Electronic Supplementary Material (ESI) for Analyst.

Ultra-clean pure shift NMR with optimal water suppression for analysis of aqueous pharmaceutical samples

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Electronic Supporting Information

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Sample information:

1) Bupivacaine HCl: 10.9 mg of bupivacaine hydrochloride from Sigma-Aldrich (lot P500128, catalog # PHR1128-1G) was diluted in 0.55 mL of a mixture of 90% H_2O/10% D_2O (v/v), and this solution was transferred to a 5 mm NMR tube.
2) Aurobasidin A (AbA): Approximately 2 mg of purified AbA from Merck & Co. Inc., Kenilworth, NJ, USA was dissolved in 150 µL of a mixture of CD_3CN:H_2O (*vide* manuscript) and transferred to a 3 mm NMR tube.

NMR parameters and instrumentation:

All data was acquired in a Avance III 600 MHz Bruker instrument equipped with a 5mm TCI cryoprobe at 308 K. 8.0 µs was used for the duration of hard 90° ^{1}H pulses for all experiments. The duration of the SAPPHIRE NOESY pre-stauration, iES and iW5 were approximatelly 1h 12 min, 44min, and 42 min, respectivelly, for the AbA sample. The duration of the double Saltire was set to 30ms, witha bandwidth of 10 kHz and flip angle of 15°, for all pure shift experiments. RSNOB pulses of 37 ms duration (50 Hz bandwidth) were used for all ES experiments. SINE.100 was used for gradient shape in all pure shift experiments, except in the double Saltire element, where RECT.1 was used. 8 scans and 4096 complex points were used in the acquisition of all SAPPHIRE experiments, with 4 increments in the SAPPHIRE dimension (TD2) and 50 chunks (TD1) of 10 ms each. The delay to keep T2 weigting constant between SAPPHIRE increments (d2) was set to 6 ms for all SAPPHIRE experiments. 4 drop points (cnst4) was used for all pure shift experiments.

Data acquisition and processing of SAPPHIRE data follow the same steps as described by Moutzouri *et. al.* [1] The interferogram FIDs were reconstructed with TopSpin 3.x macros available at https://www.nmr.chemistry.manchester.ac.uk/.The reconstruction for SAPPHIRE data is a two-step process: (i) the FID chunks are arrayed to form new FID interferograms, one per SAPPHIRE increment; (ii) each SAPPHIRE increment is added for the final averaged pure shift FID. For TopSpin 4.x the macro “sertoint.ptg” should be used before step (i) to convert the FID file into integer.

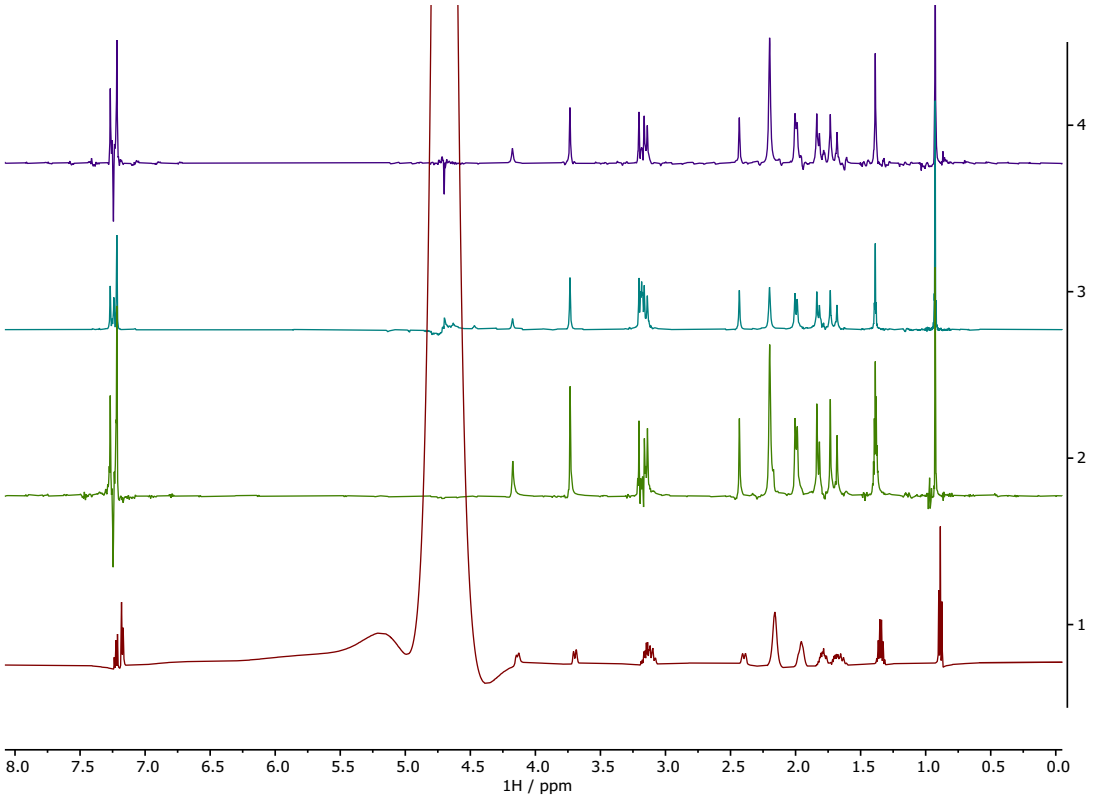

Fig. ESI 1. ^{1}H NMR pure shift spectra of bupivacaine hydrochloride in 90% H2O/10% D2O (v/v) (1) conventional ^{1}H, (2) SAPPHIRE-iW5, (3) SAPPHIRE-iES, and (4) PSYCHE-NOESY-pre-saturation.

