KJM 5250 and KJM 9250

SHSQC and SHMBC Experiments with and without Presaturation (CW (PR)) or Excitation Sculpting Solvent Suppression (ES) on AVneo800

Version 5.1

Topspin 4.3

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AVneo800 SHSQC and SHMBC Experiments

1.0 Introduction

aw coded **Neo-800 SHSQC** and **SHMBC** parameter sets are set up with 2K acquired ^{1}H points in F2 and 128 ^{13}C increments in F1.

^{1}H and ^{13}C spectral windows and their mid points should be determined before setting up S**HSQC** or **SHMBC** experiments. The **O1** frequency at which **PR** or **ES** is applied at should be determined accurately in **Hz**, rather than approximately in **ppm**.

Topspin's **getprosol** and **pulsecal** commands should be used to read in **prosol Table** stored **pulse times** and **powers** and adjust them based on your samples solvent and matrix /buffer effects. Optionally, for concentrated samples, but not low level samples, **pulsecal 13c** can be used to adjust ^{13}C pulse times and powers.

Neo-800 aw coded **shsqc135** pp's have been derived from Topspin's **hsqcedetgpsisp2.3** pp with the addition of auto-calculation of **d21** and **d24** from **cnst**2 (= the ^{1}J ^{13}C-^{1}H coupling constant: default value = 145 Hz) and the removal of an optional **p28** trim pulse.

A set of **shsqc135.5q3** experiments with all of their f2 channel **Crp** type pulses replaced by **555 usec** prosol Table linked **Q3.surbop.1** pulses is included in this user guide. The ^{13}C spectral window of these experiments is slightly less than that of **shsqc135,m** experiments.

shmbcq5 experiments are derived from Topspin's **hmbcgplpndqf** experiment with two of its 90 degree ^{13}C f2 channel pulses replaced by prosol table linked **Q5.1000** pulses.

Constant time (CT) **aw** coded **shmbcct** parameter sets are set up with **min/max ^{1}J** coupling constants of **120 Hz** and **170** Hz respectively and an **8 Hz** ^{n}J selection filter .

1.1 Processing

SHSQC45 and SHQC135 experiments are phase sensitive experiments which should be phased before optionally using the **abs1** and **abs2** commands. Low level ^{2}J correlations and some correlations outside the set up ^{13}C SW (F1) range may be observed in S**HSQC** spectra.

SHMBCQ5 spectra are magnitude mode (QF) spectra (phasing not required) and are transformed with **xfb**.

Constant time **SHMBCCT** spectra acquired in echo-antiecho mode are transformed with **xfb** *and* **xf2m.**

The ^{13}C axis resolution of **SHSQC** and **SHMBC** spectra acquired using 128 increments and linearly processed with 512 or 1024 ^{13}C axis points is typically 3-4 times greater than that of standard full window **HSQC** and **HMBC** spectra acquired with 160-256 or more increments.

2.0 SHSQC Experiments and Parameter Sets

The following ^{1}H detected **SHSQC** experiments and parameter sets have been set up on the **Neo-800** spectrometer.

2.1	**shsqc45**	narrow window experiment
2.2	**shsqc135**	narrow window experiment
2.3	**shsqc135pr**	with PR presaturation
2.4	**shsqc135es**	with ES peak suppression
2.5	**shsqc135.m**	medium window experiment
2.6	**shsqc135pr.m**	with PR presaturation
2.7	**shsqc135es.m**	with ES peak suppression
2.8	**shsqc135espr.m**	with ES + PR peak suppression
2.9	**shsqc135.w**	wider window experiment
2.10	**shsqc135pr.w**	with PR presaturation
2.11	**shsqc135es.w**	with ES peak suppression
2.12	**shsqc135.5q3**	medium window experiment
2.13	**shsqc135pr.5q3**	with PR presaturation
2.14	**shsqc135es.5q3**	with ES peak suppression

3.0 SHMBC Experiments and Parameter Sets

The following ^{1}H detected **SHMBC** experiments and parameter sets have been set up on the **Neo-800** spectrometer.

3.1	**shmbcq5**	narrow window experiment
3.2	**shmbcq5pr**	with PR presaturation
3.3	**shmbcq5.m**	medium window experiment
3.4	**shmbcq5pr.m**	with PR presaturation
3.5	**shmbcct**	narrow window experiment
3.6	**shmbcctpr**	with PR presaturation
3.7	**shmbcctes**	with ES peak suppression
3.8	**shmbcct.m**	medium window experiment
3.9	**shmbcctpr.m**	with PR presaturation
3.10	**shmbcctes.m**	with ES peak suppression
3.11	**shmbcctespr.m**	with ES + PR peak suppression
3.12	**shmbcct.w**	wider window experiment
3.13	**shmbcctpr.w**	with PR presaturation
3.14	**shmbcctes.w**	with ES peak suppression

4.0 Appendix How to offset ES from O1 in ESPR experiments

2.1 SHSQC45 Spectrum

Parameter set: **awshsqc45 (+ getprosol + pulsecal)**
Pulse program: **awshsqcetgpsisp2.2-45**
d24 is automatically calculated from **cnst2**
SW(^{13}C) = **15 ppm,** excitation band width is **8-10 ppm**

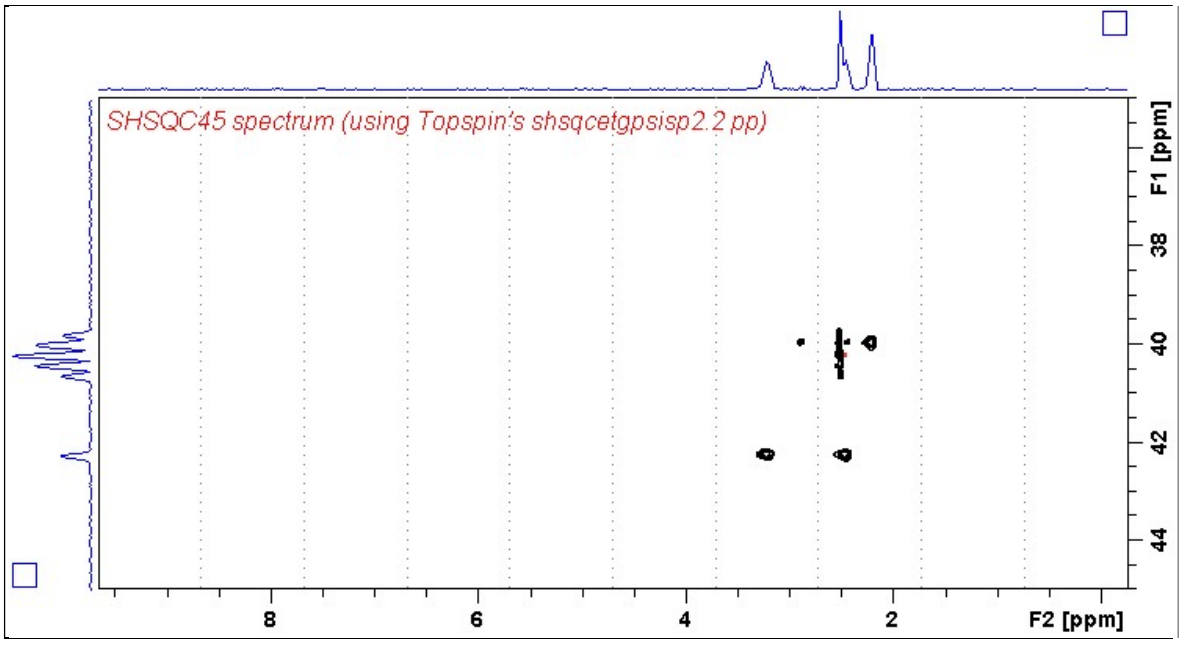
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check gradients and shaped pulses are OK, including a prosol Table defined
p43:sp32 Q3_surbop.1 pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with**: SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC45 spectrum of quinine in D_6-DSMO centered at 40 ppm.

2.2 SHSQC135 Spectrum

Parameter set: **awshsqc135 (+ getprosol + pulsecal)**
Pulse program: **awshsqc135**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **15 ppm;** excitation band width is **8-10 ppm**

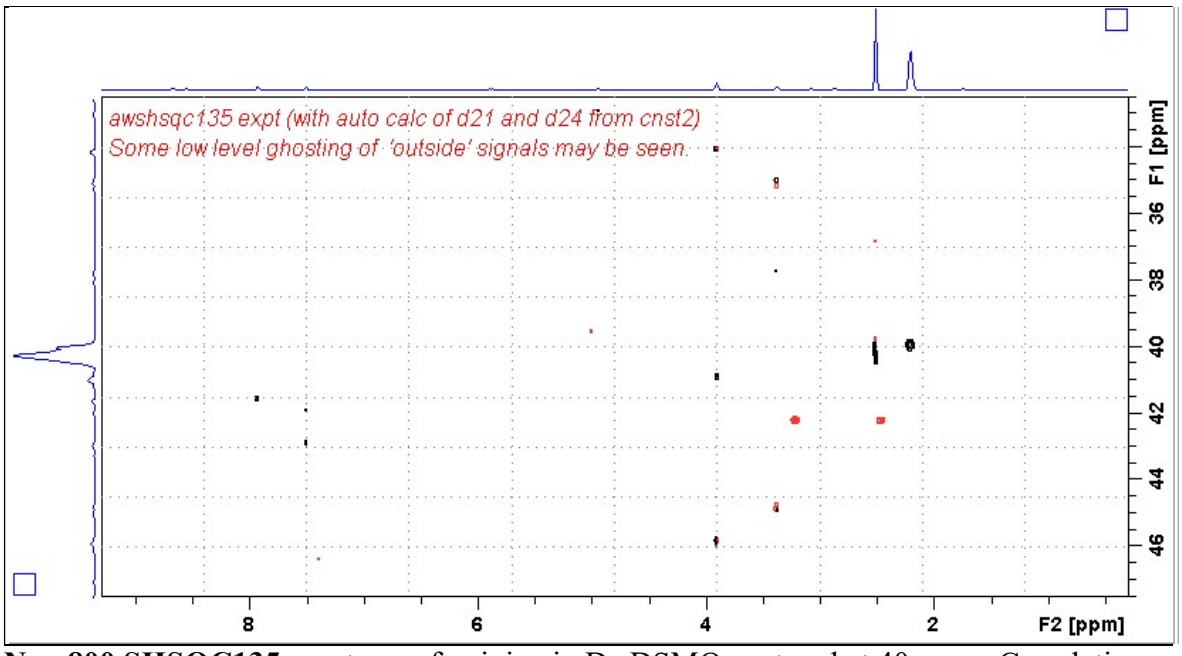
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
p43:sp32 Q3_surbop.1 pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with**: SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135 spectrum of quinine in D_6-DSMO centered at 40 ppm. Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

2.3 SHSQC135pr Spectrum

Parameter set: **awshsqc135pr (+ getprosol + pulsecal)**
Pulse program: **awshsqc135pr**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **15 ppm,** excitation band width is **8-10 ppm**

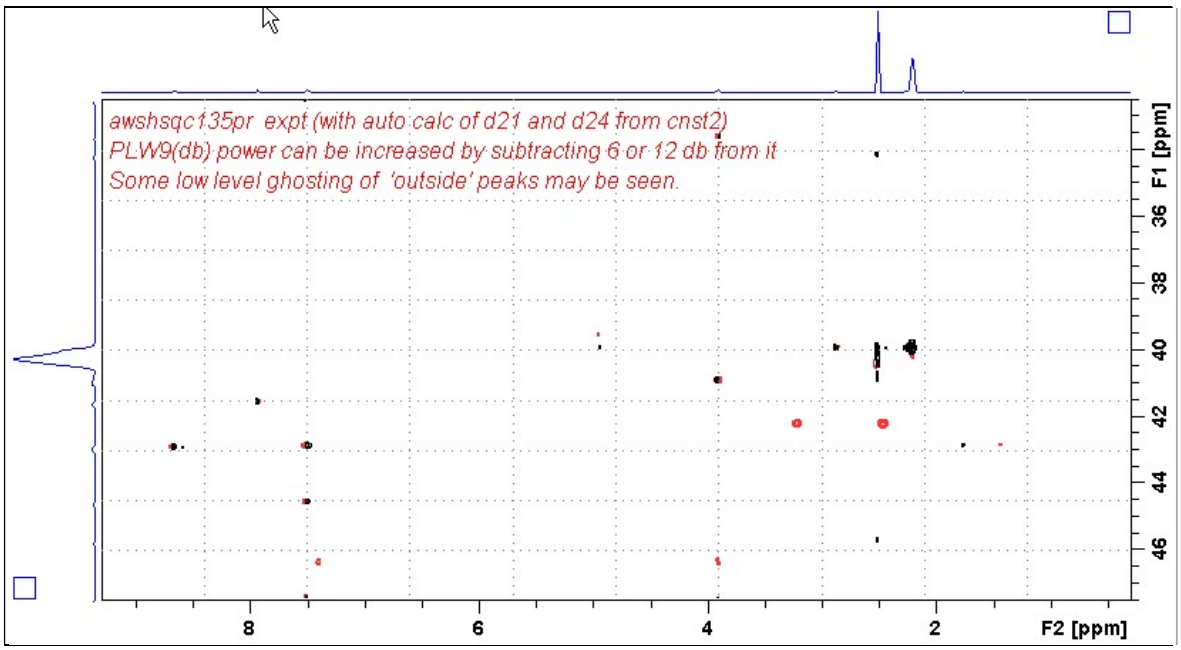
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **PR**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = **128 points.**

