.2 s	1 min 34 s	1.2 s	26 min 45 s
1.4 s	1 min 36 s	1.4 s	27 min 11 s
1.6 s	1 min 37 s	1.6 s	27 min 38 s
1.8 s	1 min 39 s	1.8 s	28 min 4 s
2.0 s	1 min 40 s	2.0 s	28 min 30 s
2.2 s	1 min 42 s	2.2 s	28 min 57 s
2.4 s	1 min 44 s	2.4 s	29 min 23 s
Total experimental time	**20 min 22 s**	Total experimental time	**5 h 47 min 42 s**

Experimental details of CPMG and CPMG-PSYCHE recorded for estradiol

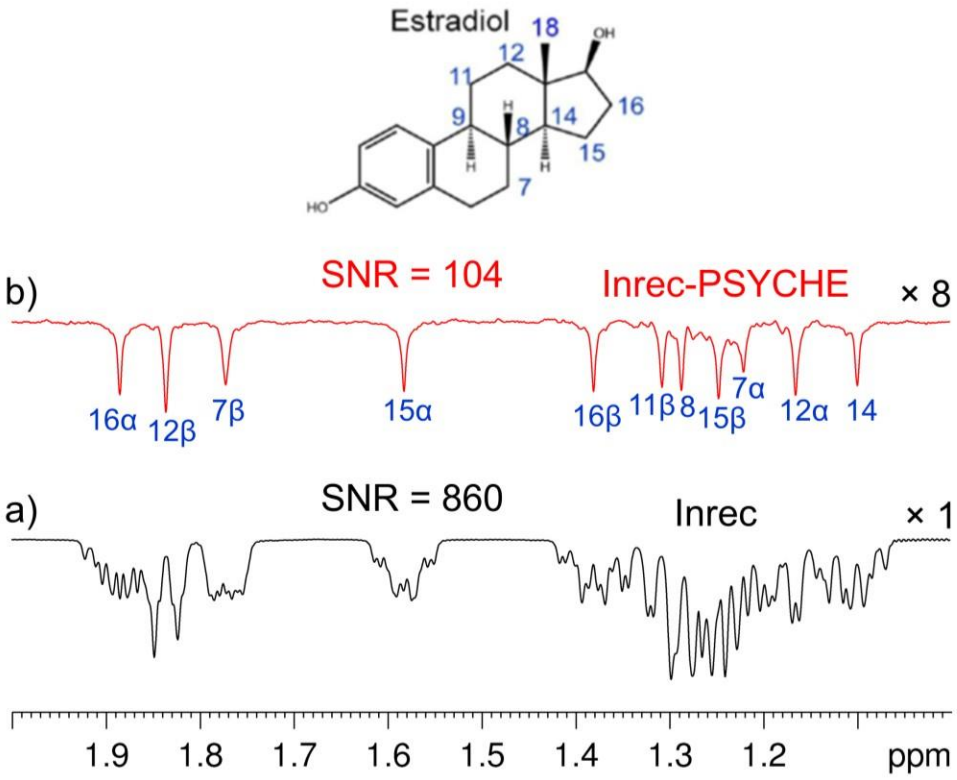
Spectral width: 7000 Hz (F2) and 50 Hz (F1)
Number of data points (F2): 8192
Number of decoupling chunks (F1): 32
Recycle delay: 10 s
Number of scans/ Dummy scans: 4/ 4
τe : 1 ms

CPMG			**CPMG-PSYCHE**		
Number of loops (m)	Delay $\tau = 2\tau_e m$	Experimental time	Number of loops (m)	Delay $\tau = 2\tau_e m$	Experimental time
100	0.2 s	1 min 26 s	100	0.2 s	24 min 33 s
200	0.4 s	1 min 28 s	200	0.4 s	25 min 0 s
300	0.6 s	1 min 29 s	300	0.6 s	25 min 26 s
400	0.8 s	1 min 31 s	400	0.8 s	25 min 53 s
500	1.0 s	1 min 33 s	500	1.0 s	26 min 20 s
600	1.2 s	1 min 34 s	600	1.2 s	26 min 46 s
700	1.4 s	1 min 36 s	700	1.4 s	27 min 13 s
800	1.6 s	1 min 37 s	800	1.6 s	27 min 39 s
900	1.8 s	1 min 39 s;	900	1.8 s	28 min 6 s
1000	2.0 s	1 min 41 s	1000	2.0 s	28 min 33 s
1200	2.4 s	1 min 44 s	1200	2.4 s	29 min 26 s
Total experimental time		**16 min 18 s**	Total experimental time		**4 h 54 min 55 s**