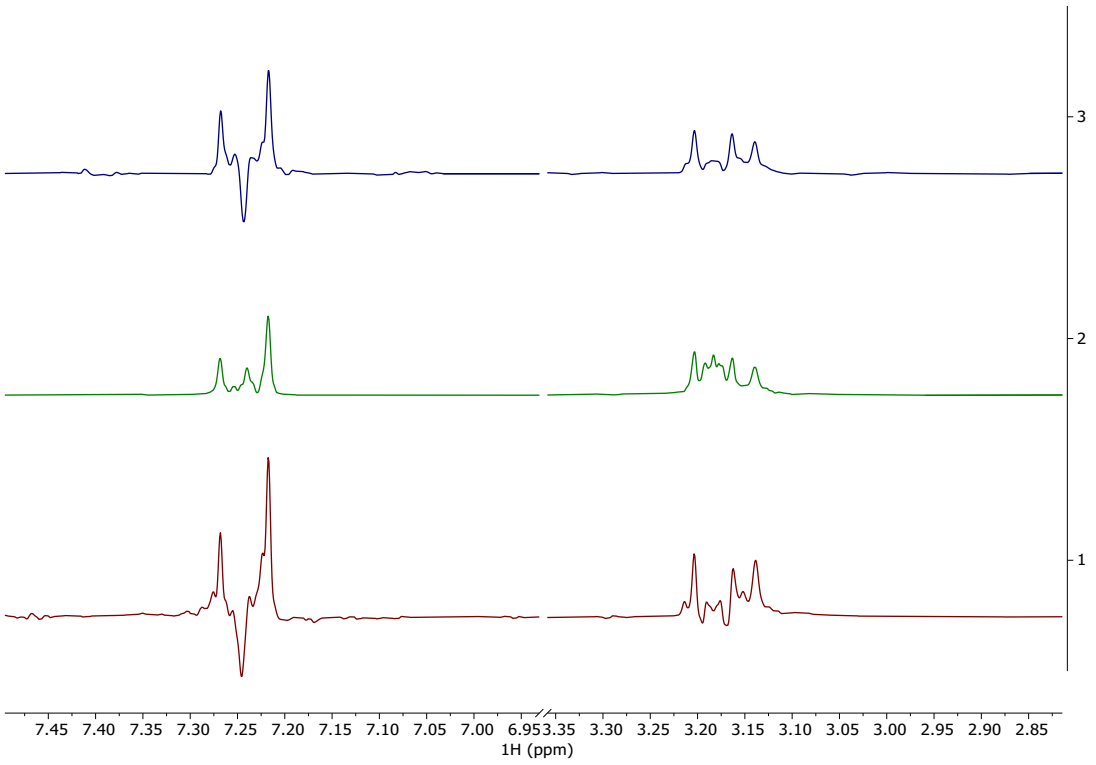

Fig. ESI 2. Zoom of Fig. ESI 1 for strongly coupled signals. (1) SAPPHIRE-iW5, (2) SAPPHIRE-iES, and (3) PSYCHE-NOESY-pre-saturation.