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **2 sec** or other time of your choice.
PLW9(db) = **PR** power applied during **D1**. If required the **PR** power can be increased by *subtracting* 6 or 12 db from its prosol Table value.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Check that gradients and shaped pulses are OK, including a prosol Table defined
p43:sp32 Q3_surbop.1 pulse

Set **receiver gain** using **RGA** *(Important!).*

Process with**:** **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135pr spectrum of quinine in D_6-DSMO centered at 40 ppm. Presaturation was applied at the HOD line frequency (3.35 ppm). Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

2.4 SHSQC135es Spectrum

Parameter set: **awshsqc135es (+ getprosol + pulsecal)**
Pulse program: **awshsqc135es**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **15 ppm,** excitation band width is **8-10 ppm**

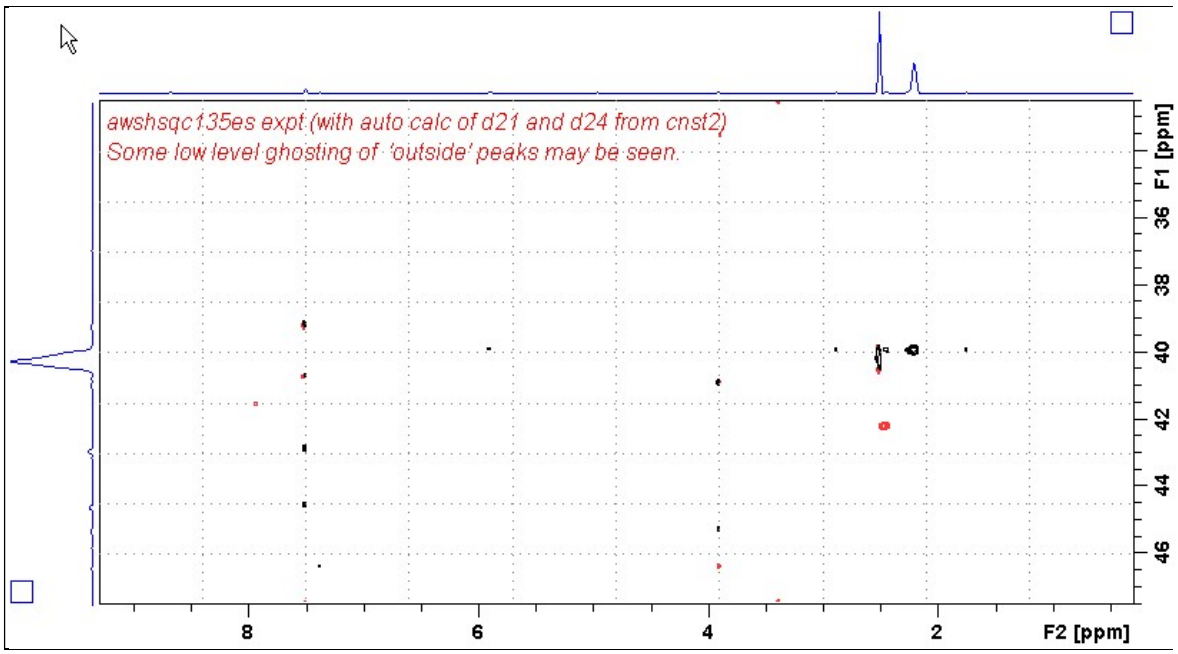
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **ES**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = 128-256 (your choice).

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
2000 usec p40:sp10 Sinc1.1000 ES pulse and a **p43:sp32 Q3_surbop.1** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with**: SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135es spectrum of quinine in D_6-DSMO centered at 40 ppm. **ES** was applied at 3.35 ppm (= the HOD line). ^{1}H signals /correlations located 0.2-0.3 ppm either side of the **ES** suppressed line have reduced intensity. Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

2.5 SHSQC135.m Spectrum

Parameter set: **awshsqc135.m (+ getprosol + pulsecal)**
Pulse program: **awshsqc135.m**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **40 ppm;** excitation band width is ~ **30-34 ppm**

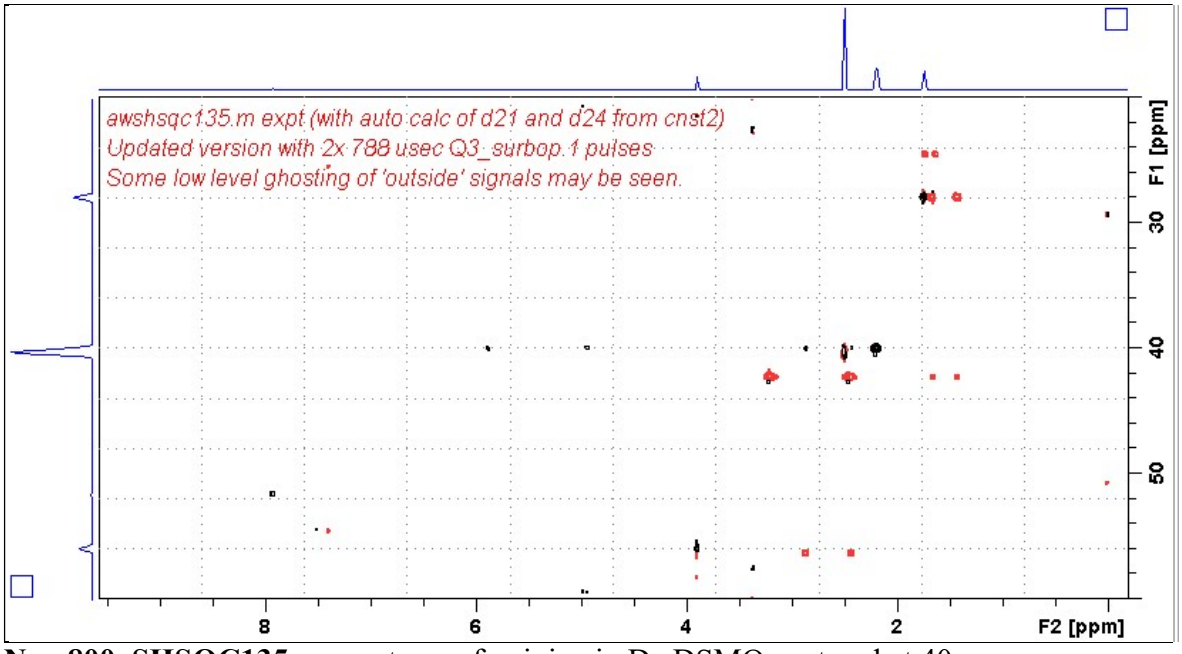
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
p24:sp16 Q3_surbop.1 pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135.m spectrum of quinine in D_6-DSMO centered at 40 ppm.
Correlations at the edges of the ^{13}C spectral window have reduced intensity.

2.6 SHSQC135pr.m Spectrum

Parameter set: **awshsqc135pr.m (+ getprosol + pulsecal)**
Pulse program: **awshsqc135pr.m**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **40 ppm;** excitation band width is **30-34 ppm**

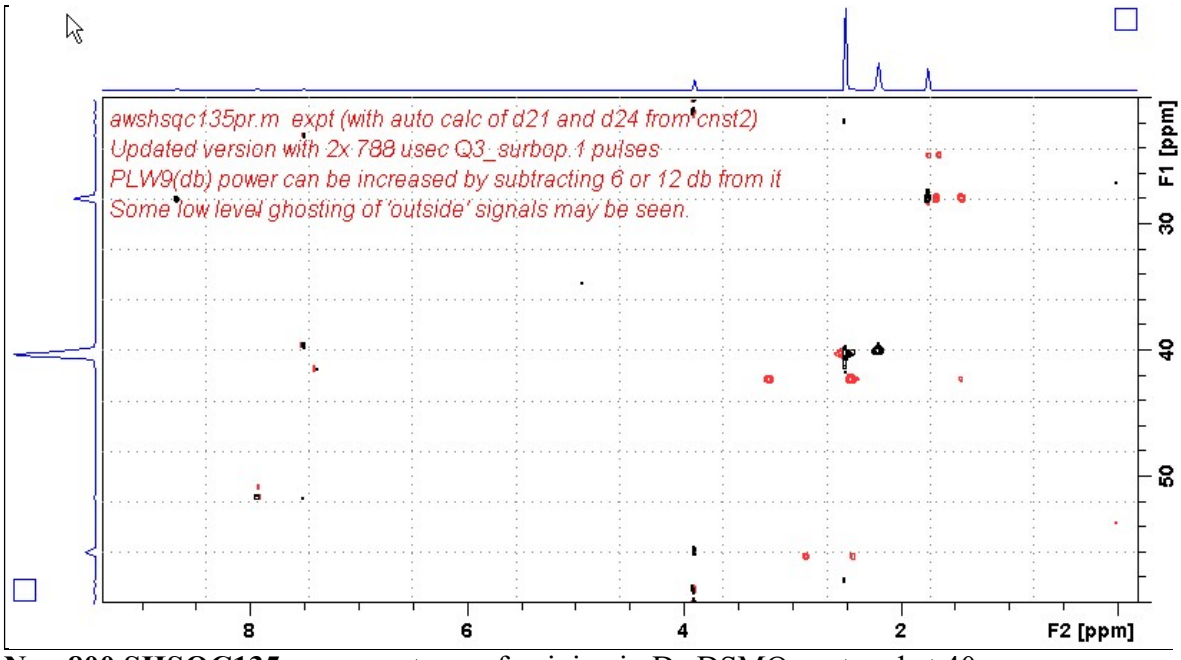
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **PR**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = 128-256 (your choice)**.**

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **2 sec** or other time of your choice.
PLW9(db) = **PR** power applied during **D1**. If required the **PR** power can be increased by *subtracting* 6 or 12 db from its prosol Table value.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined **p24:sp16 Q3_surbop.1** pulse.

.
Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135pr.m spectrum of quinine in D_6-DSMO centered at 40 ppm. Presaturation was applied at the HOD line frequency (3.35 ppm). Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

2.7 SHSQC135es.m Spectrum

Parameter set: **awshsqc135es.m (+ getprosol + pulsecal)**
Pulse program: **awshsqc135es.m**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **40 ppm;** excitation band width is **30-34 ppm**

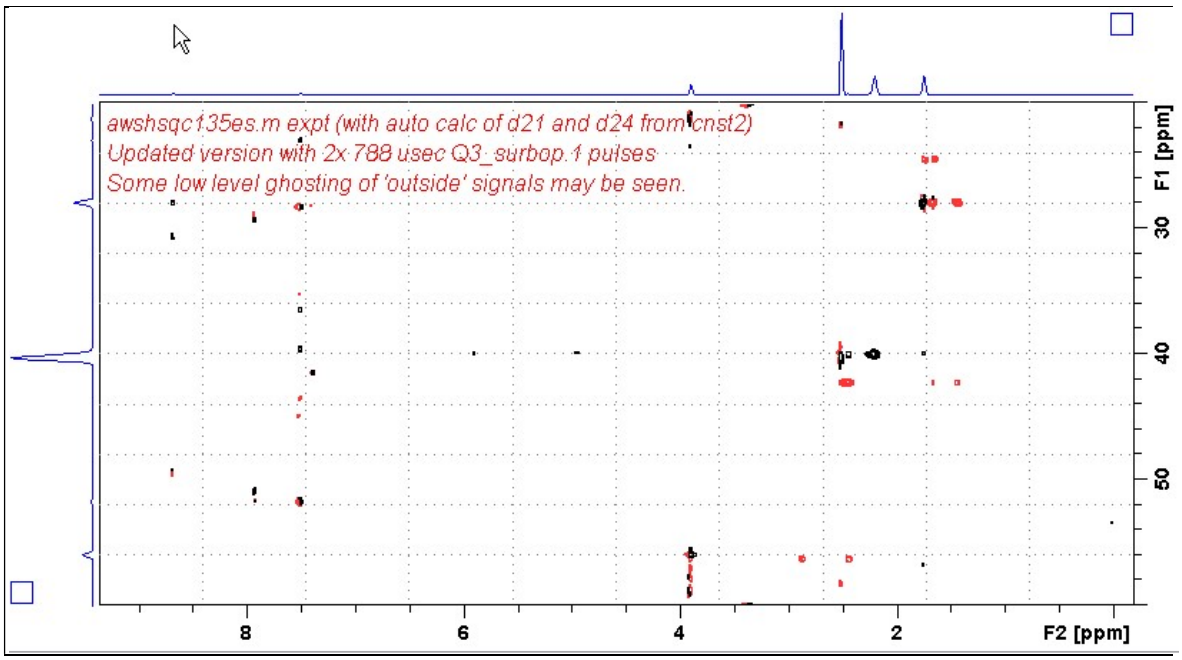
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **ES**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = 128-256 (your choice).