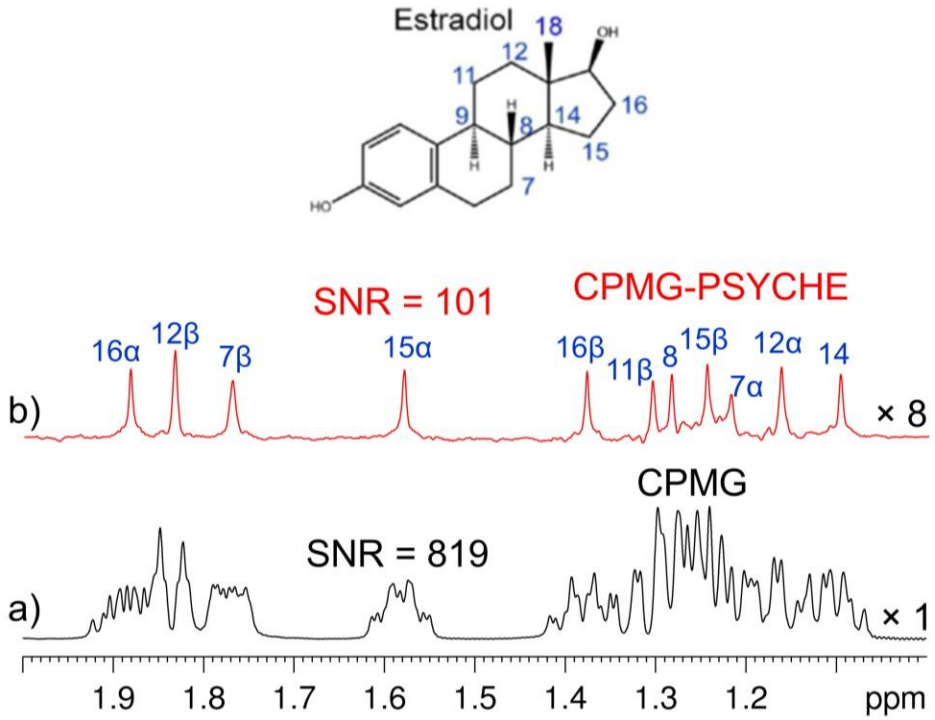
Experimental details of Inrec-PSYCHE/ CPMG-PSYCHE recorded for Naringin/ Naringin+HSA

Spectral width: 7000 Hz (F2) and 50 Hz (F1)
Number of data points (F2): 8192
Number of decoupling chunks (F1): 32
Recycle delay: 10 s
Number of scans/ Dummy scans: 4/ 4
τe : 1 ms

Inrec-PSYCHE		**CPMG-PSYCHE**		
Delay τ	Experimental time	Number of loops (m)	Delay $\tau = 2\tau_e m$	Experimental time
0.005 s	24 min 7 s	4	0.008 s	24 min 8 s
0.1 s	24 min 20 s	50	0.1 s	24 min 20 s
0.3 s	24 min 46 s	100	0.2 s	24 min 33 s
0.4 s	24 min 59 s	200	0.4 s	25 min 0 s
0.75 s	25 min 46 s	400	0.8 s	25 min 53 s
2.0 s	28 min 31 s	600	1.2 s	26 min 46 s
5.0 s	35 min 7 s	1000	2.0 s	28 min 33 s
Total experimental time	**3 h 7 min 36 s**	Total experimental time		**3 h 1 min 13 s**



Supporting Figure-1: Comparison of the Inrec spectra recorded (at τ =0 s) for estradiol molecule (10 mg dissolved in 0.5 ml of DMSO-D_6) in conventional (a) and PSYCHE-decoupling (b) schemes. Herein, SNR values are calculated for the well separated H15α resonance of estradiol, which reveals that the measured SNR values of Inrec-PSYCHE is about ~12 % with respect to the conventional-Inrec. However, in reality, the SNR of Inrec-PSYCHE per unit measurement time would be only about ~2% when compared to the conventional-Inrec.



Supporting Figure-2: Comparison of the CPMG spectra recorded (at τ =0 s) for estradiol molecule (10 mg dissolved in 0.5 ml of DMSO-D_6) in conventional (a) and PSYCHE-decoupling (b) schemes. Herein, SNR values are calculated for the well separated H15α resonance of estradiol, which reveals that the measured SNR values of CPMG-PSYCHE is about ~12 % with respect to the conventional-CPMG. However, in reality, the SNR of CPMG-PSYCHE per unit measurement time would be only about 2% when compared to the conventional-CPMG.

Pulse sequence of Inrec-PSYCHE

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

define delay tauA
define delay tauB

"in0=inf1/2"
"p2=p1*2"
"p12=p11+d18"
"tauA=in0/2-p16-d16-50u"
"tauB=(dw*2*cnst4)+d16+50u"
"d12=10u"

"acqt0=-p1*2/3.1416"

1 ze
2 30m pl1:f1
  d1
  p2 ph1
  d7
  p1 ph2
d0
tauA
50u UNBLKGRAD
p16:gp1
d16
p2 ph5
50u
p16:gp1
d16
tauA
p17:gp2
d17
10u pl0:f1
tauB
( center (p12:gp12) (p11:sp11 ph4):f1 )
d16
p17:gp2
d17
d0
50u BLKGRAD
4 go=2 ph31
 30m mc #0 to 2 F1QF(id0)
exit

ph1=0 2
ph2=0 0 2 2 1 1 3 3
ph4=0
ph5=0
ph31=0 0 2 2 1 1 3 3
```

Pulse sequence of CPMG-PSYCHE

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

define delay tauA
define delay tauB

"in0=inf1/2"
"p2=p1*2"
"p12=p11+d18"
"tauA=in0/2-p16-d16-50u"
"tauB=(dw*2*cnst4)+d16+50u"
"d12=10u"

1 ze
2 30m pl1:f1
  d1
  p1 ph1
3 d20
  p2 ph2
  d20
  lo to 3 times l4
d0
tauA
50u UNBLKGRAD
p16:gp1
d16
p2 ph3
50u
p16:gp1
d16
tauA
p17:gp2
d17
10u pl0:f1
tauB
( center (p12:gp12) (p11:sp11 ph4):f1 )
d16
p17:gp2
d17
d0
50u BLKGRAD

4 go=2 ph31
 30m mc #0 to 2 F1QF(id0)
exit

ph1=0 0 2 2 1 1 3 3
ph2=1 3 1 3 0 2 0 2
ph3=0
ph4=0
ph31=0 0 2 2 1 1 3 3
```