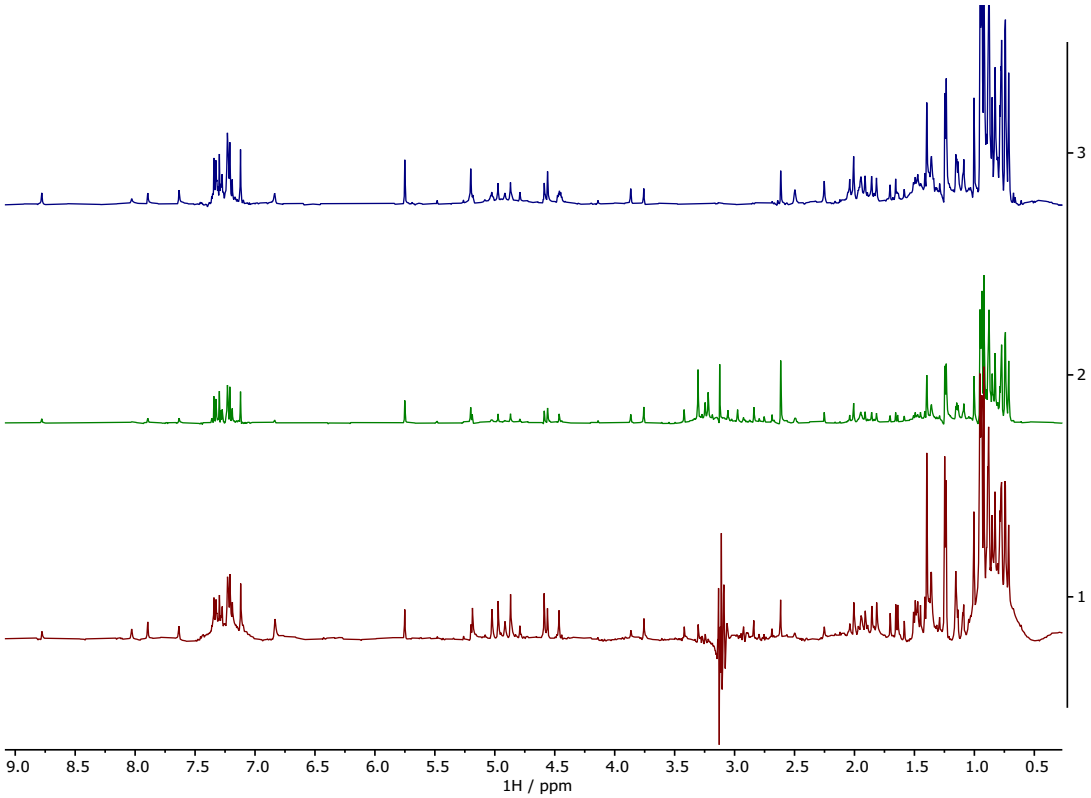

Fig. ESI 3. Full ^{1}H NMR pure shift spectra of Aureobasidin A 10% H_2O/90% CD_3CN for: (1) SAPPHIRE-NOESY-pre-saturation, (2) SAPPHIRE-iES, and (3) SAPPHIRE-iW5.

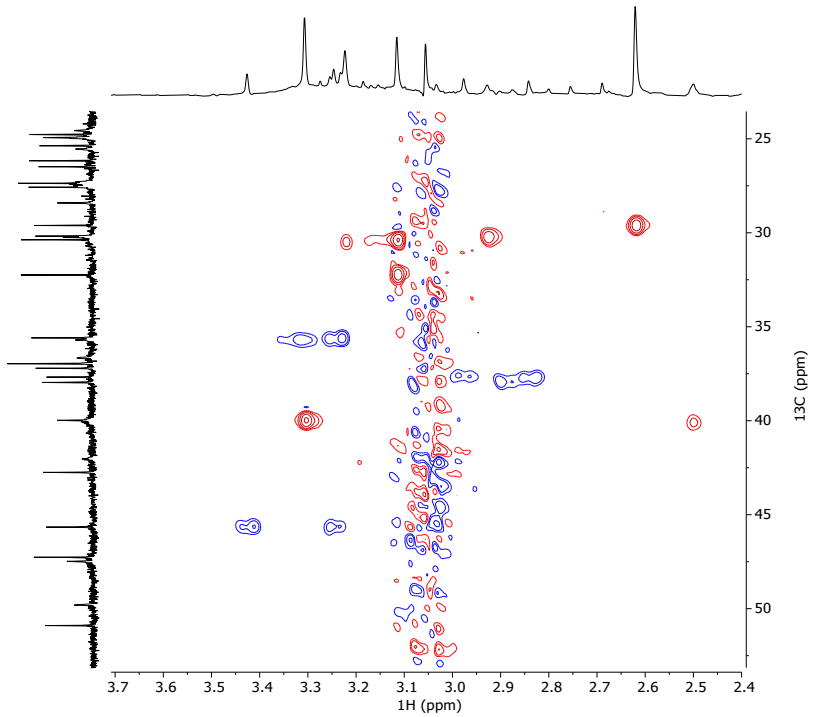

Fig ESI 4. HSQC real-time pure shift with multiplicity editing of Aureobasidin A in 90% H_2O/10% D_2O (v/v). Vertical projection was replaced by $^{13}C\{^{1}H\}$ spectrum and top projection was replaced by SAPPHIRE-iES