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
2000 usec p12:sp1 Sinc1.1000 ES pulse and a **p24:sp16 Q3_surbop.1** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) =512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135es.m spectrum of quinine in D_6-DSMO centered at 40 ppm. **ES** was applied at 3.35 ppm (= the HOD line). ^{1}H signals /correlations located 0.2-0.3 ppm either side of the **ES** suppressed line have reduced intensity. Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

2.8 SHSQC135espr.m Spectrum

Parameter set: **awshsqc135espr.m (+ getprosol + pulsecal)**
Pulse program: **awshsqc135espr.m**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **40 ppm;** excitation band width is **30-34 ppm**

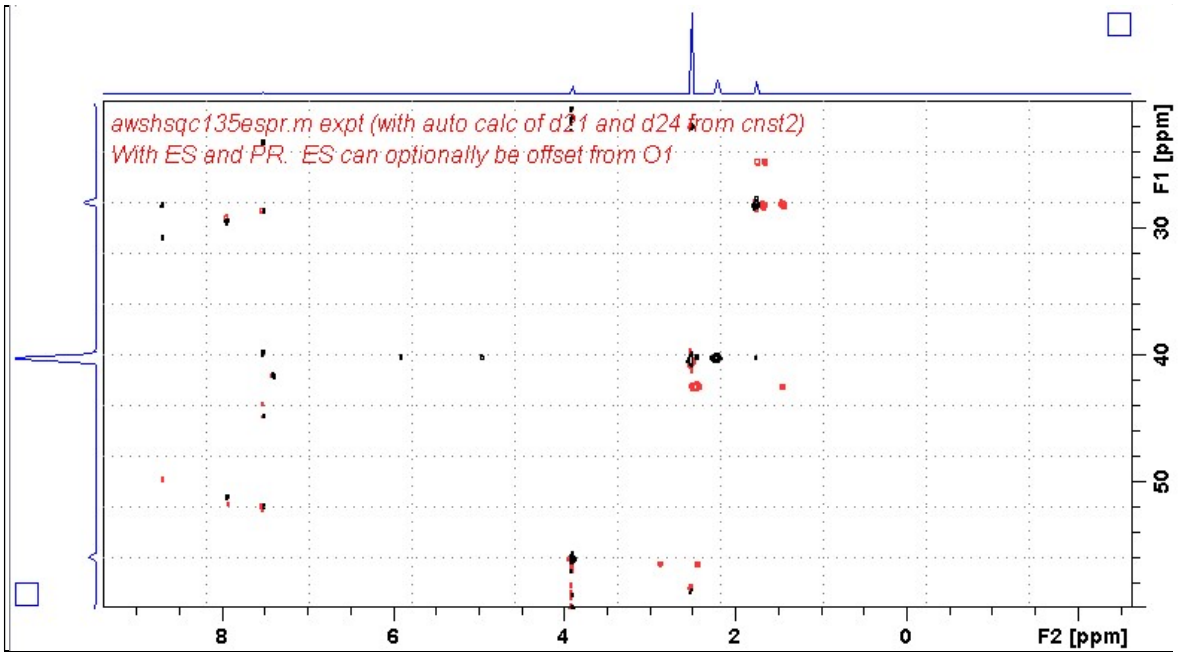
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **ES** and **PR**).
ES can optionally be offset from **PR** as described in the Appendix.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = 128-256 (your choice).

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **2 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).
PLW9(db) = **PR** power applied during **D1**. If required the **PR** power can be increased by *subtracting* 6 or 12 db from its prosol Table value.

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined **2000 usec p12:sp1 Sinc1.1000 ES** pulse and a **p24:sp16 Q3_surbop.1** pulse.
ES can optionally be offset from **PR** at **O1** as described in the Appendix.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) =512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135espr.m spectrum of quinine in D_6-DSMO centered at 40 ppm. **ES** + PR was applied at 3.35 ppm (= the HOD line). ^{1}H signals /correlations located 0.2-0.3 ppm either side of the **ES** suppressed line have reduced intensity. Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

2.9 SHSQC135.w Spectrum

Parameter set: **awshsqc135.w (+ getprosol + pulsecal)**
Pulse program: **awshsqc135.w**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **60 ppm;** excitation band width is **45-50 ppm**

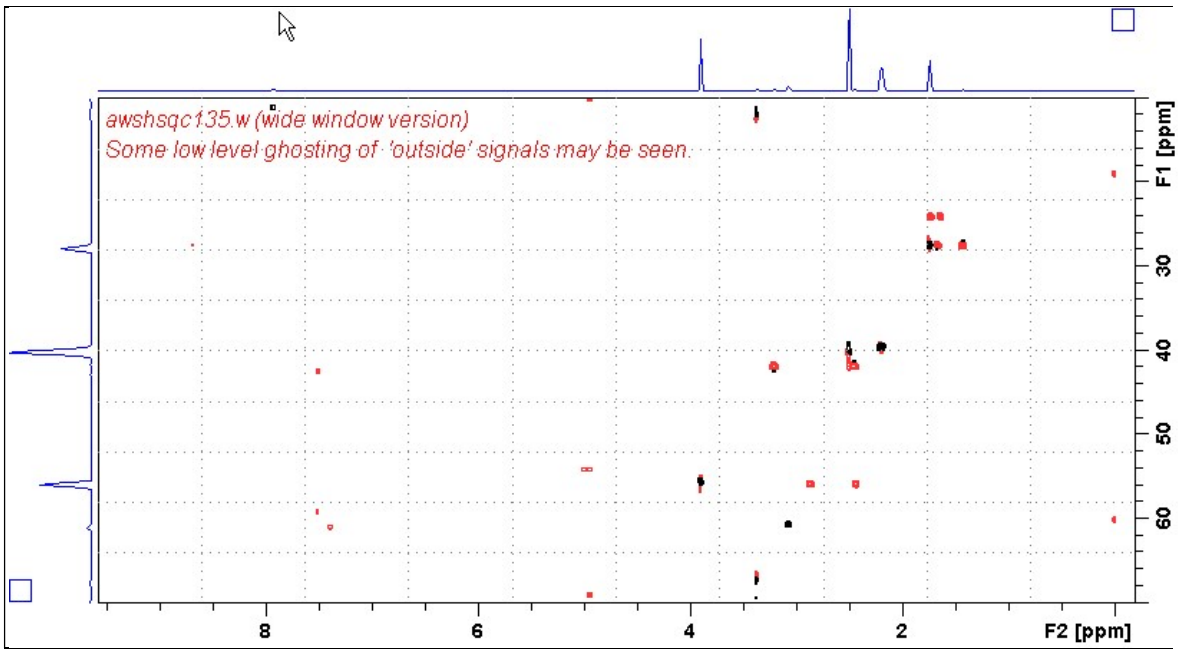
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
p33:sp23 Q3_surbop.1 pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135.w spectrum of quinine in D_6-DSMO centered at 40 ppm.
Correlations at the edges of the ^{13}C spectral window have reduced intensity.

2.10 SHSQC135pr.w Spectrum

Parameter set: **awshsqc135pr.w (+ getprosol + pulsecal)**
Pulse program: **awshsqc135pr.w**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **60 ppm;** excitation band width is **45-50 ppm**

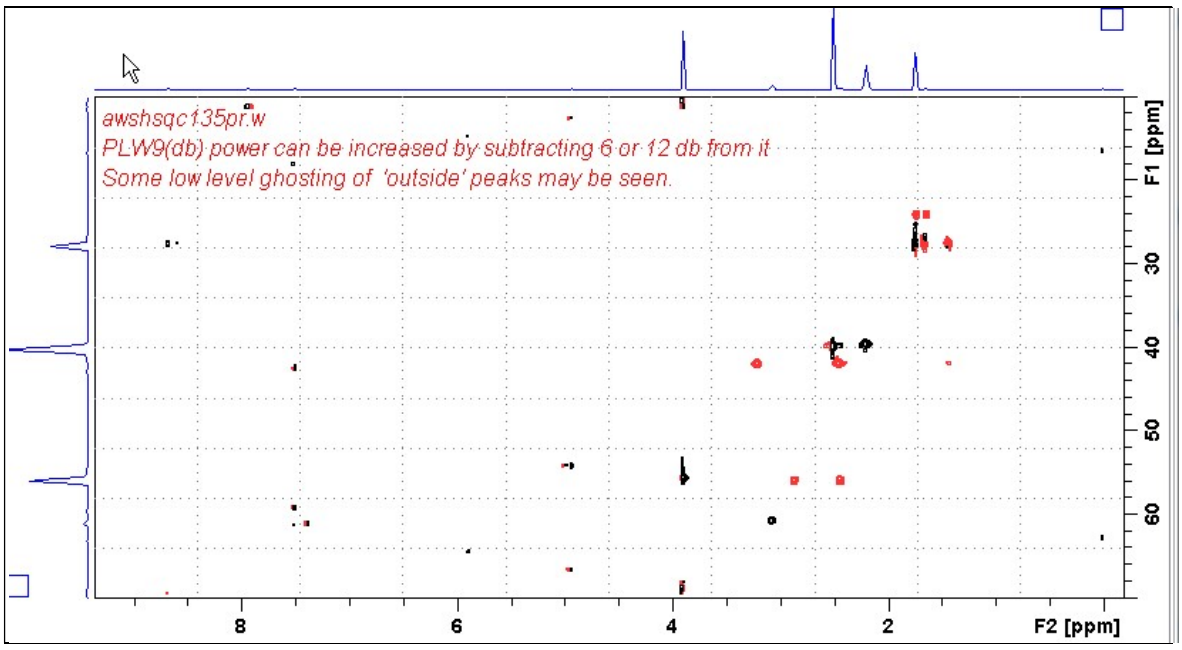
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **PR**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **2 sec** or other time of your choice.
PLW9(db) = **PR** power applied during **D1**. If required the **PR** power can be increased by *subtracting* 6 or 12 db from its prosol Table value.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Check that gradients and shaped pulses are OK, including a prosol Table defined **p33:sp323** Q3 type pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135pr.w spectrum of quinine in D_6-DSMO centered at 40 ppm. Presaturation was applied at the HOD line frequency (3.35 ppm). Correlations at the edges of the ^{13}C spectral window have reduced intensity.