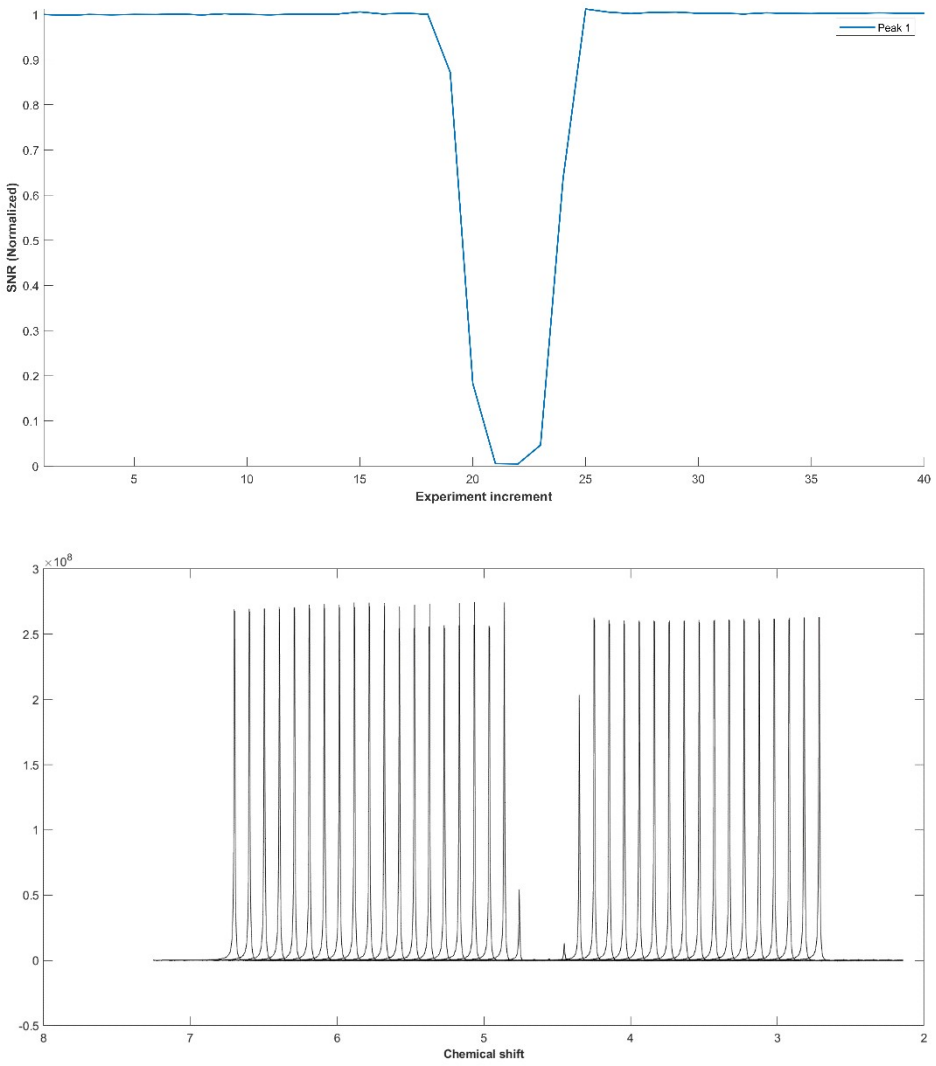

Fig ESI 5. Suppression profiles for the PSYCHE-SAPPHIRE-iES experiment

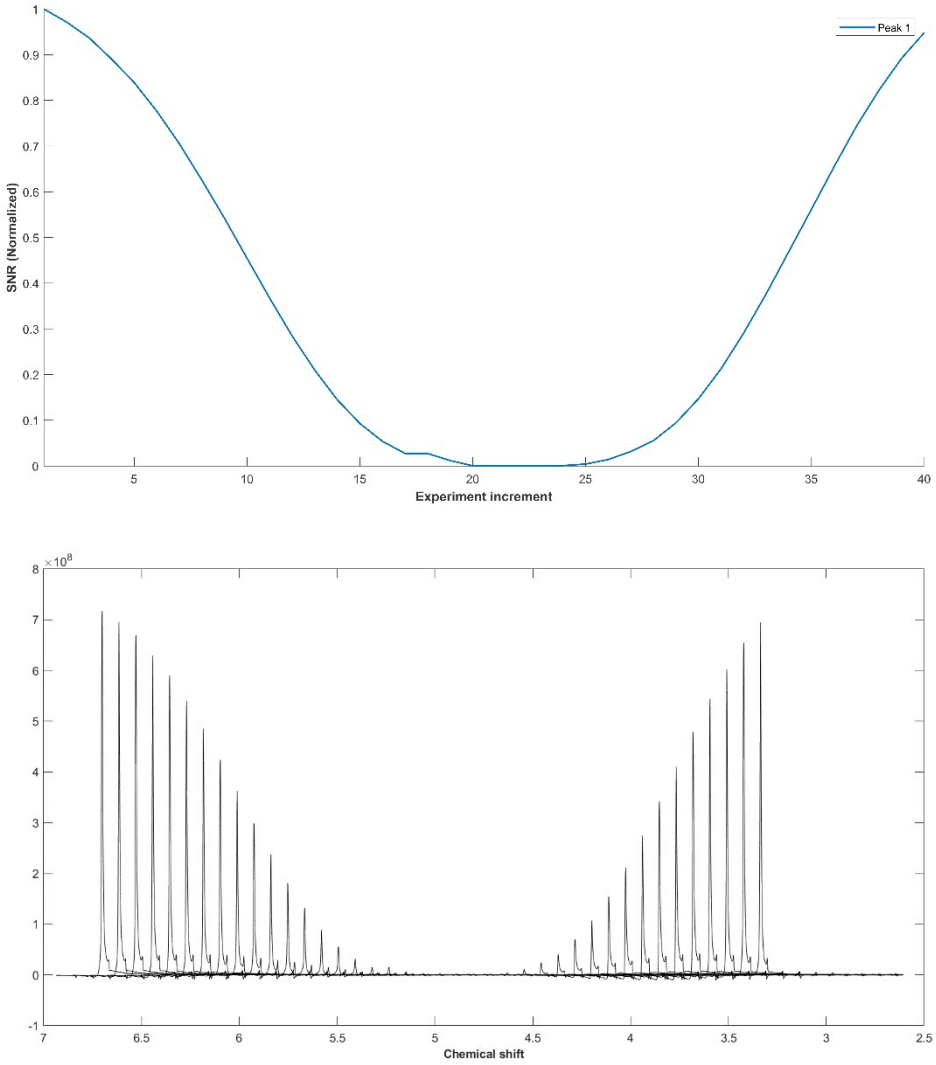

Fig ESI 6. Suppression profiles for the PSYCHE-SAPPHIRE-iW5 experiment

```
;sapphire_es
; updated 21/06/2022 RAHWAY
;
;   Guilherme Dal Poggetto, PhD
;   email: guilherme.dal.poggetto@merck.com
;   Analytical Enabling Capabilities - Rahway, NJ
;
;       Sideband Averaging with Periodic PHase
;       Incrementation of Residual J Evolution
;       for the acquisition of clean PSYCHE pure shift spectra
; with excitation sculpting
;
;       The pulse sequence involves a 3D acquisition scheme.
;       F3 is the direct dimension. F1 is the incremented dimension
for the reconstruction of the pure shift interferogram.
;       F2 is the incremented dimension for the J-evolution.
;
;       The data can be reconstructed using the two following AU
programs (downloaded from: http://nmr.chemistry.manchester.ac.uk)
;               1) pm_pshift (produces pure shift spectra for each
different J-evolution time, adjusting the length of the first chunk
appropriately)
;               2) pm_fidadd (averages the pure shift spectra acquired
with differente J-evolution times)
;
;$CLASS=HighRes
;$DIM=3D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

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

define delay tauA
define delay tauAA
define delay tauB
define delay tauBB
define delay tauBBB
define delay tauBBBB
define delay tauC
define delay tauD

"p2=p1*2"

"l0=0"
"l8=0"

"in0=inf1/2"
"in10=inf2"

"d0=inf1/2"
"d10=inf2"
```

```
"d30=in0/2"
"d40=in0/2-in10"

"cnst5=(td2/2)+1"

"tauA=0"
"tauAA=inf1/4"
"tauB=d2-p17-2*d16-20u"
"tauBB=d2-p17-2*d16-20u-inf2"
"tauBBB=d2-p17-2*d16-20u"
"tauBBBB=d2-p17-2*d16-20u+inf2"
"tauC=inf2"
"tauD=(dw*2*cnst4)"

"cnst50=(cnst20/360)*sqrt((2*cnst21)/(p40/2000000))"
"p30=1000000.0/(cnst50*4)"

"cnst31= (p30/p1) * (p30/p1)"
"spw40=plw1/cnst31"

"p10=p40"

;%%%%%%%%%% WaveMaker Parameters %%%%%%%%%%
"d11=30m+1s/(cnst12)-1s/(cnst12)"
"d11=30m+1s/(cnst13)-1s/(cnst13)"
;sp12:wvm:gdp_rsnob:f1 rsnob(cnst12 Hz, cnst13 ppm; PA=0.5,
NPOINTS=5000);

"d11=30m"

"acqt0=0"
baseopt_echo
aqseq 312

1 ze
2 50m
        d1 pl1:f1
3 50u UNBLKGRAD


 if "l8 < cnst5"
   {
               "tauA=(l8*in10)"
               "tauB=d2-p17-2*d16-20u-(l8*in10)"
               "d30=(in0/2+(l8*in10))+((l0-1)*in0)"
               "tauBBB=(d2-p17-2*d16-20u)-(l8*in10)"

               p1 ph1

               if "l0==0"
                       {
                               tauA
                       }
               else
```

```
        {
                tauAA
        }
                p16:gp1
                d16
                8u
                p2 ph2
                4u pl0:f1
        (p12:sp12 ph5):f1
                4u pl1:f1
                p16:gp1
                d16

if "l0==0"
        {
                tauA
        }
else
        {
                tauAA
        }


if "l0==0"
        {

        }
else
        {
                d30
        }

if "l0==0"
        {
                tauB
        }
else
        {
                tauBBB
        }

                d16
                p17:gp2
                d16
        20u pl0:f1
                ;
        ( center (p40:sp40 ph3):f1 (p10:gp10) )
                ;
        20u pl1:f1
                d16
                p17:gp2
                d16

if "l0==0"
```

```
                        {
                                tauB
                        }
        else
                        {
                                tauBBB
                        }

                                tauD
                                p18:gp3
                                d16 pl0:f1
                                4u
                        (p12:sp12 ph6):f1
                                4u pl1:f1
                                p2 ph4
                                8u
                                p18:gp3
                                d16 BLKGRAD
                if "l0==0"
                        {

                        }
                else
                        {
                                d30
                        }


lab1, goto lab7

        }

else
                {

                "tauC=(in10)+((l8-cnst5)*in10)"
                "tauBB=(d2-p17-2*d16-20u-in10)-((l8-cnst5)*in10)"
                "d40=((in0/2-in10)-((l8-cnst5)*in10))+((l0-1)*in0)"
                "tauBBBB=(d2-p17-2*d16-20u+in10)+((l8-cnst5)*in10)"

                p1 ph1
                if "l0==0"
                        {

                        }
        else
                        {
                                tauAA
                        }
                                p16:gp1
                                d16
                                8u
                                p2 ph2
                                4u pl0:f1
```

```
                (p12:sp12 ph5):f1
                        4u pl1:f1
                        p16:gp1
                        d16
         if "l0==0"
                {

                }
else
                {
                        tauAA
                }

 if "l0==0"
                {

                }
        else
                {
                        d40
                }

        if "l0==0"
                {
                        tauBB
                }
else
                {
                        tauBBBB
                }

                        d16
                        p17:gp2
                        d16
                20u pl0:f1
                        ;
                ( center (p40:sp40 ph3):f1 (p10:gp10) )
                        ;
                20u pl1:f1
                        d16
                        p17:gp2
                        d16
        if "l0==0"
                {
                        tauBB
                }
else
                {
                        tauBBBB
                }

         tauD

        if "l0==0"
```

```
                        {
                                tauC
                        }
        else
                        {

                        }

                                p18:gp3
                                d16 pl0:f1
                                4u
                        (p12:sp12 ph6):f1
                                4u pl1:f1
                                p2 ph4
                                8u
                                p18:gp3
                                d16 BLKGRAD
        if "l0==0"
                        {
                                tauC
                        }
        else
                        {

                        }

   if "l0==0"
                        {

                        }
                else
                        {
                                d40
                        }



lab2, goto lab7
         }

lab7, go=2 ph31
50m mc #0 to 2
        F1QF(calclc(l0,1))
  F2QF(calclc(l8,1))
exit


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