2.11 SHSQC135es.w Spectrum

Parameter set: **awshsqc135esw (+ getprosol + pulsecal)**
Pulse program: **awshsqc135es.w**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **60 ppm;** excitation band width is **45-50 ppm**

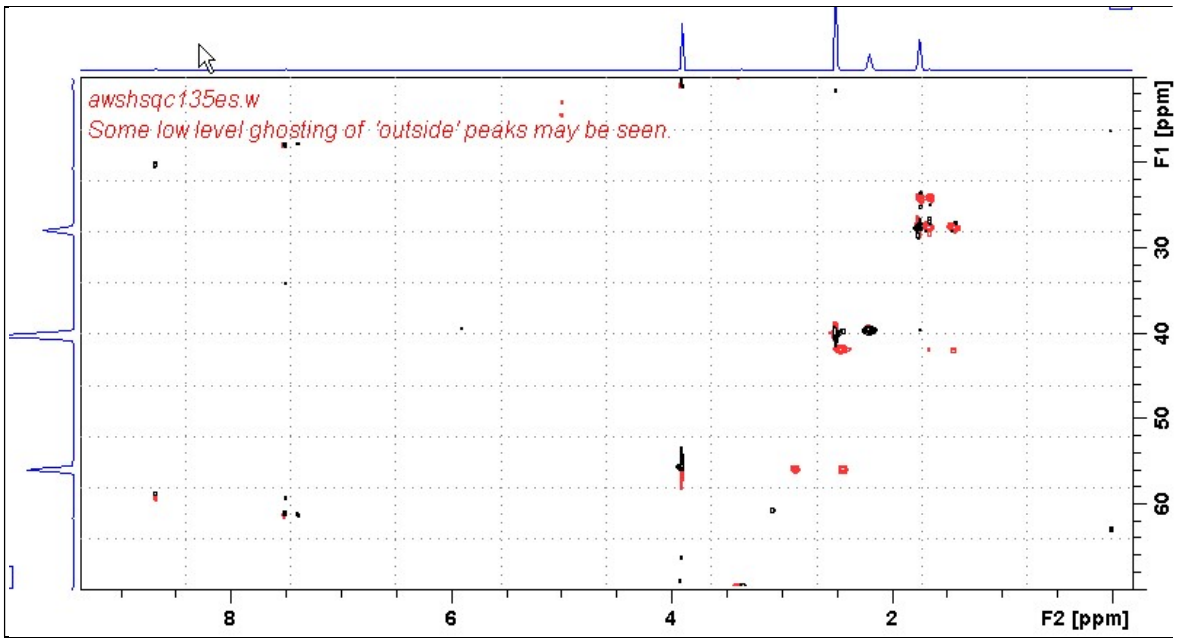
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **ES**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
2000 usec p12:sp1 Sinc1.1000 ES pulse and a **p33:sp23 Q3_surbop.1** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135es.w spectrum of quinine in D_6-DSMO centered at 40 ppm. **ES** was applied at 3.35 ppm (= the HOD line). ^{1}H signals /correlations located 0.2-0.3 ppm either side of the **ES** suppressed line have reduced intensity. Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

2.12 SHSQC135.5q3 Spectrum

Parameter set: **awshsqc135.5q3 (+ getprosol + pulsecal)**
Pulse program: **awshsqc135.5q3**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **40 ppm;** excitation band width is ~ **28-32 ppm**

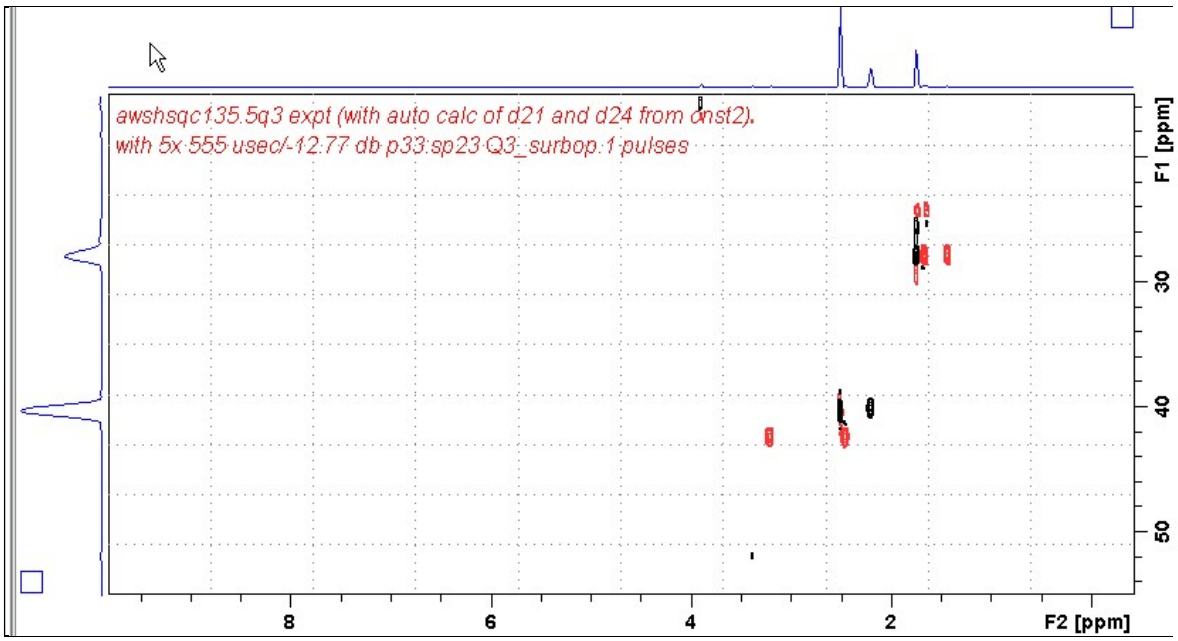
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a **555 usec** prosol Table defined **p33:sp23 Q3_surbop.1** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135.5q3 spectrum of quinine in D_6-DSMO centered at 35 ppm.
Correlations at the edges of the ^{13}C spectral window have reduced intensity.

2.13 SHSQC135pr.5q3 Spectrum

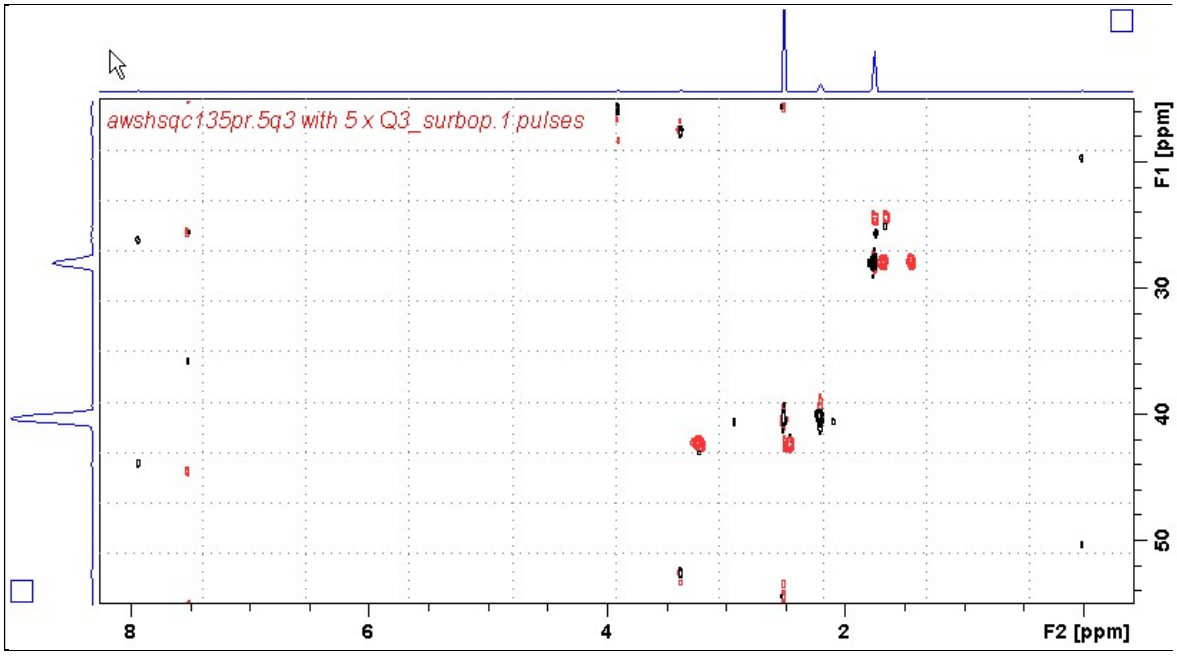
Parameter set: **awshsqc135pr.5q3 (+ getprosol + pulsecal)**
Pulse program: **awshsqc135pr.5q3**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **40 ppm,** excitation band width is **28-32 ppm**

Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **PR**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = **128 points**.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **2 sec** or other time of your choice.
PLW9(db) = **PR power** applied during **D1**. If required the **PR power** can be increased by *subtracting* 6 or 12 db from its prosol Table value.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined **p33:sp23 Q3_surbop.1** pulse.
.
Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135pr.5q3 spectrum of quinine in D_6-DSMO centered at 35 ppm. Presaturation was applied at the DMSO line frequency (2.51 ppm). Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

2.14 SHSQC135es.5q3 Spectrum

Parameter set: **awshsqc135es.5q3 (+ getprosol + pulsecal)**
Pulse program: **awshsqc135es.5q3**
d21 and **d24** are automatically calculated from **cnst2**
SW(^{13}C) = **40 ppm;** excitation band width is **28-32 ppm**

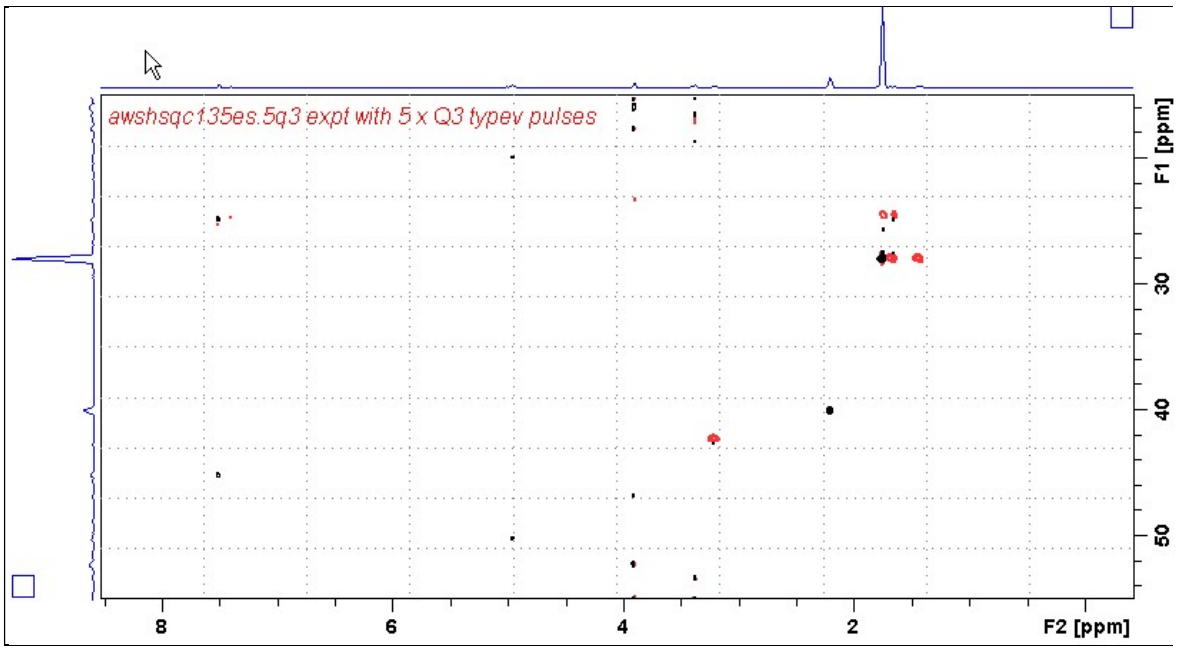
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **ES**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = **128 points.**

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
2000 usec p12:sp1 Sinc1.1000 ES pulse and a **p33:sp23 Q3_surbop.1** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) =512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb, manual phasing and **abs1** + **abs2**



Neo-800 SHSQC135es.5q3 spectrum of quinine in D_6-DSMO centered at 35 ppm. **ES** was applied at the DMSO line (2.51 ppm). ^{1}H signals /correlations located 0.2-0.3 ppm either side of the **ES** suppressed line have reduced intensity. Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

3.1 SHMBCQ5 Spectrum

Parameter set: **awshmbcq5 (+ getprosol + pulsecal)**
Pulse program: **awshmbccq5**
SW(^{13}C) = **20 ppm,** excitation band width is **12-14 ppm**

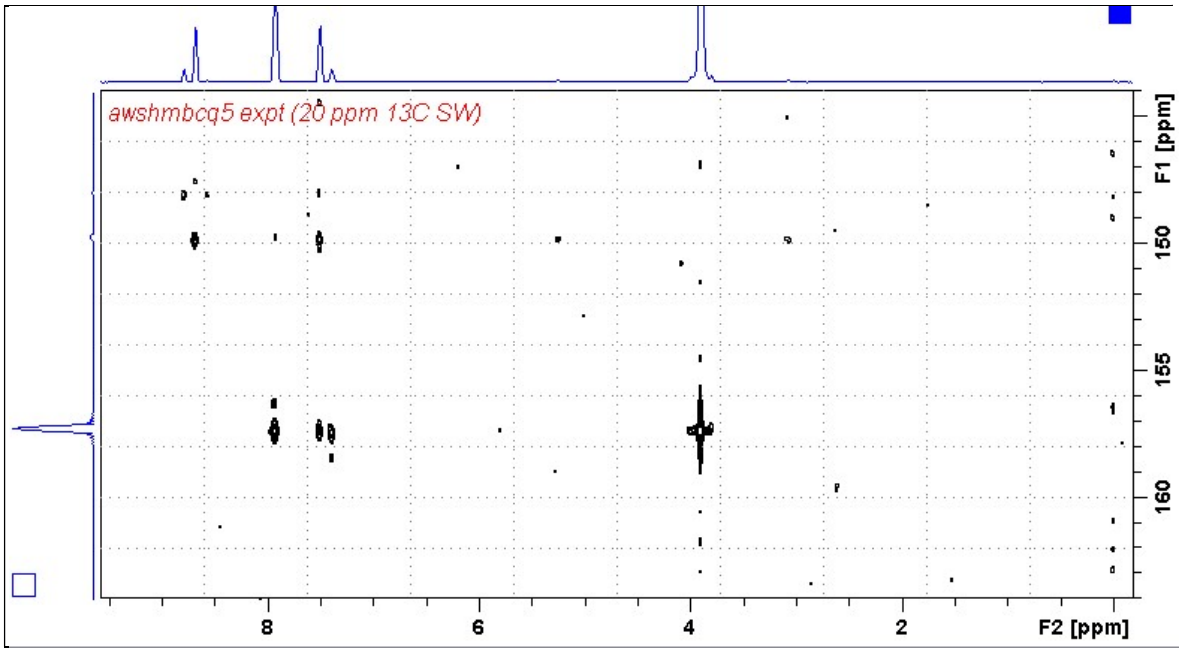
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay =**1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg 125-160 Hz).
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
p35:sp27 Q5.1000 pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = SINE
SSB(F2) = SSB(F1) = 0
xfb *and* **abs1 + abs2**



Neo-800 SHMBCQ5 spectrum of quinine in D_6-DMSO centered at 154 ppm.
Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

3.2 SHMBCQ5pr Spectrum

Parameter set: **awshmbcctpr (+ getprosol + pulsecal)**
Pulse program: **awshmbcctpr**
SW(^{13}C) = **20 ppm,** excitation band width is **12-14 ppm**

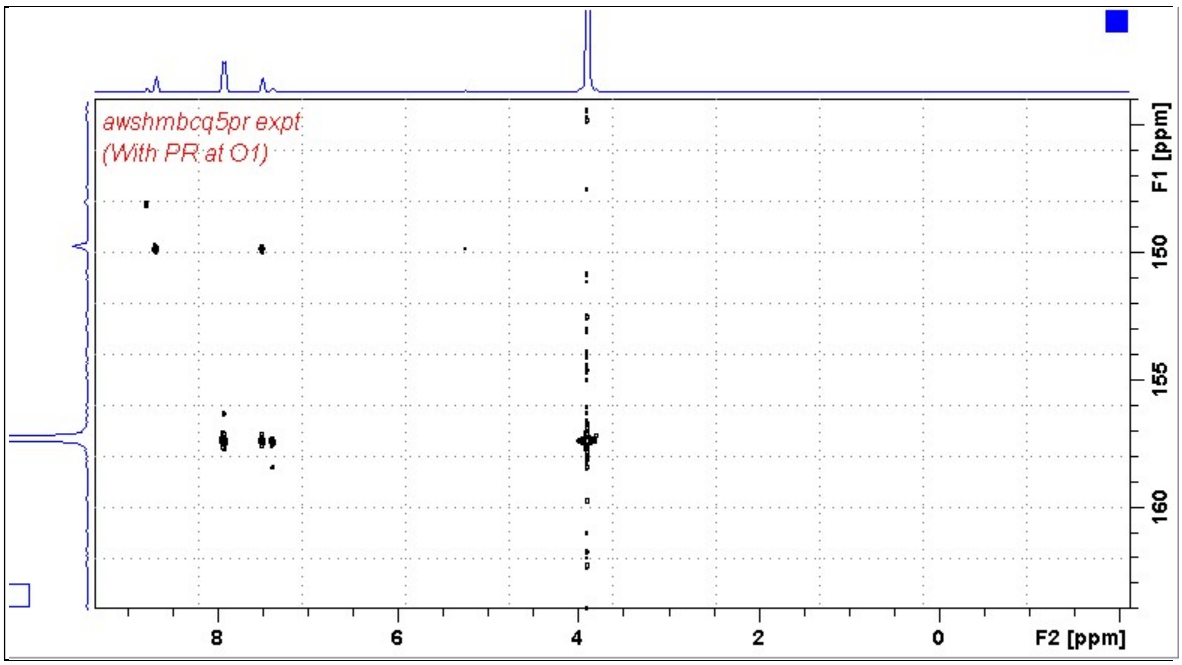
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **PR**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = 128-256 (your choice).

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **2 sec** or other time of your choice
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg 125-160 Hz).
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).
PLW9(db) = **PR** power applied during **D1**. If required the **PR** power can be increased by *subtracting* 6 or 12 db from its prosol Table value.

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined **p35:sp27 Q5.1000** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 1K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = SINE
SSB(F2) = SSB(F1) = 0
xfb *and* **abs1 + abs2**



Neo-800 SHMBCQ5pr spectrum of quinine in D_6-DMSO centered at 154 ppm. Presaturation was applied at the HOD line frequency (3.35 ppm). Correlations at the edges of the ^{13}C spectral window have reduced intensity.

3.3 SHMBCQ5.m Spectrum

Parameter set: **awshmbcq5.m (+ getprosol + pulsecal)**
Pulse program: **awshmbccq5.m**
SW(^{13}C) = **40 ppm,** excitation band width is **30-34 ppm**

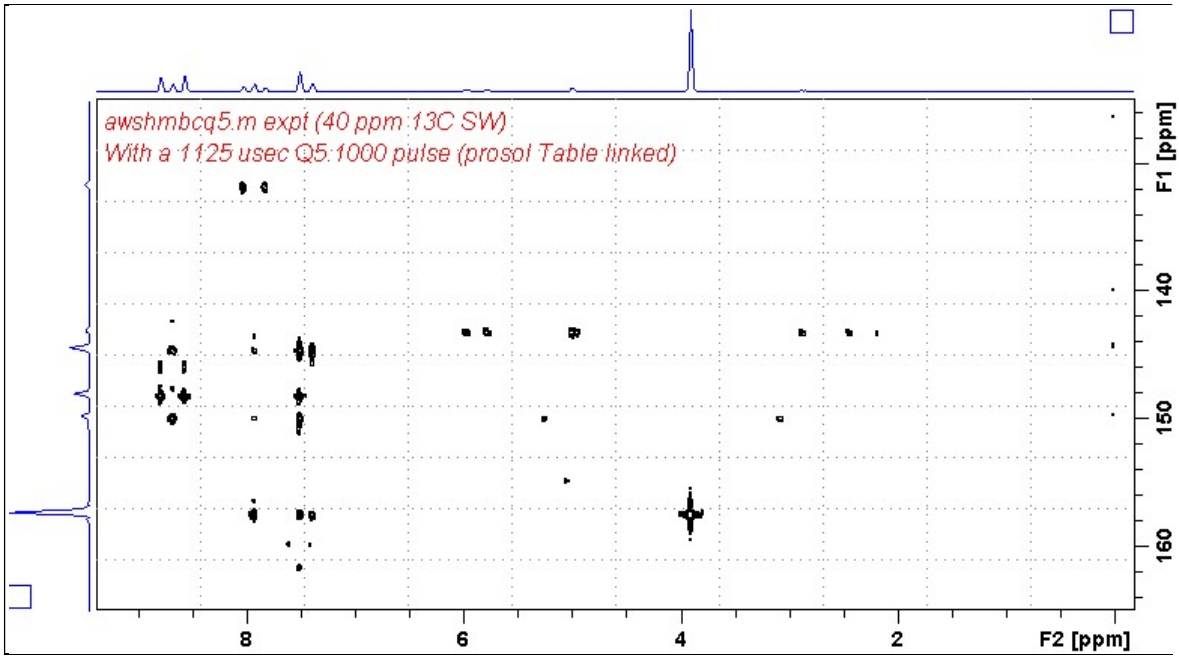
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay =**1.5 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg 125-160 Hz).
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
p23:sp10 Q5.1000 pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = SINE
SSB(F2) = SSB(F1) = 0
xfb *and* **abs1 + abs2**



Neo-800 SHMBCQ5.m spectrum of quinine in D_6-DMSO centered at 145 ppm.
Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

3.4 SHMBCQ5pr.m Spectrum

Parameter set: **awshmbcctpr (+ getprosol + pulsecal)**
Pulse program: **awshmbcctpr**
SW(^{13}C) = **40 ppm,** excitation band width is **30-34 ppm**

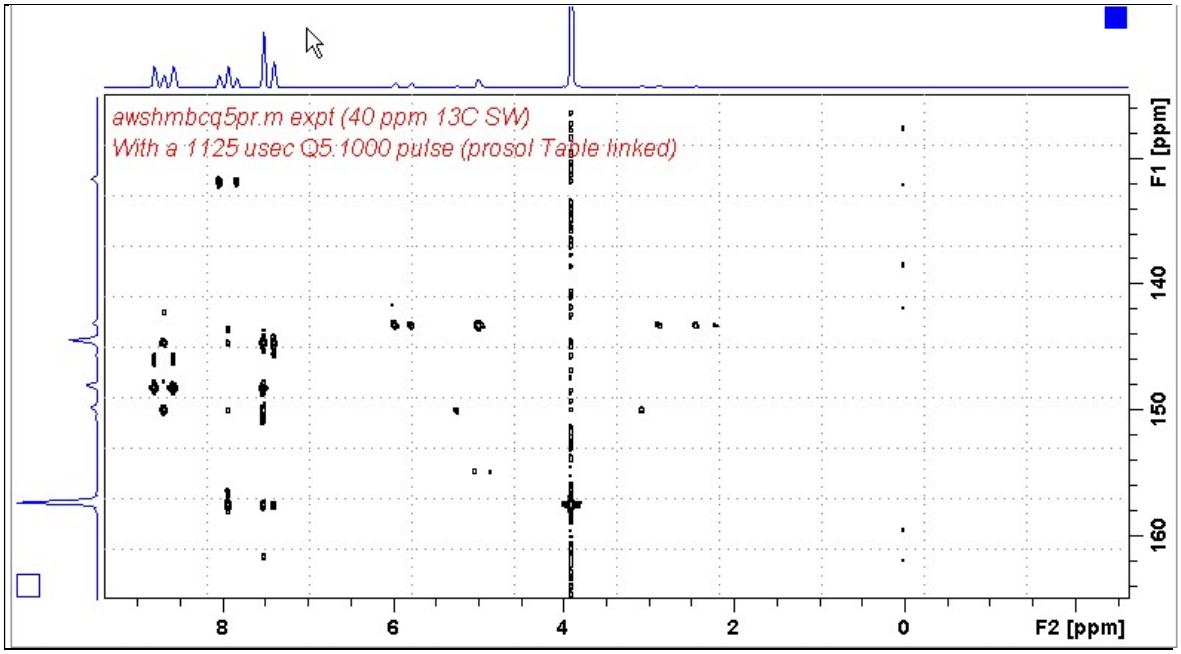
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **PR**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = 128-256 (your choice).

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **2 sec** or other time of your choice.
CNST2 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg 125-160 Hz).
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).
PLW9(db) = **PR power** applied during **D1**. If required the **PR power** can be increased by *subtracting* 6 or 12 db from its prosol Table value.