```
;POWER LEVEL
;pl0  : zero power (0W)
;pl1  : power level for pulse (default)
;spw40 : power level of PSYCHE selective pulse

;PULSE DURATION
;p1: high power 90 pulse width
;p2: high power 180 pulse width
;p10 : duration of weak gradient during PSYCHE pulse element
;p12 : duration of water excitation sculpting
;p40 : duration of double-chirp PSYCHE pulse element

;PULSE SHAPE
;spnam12 : file name for the  180 water excitation sculpting
;spnam40: file name for PSYCHE pulse element

;GRADIENT DURATION
;p16: CTP gradient pulse width
;p17: CTP gradient pulse width
;p18: CTP gradient pulse width

;GRADIENT SHAPE
;gpnam1: SINE.100
;gpnam2: SINE.100
;gpnam3: SINE.100
;gpnam10: RECT.1

;GRADIENT STRENGTH
;gpz1  : CTP gradient [77%]
;gpz2  : CTP gradient [49%]
;gpz3  : CTP gradient [63%]
;gpz10 : weak gradient during PSYCHE element (1-4%)
;gpz10 : weak gradient during PSYCHE element (1-4%)

;DELAYS
;d1: relaxation delay; 1-5 * T1
;d16: gradient stabilisation delay
;d2: delay to keep the T2 weighting constant between the pure shift
experiments acquired with different evolution time [greater than
1/4SW1+p16+2*d16]


;CONSTANTS
;cnst4: number of points to drop when collecting FID
;cnst5:(td2/2)+1
;cnst12: bandwidth for selective inversion pulse (in Hz)
;cnst13: chemical shift for selective inversion pulse (in ppm)
;cnst20: desired flip angle for PSYCHE pulse element (degree)
(normally 10-25)
;cnst21: bandwidth of each chirp in PSYCHE pulse element (Hz)
(normally 10000)
```

```
;OTHERS
;td1: number of chunks to be acquired
;td2: number of different J evolution times to be averaged (N)
;ns: 8 * n, total number of scans
;ds: 8, number of dummy scans
;sw1: sw3/n (n must be an integer number)
;sw2: 2*N*sw1 where N is the steps in the SAPPHIRE suppression (this
pulse sequence works when N is an even number)
;2sw3/sw2 should be integer
;in10: 1/sw2
;l8: loop counter for F2 dimension
;l0: loop counter for F1 dimension
;FnMODE1: QF
;FnMODE2: QF
```

```
;sapphire_W5
```

```
; updated 07/06/2022 RAHWAY
;
;   Guilherme Dal Poggetto, PhD
;   email: guilherme.dal.poggetto@merck.com
;   Analytical Enabling Capabilities - Rahway, NJ
;
;       Sideband Averaging with Periodic PHase
;       Incrementation of Residual J Evolution
;       for the acquisition of clean PSYCHE pure shift spectra
;       Hard 180o pulses were replaced by W5 water-saturation
;
;       The pulse sequence involves a 3D acquisition scheme.
;       F3 is the direct dimension. F1 is the incremented dimension
for the reconstruction of the pure shift interferogram.
;       F2 is the incremented dimension for the J-evolution.
;
;       The data can be reconstructed using the two following AU
programs (downloaded from: http://nmr.chemistry.manchester.ac.uk)
;               1) pm_pshift (produces pure shift spectra for each
different J-evolution time, adjusting the length of the first chunk
appropriately)
;               2) pm_fidadd (averages the pure shift spectra acquired
with differente J-evolution times)
;
;$CLASS=HighRes
;$DIM=3D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

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

define delay tauA
define delay tauAA
define delay tauB
define delay tauBB
define delay tauBBB
define delay tauBBBB
define delay tauC
define delay tauD

"p2=p1*2"

"l0=0"
"l8=0"

"in0=inf1/2"
"in10=inf2"

"d0=inf1/2"
"d10=inf2"
"d30=in0/2"
```

```
"d40=in0/2-in10"

"cnst5=(td2/2)+1"

"tauA=0"
"tauAA=inf1/4"
"tauB=d2-p17-2*d16-20u"
"tauBB=d2-p17-2*d16-20u-inf2"
"tauBBB=d2-p17-2*d16-20u"
"tauBBBB=d2-p17-2*d16-20u+inf2"
"tauC=inf2"
"tauD=(dw*2*cnst4)"