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined **p23:sp10 Q5.1000** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = SINE
SSB(F2) = SSB(F1) = 0
xfb *and* **abs1 + abs2**



Neo-800 SHMBCQ5pr.m spectrum of quinine in D_6-DMSO centered at 145 ppm. Presaturation was applied at the HOD line frequency (3.35 ppm). Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

3.5 SHMBCCT Spectrum

Parameter set: **awshmbcct (+ getprosol + pulsecal)**
Pulse program: **shmbcctetgpl2nd**
SW(^{13}C) = **15 ppm,** excitation band width is **8-10 ppm**

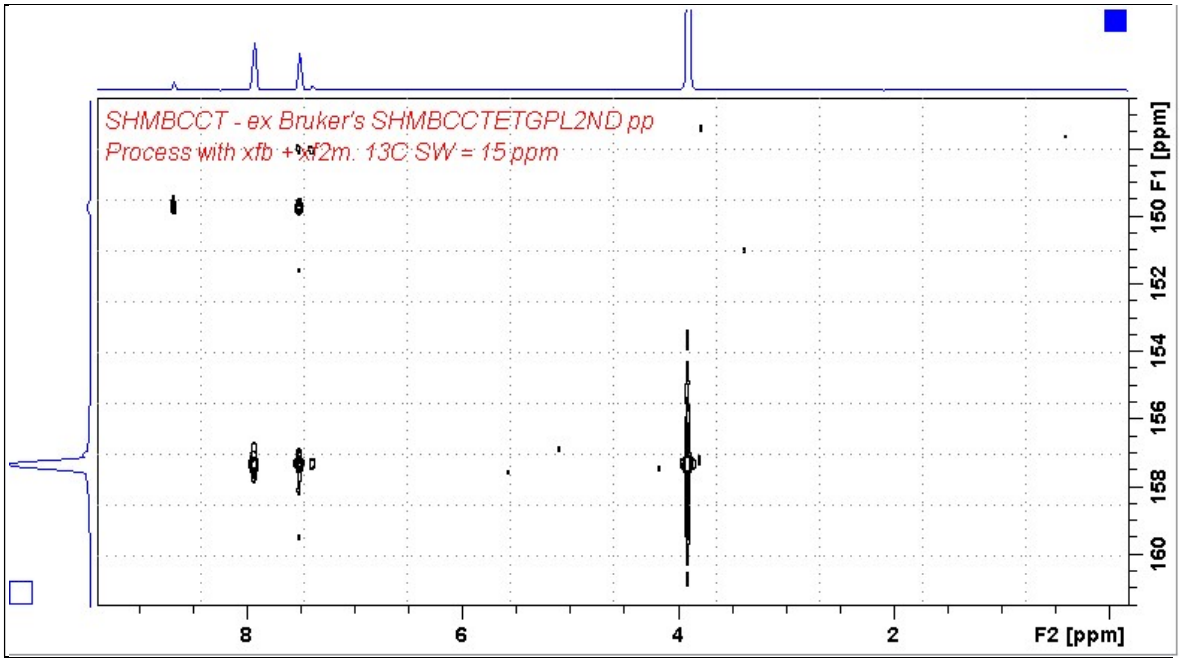
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay =**1.5 sec** or other time of your choice.
CNST6 = **120 Hz**, **CNST7 = 170 Hz** = min/max ^{1}J coupling constants.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
p43:sp32 Q3_surbop.1 pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb *and* **xf2m (***and* **abs1 + abs2)**



Neo-800 SHMBCCT spectrum of quinine in D_6-DMSO centered at 154 ppm.
Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

3.6 SHMBCCTpr Spectrum

Parameter set: **awshmbcctpr (+ getprosol + pulsecal)**
Pulse program: **awshmbcctpr**
SW(^{13}C) = **15 ppm,** excitation band width is **8-10 ppm**

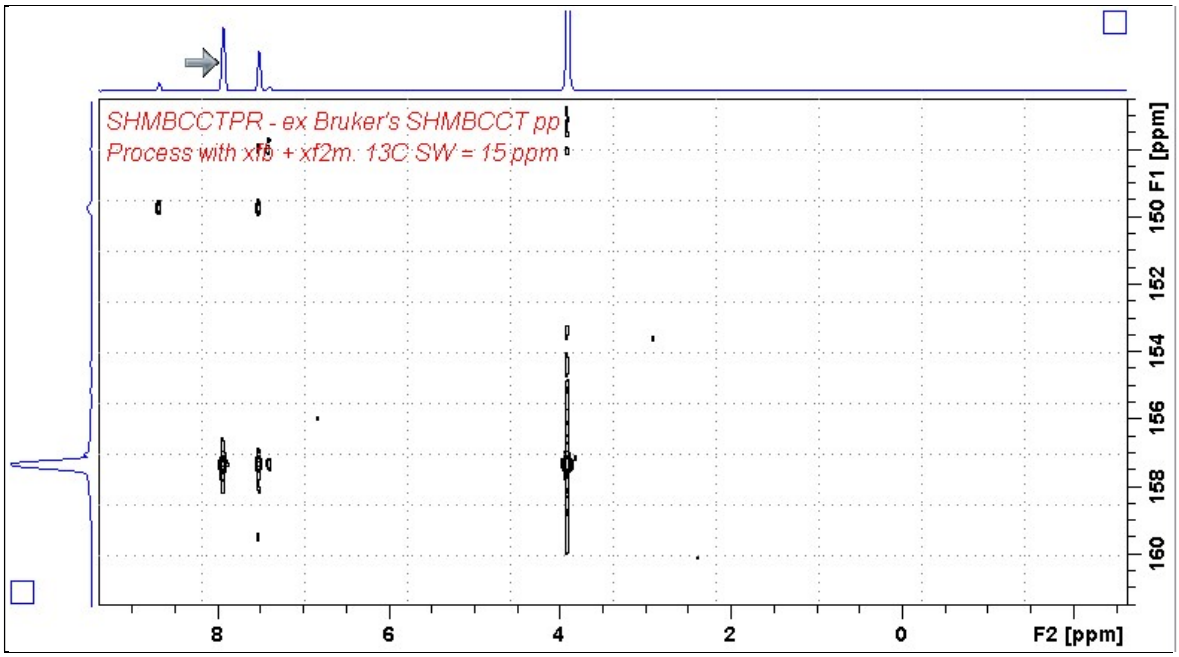
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **PR**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = 128-256 (your choice).

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **2 sec** or other time of your choice.
CNST6 = **120 Hz**, **CNST7 = 170 Hz** = min/max ^{1}J coupling constants.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).
PLW9(db) = **PR** power applied during **D1**. If required the **PR** power can be increased by *subtracting* 6 or 12 db from its prosol Table value.

Check that gradients and shaped pulses are OK, including a prosol Table defined
p43:sp32 Q3_surbop.1 pulse

Set **receiver gain** using **RGA** *(Important!).*

Process with: SI(F2) = 2K**, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb *and* **xf2m (***and* **abs1 + abs2)**



Neo-800 SHMBCCTpr spectrum of quinine in D_6-DMSO centered at 154 ppm. Presaturation was applied at the HOD line frequency (3.35 ppm). Correlations at the edges of the ^{13}C spectral window have reduced intensity.

3.7 SHMBCCTes Spectrum

Parameter set: **awshmbcctes (+ getprosol + pulsecal)**
Pulse program: **awshmbcctes**
SW(^{13}C) = **15 ppm,** excitation band width is **8-10 ppm**

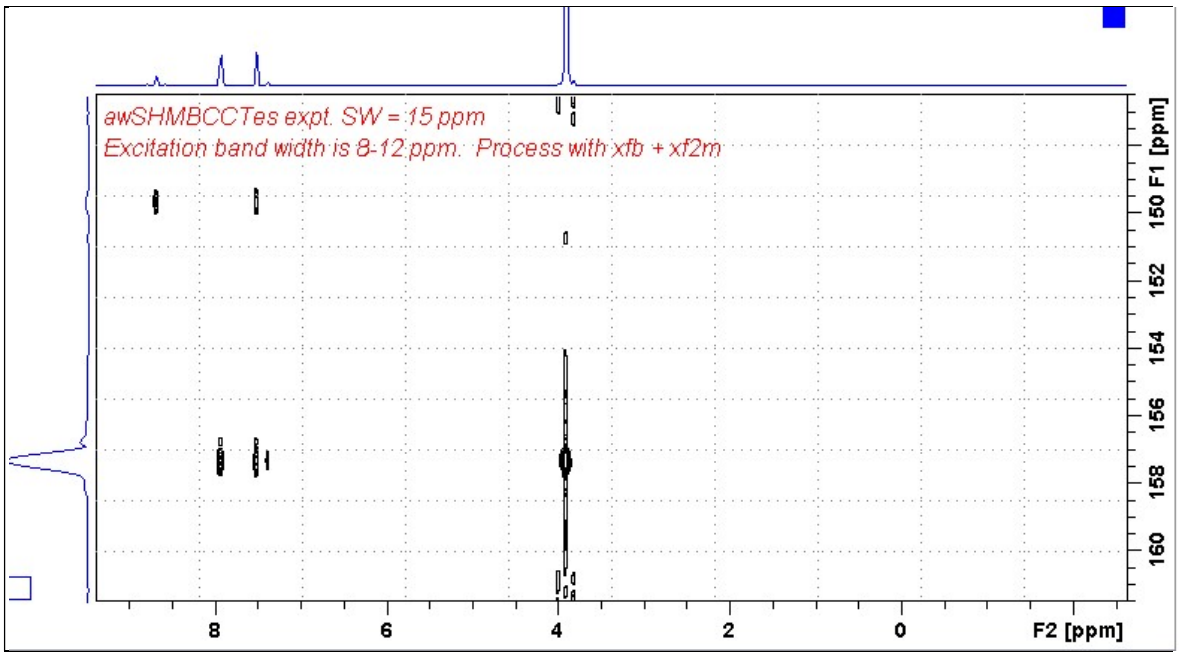
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **ES**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = **128 points**

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay =**1.5 sec** or other time of your choice.
CNST6 = **120 Hz**, **CNST7 = 170 Hz** = min/max ^{1}J coupling constants.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
2000 usec p40:sp10 Sinc1.1000 ES pulse and a **p43:sp32 Q3_surbop.1** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: SI(F2) = 2K**, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb *and* **xf2m (***and* **abs1 + abs2)**



Neo-800 SHMBCCTes spectrum of quinine in D_6-DSMO centered at 154 ppm. **ES** was applied at 3.35 ppm (= the HOD line). ^{1}H signals /correlations located 0.2- 0.3 ppm either side of the **ES** suppressed line have reduced intensity. Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

3.8 SHMBCCT.m Spectrum

Parameter set: **awshmbcct.m (+ getprosol + pulsecal)**
Pulse program: **awshmbcct.w**
SW(^{13}C) = **40 ppm,** excitation band width is **28-32 ppm**

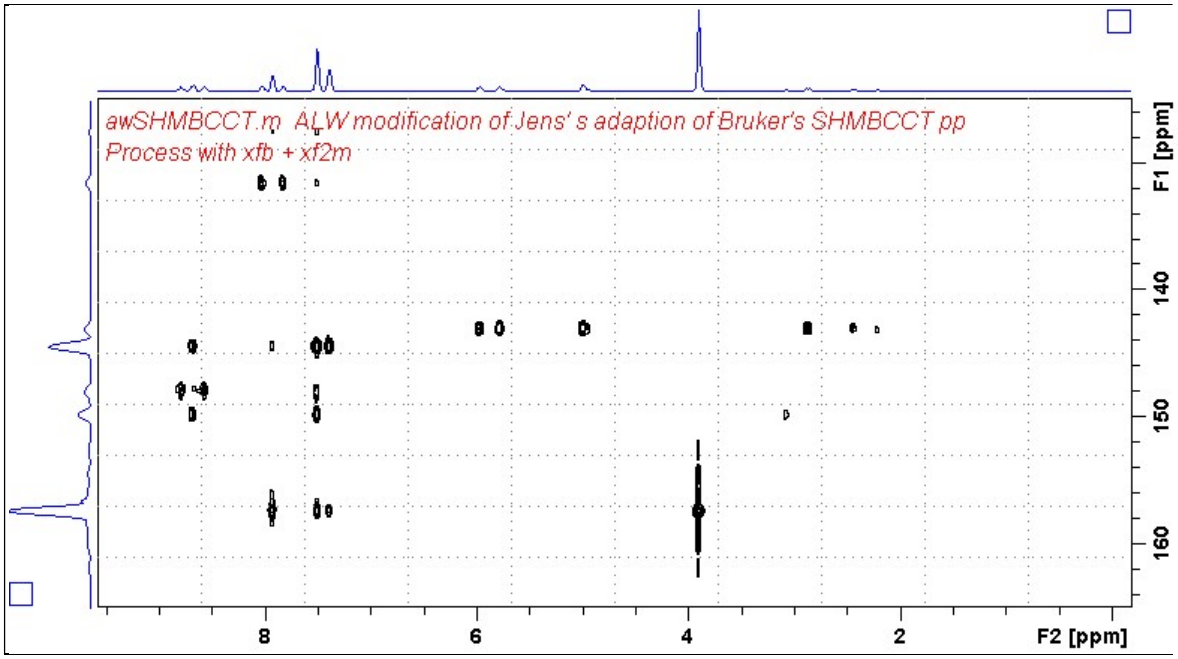
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay =**1.5 sec** or other time of your choice.
CNST6 = **120 Hz**, **CNST7 = 170 Hz** = min/max ^{1}J coupling constants.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
p24:sp16 Q3_surbop.1 pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb *and* **xf2m (***and* **abs1 + abs2)**



Neo-800 SHSQCCT.m spectrum of quinine in D_6-DSMO centered at 145 ppm.
Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**
SHMBCCTPR (Constant time mode SHMBC experiment)

3.9 SHMBCCTpr.m Spectrum

Parameter set: **awshmbcctpr.m (+ getprosol + pulsecal)**
Pulse program: **awshmbcctpr.m**
SW(^{13}C) = **40 ppm,** excitation band width is **28-32 ppm.**