"cnst50=(cnst20/360)*sqrt((2*cnst21)/(p40/2000000))"
"p30=1000000.0/(cnst50*4)"

"cnst31= (p30/p1) * (p30/p1)"
"spw40=plw1/cnst31"

"p10=p40"

"d11=d11+cnst7*d11-cnst7*d11"
"d11=d11+cnst29*d11-cnst29*d11"
"cnst28=o1"
"cnst30=(cnst29*bf1)-cnst28"
"cnst27=0"

"p27=1000000.0/(cnst6*4)"
"cnst46= (p27/p1) * (p27/p1)"
"plw18=plw1/cnst46"
"cnst7=18*d19+5.95*p27+4*d12"

"d11=30m"
"d12=20u"
"acqt0=0"
baseopt_echo

aqseq 312

1 ze
2 50m
        d1 pl1:f1
3 50u UNBLKGRAD


 if "l8 < cnst5"
   {
               "tauA=(l8*in10)"
               "tauB=d2-p17-2*d16-20u-(l8*in10)"
               "d30=(in0/2+(l8*in10))+((l0-1)*in0)"
               "tauBBB=(d2-p17-2*d16-20u)-(l8*in10)"

               p1 ph1
```

```
if "l0==0"
        {
                tauA
        }
else
        {
                tauAA
        }
                p16:gp1
                d16 pl18:f1
                d12 fq=cnst30:f1
                d12
                p27*0.087 ph2
                d19*2
                p27*0.206 ph2
                d19*2
                p27*0.413 ph2
                d19*2
                p27*0.778 ph2
                d19*2
                p27*1.491 ph2
                d19*2
                p27*1.491 ph3
                d19*2
                p27*0.778 ph3
                d19*2
                p27*0.413 ph3
                d19*2
                p27*0.206 ph3
                d19*2
                p27*0.087 ph3
                d12 fq=cnst27:f1
                d12 pl1:f1
                p16:gp1
                d16

if "l0==0"
        {
                tauA
        }
else
        {
                tauAA
        }


if "l0==0"
        {

        }
else
        {
                d30
        }
```

```
        if "l0==0"
                {
                        tauB
                }
        else
                {
                        tauBBB
                }

                        d16
                        p17:gp2
                        d16
                20u pl0:f1
                        ;
                ( center (p40:sp40 ph4):f1 (p10:gp10) )
                        ;
                20u pl1:f1
                        d16
                        p17:gp2
                        d16

        if "l0==0"
                {
                        tauB
                }
else
                {
                        tauBBB
                }

                        tauD
                        p18:gp3
                        d16 pl18:f1
                        d12 fq=cnst30:f1
                        d12
                        p27*0.087 ph5
                        d19*2
                        p27*0.206 ph5
                        d19*2
                        p27*0.413 ph5
                        d19*2
                        p27*0.778 ph5
                        d19*2
                        p27*1.491 ph5
                        d19*2
                        p27*1.491 ph6
                        d19*2
                        p27*0.778 ph6
                        d19*2
                        p27*0.413 ph6
                        d19*2
                        p27*0.206 ph6
                        d19*2
```

```
                                p27*0.087 ph6
                                d12 fq=cnst27:f1
                                d12 pl1:f1
                                p18:gp3
                                d16 BLKGRAD
                        if "l0==0"
                                {

                                }
                        else
                                {
                                        d30
                                }


lab1, goto lab7

        }

else
                        {

                        "tauC=(in10)+((l8-cnst5)*in10)"
                        "tauBB=(d2-p17-2*d16-20u-in10)-((l8-cnst5)*in10)"
                        "d40=((in0/2-in10)-((l8-cnst5)*in10))+((l0-1)*in0)"
                        "tauBBBB=(d2-p17-2*d16-20u+in10)+((l8-cnst5)*in10)"

                        p1 ph1
                        if "l0==0"
                                {

                                }
         else
                                {
                                        tauAA
                                }
                                        p16:gp1
                                        d16 pl18:f1
                                        d12 fq=cnst30:f1
                                        d12
                                        p27*0.087 ph2
                                        d19*2
                                        p27*0.206 ph2
                                        d19*2
                                        p27*0.413 ph2
                                        d19*2
                                        p27*0.778 ph2
                                        d19*2
                                        p27*1.491 ph2
                                        d19*2
                                        p27*1.491 ph3
                                        d19*2
                                        p27*0.778 ph3
                                        d19*2
```

```
                        p27*0.413 ph3
                        d19*2
                        p27*0.206 ph3
                        d19*2
                        p27*0.087 ph3
                        d12 fq=cnst27:f1
                        d12 pl1:f1
                        p16:gp1
                        d16
        if "l0==0"
                {

                }
else
                {
                        tauAA
                }

 if "l0==0"
                {

                }
       else
                {
                        d40
                }

       if "l0==0"
                {
                        tauBB
                }
else
                {
                        tauBBBB
                }

                        d16
                        p17:gp2
                        d16
                20u pl0:f1
                        ;
                ( center (p40:sp40 ph4):f1 (p10:gp10) )
                        ;
                20u pl1:f1
                        d16
                        p17:gp2
                        d16
       if "l0==0"
                {
                        tauBB
                }
else
                {
                        tauBBBB
```