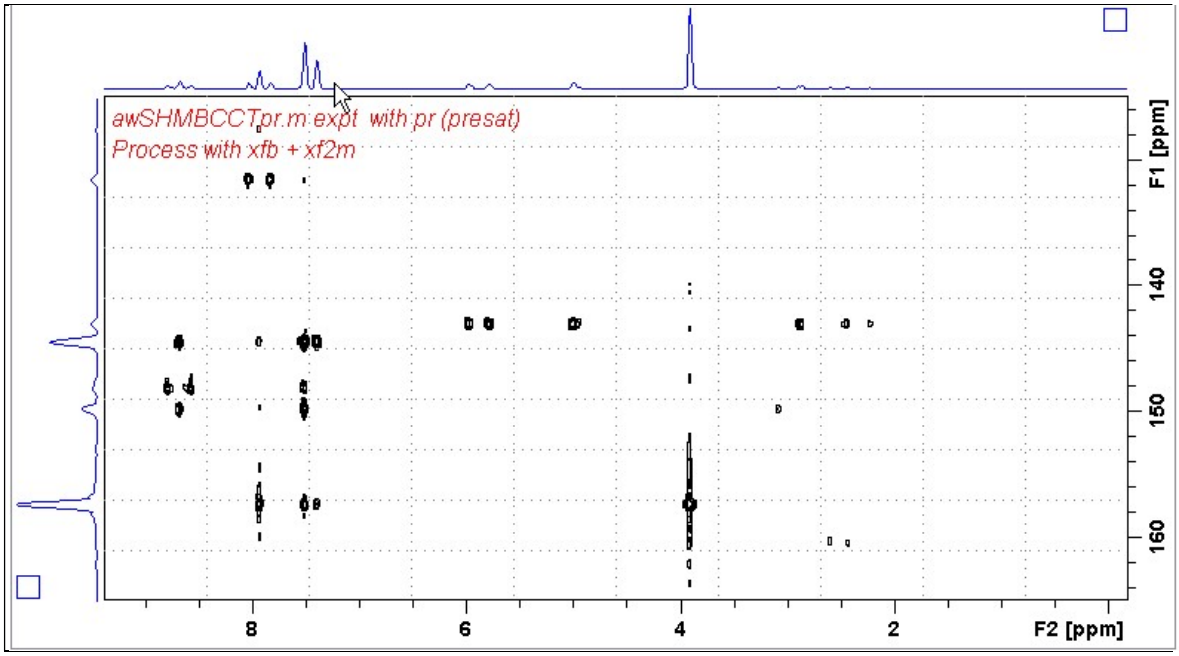
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **PR**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, **TD(F1)** = **128 points.**

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay =**2 sec** or other time of your choice.
CNST6 = **120 Hz**, **CNST7 = 170 Hz** = min/max ^{1}J coupling constants.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).
PLW9(db) = **PR power** applied during **D1**. If required the **PR power** can be increased by *subtracting* 6 or 12 db from its prosol Table value.

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined **p24:sp16 Q3_surbop.1** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb *and* **xf2m (***and* **abs1 + abs2)**



Neo-800 SHMBCCTpr.m spectrum of quinine in D_6-DSMO centered at 145 ppm. Presaturation was applied at the HOD line frequency (3.35 ppm). Correlations at the edges of the ^{13}C spectral window have reduced intensity.

3.10 SHMBCCTes.m Spectrum

Parameter set: **awshmbcctpr.w (+ getprosol + pulsecal)**
Pulse program: **awshmbcctpr.w**
SW(^{13}C) = **40 ppm,** excitation band width is **28-32 ppm**

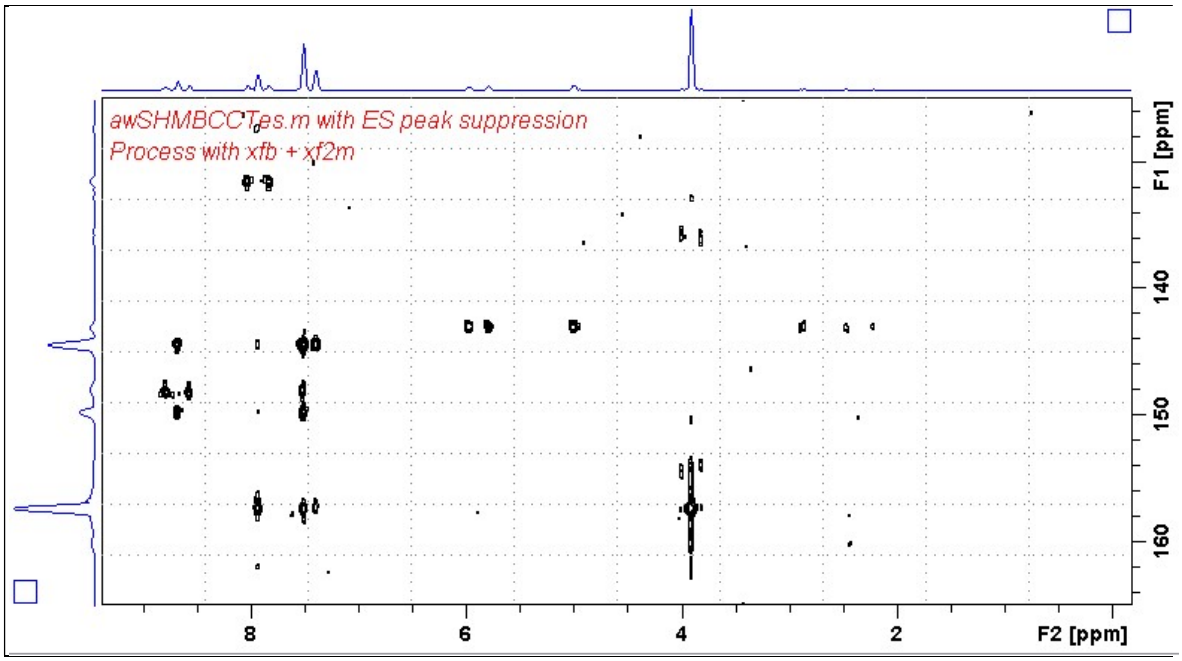
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **ES**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay =**1.5 sec** or other time of your choice.
CNST6 = **120 Hz**, **CNST7 = 170 Hz** = min/max ^{1}J coupling constants.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
2000 usec p12:sp1 Sinc1.1000 ES pulse and a **p24:sp16 Q3_surbop.1** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb *and* **xf2m (***and* **abs1 + abs2)**



Neo-800 SHMBCCTes.m spectrum of quinine in D_6-DSMO centered at 145 ppm. **ES** was applied at 3.35 ppm (= the HOD line). ^{1}H signals /correlations located 0.2- 0.3 ppm either side of the **ES** suppressed line have reduced intensity. Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

3.11 SHMBCCTespr.m Spectrum

Parameter set: **awshmbcctpr.w (+ getprosol + pulsecal)**
Pulse program: **awshmbcctpr.w**
SW(^{13}C) = 40 ppm, excitation band width is **28-32 ppm**

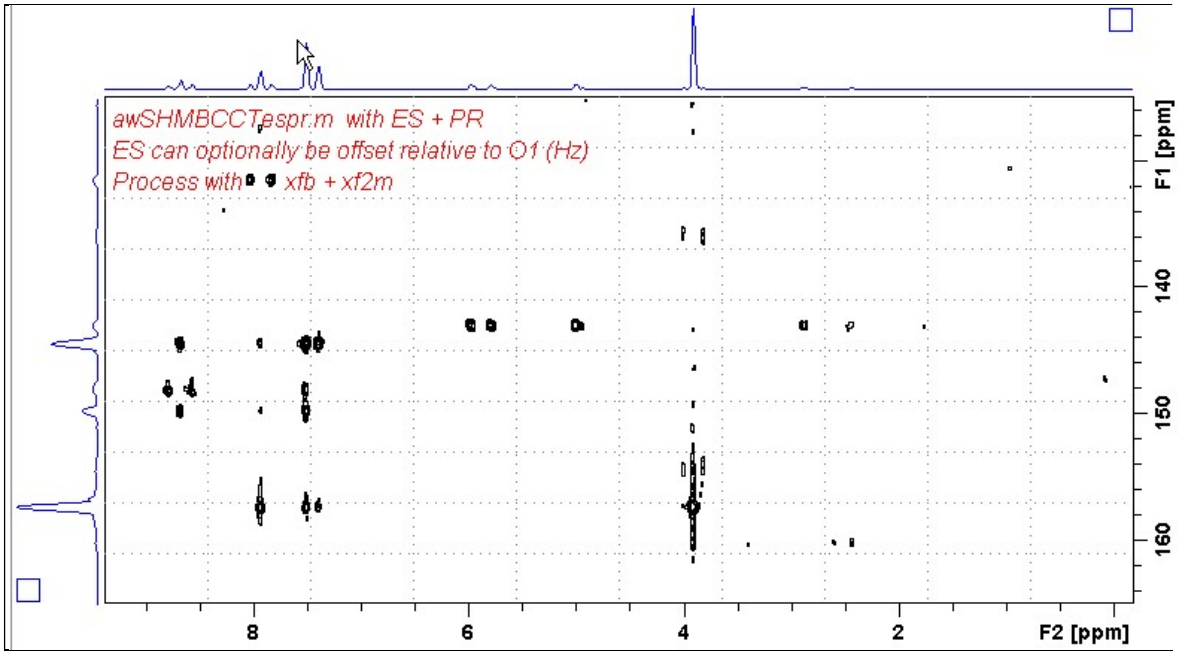
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **ES** and **PR**).
ES can optionally be offset from **PR** as described in the Appendix.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay =**2 sec** or other time of your choice.
CNST6 = 120 Hz, **CNST7 = 170 Hz** = min/max ^{1}J coupling constants.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).
PLW9(db) = PR power applied during **D1**. If required the **PR power** can be increased by *subtracting* 6 or 12 db from its prosol Table value.

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined **2000 usec p12:sp1 Sinc1.1000 ES** pulse and a **p24:sp16 Q3_surbop.1** pulse.
ES can optionally be offset from **PR** at **O1** as described in the Appendix.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb *and* **xf2m (***and* **abs1 + abs2)**



Neo-800 SHMBCCTespr.m spectrum of quinine in D_6-DSMO centered at 145 ppm. Combined **ES** + **PR** was applied at 3.35 ppm (= the HOD line). ^{1}H signals /correlations located ~ 0.3 ppm either side of the **ES** suppressed line have reduced intensity. Correlations at the edges of the ^{13}C spectral window have reduced intensity

3.12 SHMBCCT.w Spectrum

Parameter set: **awshmbcct.w (+ getprosol + pulsecal)**
Pulse program: **awshmbcct.w**
SW(^{13}C) = **60 ppm,** excitation band width is **45-50 ppm**

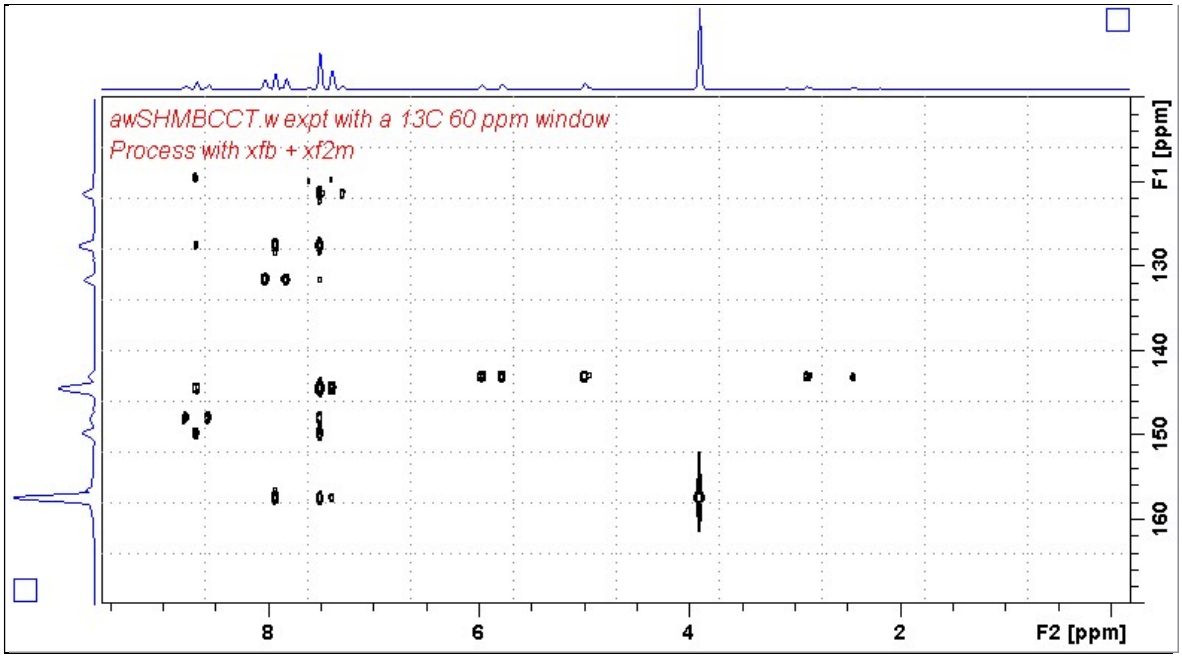
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay =**1.5 sec** or other time of your choice.
CNST6 = **120 Hz**, **CNST7 = 170 Hz** = min/max ^{1}J coupling constants.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
p33:sp23 Q3_surbop.1 pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb *and* **xf2m (***and* **abs1 + abs2)**



Neo-800 SHMBCCT.w spectrum of quinine in D_6-DSMO centered at 140 ppm.
Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

3.13 SHMBCCTpr.w Spectrum

Parameter set: **awshmbcctpr.w (+ getprosol + pulsecal)**
Pulse program: **awshmbcctpr.w**
SW(^{13}C) = 60 ppm, excitation band width is **45-50 ppm**

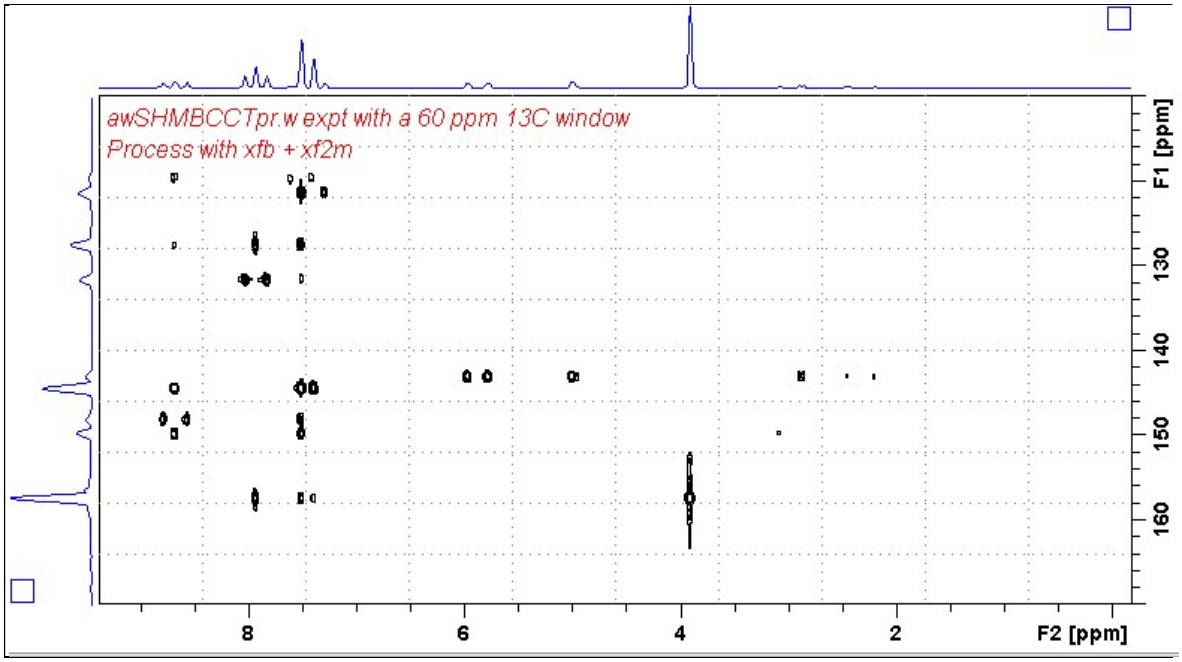
Type **eda** (enter) and enter **SW(^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **PR**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay = **2 sec** or other time of your choice.
CNST6 = 120 Hz, **CNST7 = 170 Hz** = min/max ^{1}J coupling constants.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).
PLW9(db) = **PR power** applied during **D1**. If required the **PR power** can be increased by *subtracting* 6 or 12 db from its prosol Table value.

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined **p33:sp23 Q3_surbop.1** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb *and* **xf2m (***and* **abs1 + abs2)**



Neo-800 SHMBCCTpr.w spectrum of quinine in D_6-DSMO centered at 140 ppm. Presaturation was applied at the HOD line frequency (3.35 ppm). Correlations at the edges of the ^{13}C spectral window have reduced intensity.

3.14 SHMBCCTes.w Spectrum

Parameter set: **awshmbcctes.w (+ getprosol + pulsecal)**
Pulse program: **awshmbcctes.w**
SW(^{13}C) = 60 ppm, excitation band width is **45-50 ppm**

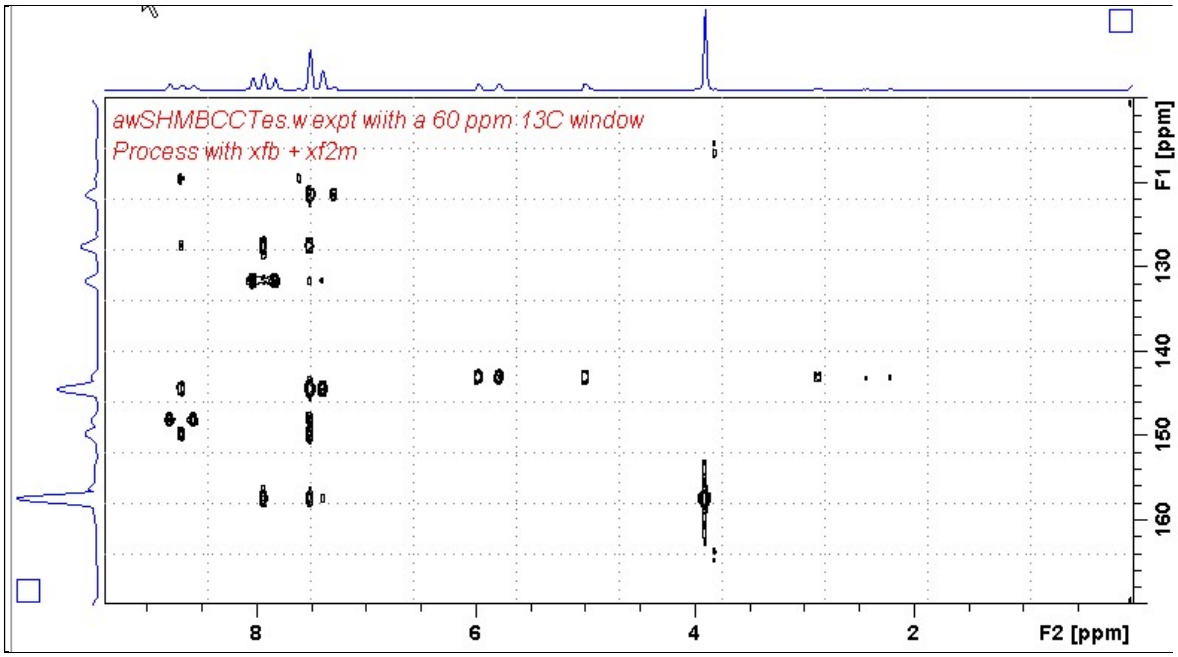
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1 = ^{1}H** spectral window midpoint in Hz (for **ES**).
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 2K, TD(F1) = 128 points.

NS = multiple of 4, 8 or 16, **DS** = 8 or 16.
D1 = repetition delay =**1.5 sec** or other time of your choice.
CNST6 = **120 Hz**, **CNST7 = 170 Hz** = min/max ^{1}J coupling constants.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).

Type **ased** (enter) and review parameters used in the job.
Check that gradients and shaped pulses are OK, including a prosol Table defined
2000 usec p12:sp1 Sinc1.1000 ES pulse and a **p33:sp23 Q3_surbop.1** pulse.

Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K, SI(F1) = 512 or 1K points**
WDW(F1) = WDW(F2) = QSINE
SSB(F2) = SSB(F1) = 2
xfb *and* **xf2m (***and* **abs1 + abs2)**



Neo-800 SHMBCCTes.w spectrum of quinine in D_6-DSMO centered at 140 ppm. **ES** was applied at 3.35 ppm (= the HOD line). ^{1}H signals /correlations located 0.2-0.3 ppm either side of the **ES** suppressed line have reduced intensity. Correlations at the edges of the ^{13}C spectral window have reduced intensity**.**

4.0 How to offset ES from O1 in an ESPR experiment

By default **ES** and **PR** are applied at **O1** (Hz) frequency in aw coded **HSQC** and **HMBCCT ESPR** experiments. Combined (double) **ES + PR** can be used to suppress a large HOD or solvent peak.

The **ES** pulse in **shmbc135espr.m** or **shmbcctespr.m** experiments is defined as an f1 (^{1}H) channel **2000 usec Sinc1.1000 p12:sp1** pulse.

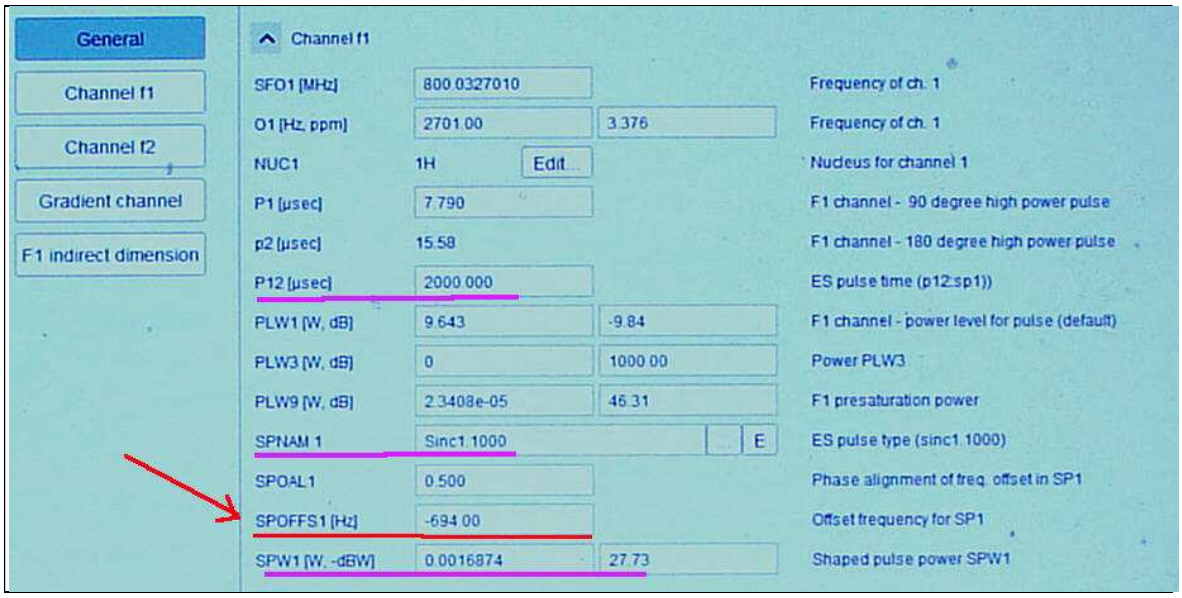
The frequency (in Hz) at which **ES** is applied can optionally be offset from **O1** (= the frequency PR is applied) so you can suppress two solvent lines by entering an **SPOFFS1(Hz)** offset value in its **ased** visible cell.

For example if, the **HOD line** occurs at **2701 Hz** and the **DMSO line** occurs at **2007 Hz**, the offset of the **DMSO line** (*to be ES suppressed*) relative to that of the **HOD line** (*PR suppressed at O1*) is calculated as:

SPOFFS1(Hz) = **ES** offset signal (Hz) - **O1** frequency (Hz)

ie **2007 Hz (DMSO) - 2701 Hz (HOD) = - 694 Hz**

The offset is negative in this case since the **DMSO line** occurs at **- 694 Hz *less*** than that of the frequency at which **PR** is applied to the **HOD line** at **O1 Hz**.



p12:sp1 (<triple> and <triple2>) **ES** pulse parameters. **The SPOFFS1(Hz)** offset value is red arrowed.

Footnote: **ES** pulses are defined as a **p12:sp1** pulses in pp's that run with *prosol relations = <triple> or <triple2>* or as **p40:sp10** pulses with *prosol relations = <default>* or *not shown/not included* as a pp line**.**