```
                        }

                 tauD

                if "l0==0"
                        {
                                tauC
                        }
        else
                        {

                        }

                                p18:gp3
                                d16 pl18:f1
                                d12 fq=cnst30:f1
                                d12
                                p27*0.087 ph5
                                d19*2
                                p27*0.206 ph5
                                d19*2
                                p27*0.413 ph5
                                d19*2
                                p27*0.778 ph5
                                d19*2
                                p27*1.491 ph5
                                d19*2
                                p27*1.491 ph6
                                d19*2
                                p27*0.778 ph6
                                d19*2
                                p27*0.413 ph6
                                d19*2
                                p27*0.206 ph6
                                d19*2
                                p27*0.087 ph6
                                d12 fq=cnst27:f1
                                d12 pl1:f1
                                p18:gp3
                                d16 BLKGRAD
        if "l0==0"
                        {
                                tauC
                        }
        else
                        {

                        }

  if "l0==0"
                        {

                        }
                else
```

```
                        {
                                d40
                        }


lab2, goto lab7
          }

lab7, go=2 ph31
50m mc #0 to 2
        F1QF(calclc(l0,1))
  F2QF(calclc(l8,1))
exit


ph1 =0 0 0 0 0 0 0 0 2 2 2 2 2 2 2 2 0 0 0 0 0 0 0 0 2 2 2 2 2 2 2 2
ph2 =0 0 1 1 0 0 1 1 0 0 1 1 0 0 1 1 0 0 1 1 0 0 1 1 0 0 1 1 0 0 1 1
ph3 =2 2 3 3 2 2 3 3 2 2 3 3 2 2 3 3 2 2 3 3 2 2 3 3 2 2 3 3 2 2 3 3
ph4 =0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 2 3 2 3 2 3 2 3 2 3 2 3 2 3 2 3
ph5 =0 0 0 0 1 1 1 1 0 0 0 0 1 1 1 1 0 0 0 0 1 1 1 1 0 0 0 0 1 1 1 1
ph6 =2 2 2 2 3 3 3 3 2 2 2 2 3 3 3 3 2 2 2 2 3 3 3 3 2 2 2 2 3 3 3 3

ph31=0 2 2 0 2 0 0 2 2 0 0 2 0 2 2 0 0 2 2 0 2 0 0 2 2 0 0 2 0 2 2 0


;POWER LEVEL
;pl0  : zero power (0W)
;pl1  : power level for pulse (default)
;pl18 : power level for 3-9-19-pulse (watergate)
;spw40 : power level of PSYCHE selective pulse

;PULSE DURATION
;p1: high power 90 pulse width
;p2: high power 180 pulse width
;p10 : duration of weak gradient during PSYCHE pulse element
;p27 : 90 degree pulse at pl18
;p40 : duration of double-chirp PSYCHE pulse element

;PULSE SHAPE
;spnam40: file name for PSYCHE pulse element

;GRADIENT DURATION
;p16: CTP gradient pulse width
;p17: CTP gradient pulse width
;p18: CTP gradient pulse width

;GRADIENT SHAPE
;gpnam1: SINE.100
;gpnam2: SINE.100
;gpnam3: SINE.100
;gpnam10: RECT.1

;GRADIENT STRENGTH
```

```
;gpz1  : CTP gradient [77%]
;gpz2  : CTP gradient [49%]
;gpz3  : CTP gradient [63%]
;gpz10 : weak gradient during PSYCHE element (1-4%)

;DELAYS
;d1: relaxation delay; 1-5 * T1
;d16: gradient stabilisation delay
;d2: delay to keep the T2 weighting constant between the pure shift
experiments acquired with different evolution time [greater than
1/4SW1+p16+2*d16]
;d19: delay for binomial water suppression
;     d19 = (1/(2*cnst10)), d = distance of next null (in Hz)


;CONSTANTS
;cnst4: number of points to drop when collecting FID
;cnst5:(td2/2)+1
;cnst6: bandwidth of WATERGATE transfer  [10k - 20k Hz]
;cnst10: distance of next null (in Hz) [2500-5000 Hz]
;cnst17: duration of W5 pulse (in sec)
;cnst20: desired flip angle for PSYCHE pulse element (degree)
(normally 10-25)
;cnst21: bandwidth of each chirp in PSYCHE pulse element (Hz)
(normally 10000)
;cnst29: solvent frequency (in ppm)

;OTHERS
;td1: number of chunks to be acquired
;td2: number of different J evolution times to be averaged (N)
;ns: 8 * n, total number of scans
;ds: 8, number of dummy scans
;sw1: sw3/n (n must be an integer number)
;sw2: 2*N*sw1 where N is the steps in the SAPPHIRE suppression (this
pulse sequence works when N is an even number)
;2sw3/sw2 should be integer
;in10: 1/sw2
;l8: loop counter for F2 dimension
;l0: loop counter for F1 dimension
;FnMODE1: QF
;FnMODE2: QF
```

REFERENCES

(1) P. Moutzouri, Y. Chen, M. Foroozandeh, P. Kiraly, A. R. Phillips, S. R. Coombes, M. Nilsson and G. A. Morris, *Chem Commun* **2017**, *53*, 10188-10191.