KJM 9250

2D-COSY, TOCSY, CLEAN-TOCSY, DIPSI2, NOESY, ROESY, ROESY2 experiments on the AVI and AVII-600 spectrometers with CW presaturation (PR) and/or Excitation Sculpturing (ES) peak suppression

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2D-COSY, TOCSY, CLEAN-TOCSY, DIPSI2, NOESY, ROESY, ROESY2 experiments on the AVI and AVII-600 spectrometers with CW presaturation (PR) and/or Excitation Sculpturing (ES) peak suppression

1.0 Introduction

1.1 Spectral Window Set up

The spectral window width and midpoint should be determined in a standard ^{1}H NMR spectrum before setting up a 2D-COSY, TOCSY, etc experiment.

The smaller the spectral window the higher the resolution of the resulting spectrum. There should be no signals within 0.5 ppm of the upper or lower limits of the spectral window.

1.2 Presaturation Frequencies

The frequencies of signals to be **ES** suppressed and/or **CW** presaturated should be determined in **Hz** a standard ^{1}H spectrum *before* running a 2D experiment.

CW presaturation on **F1** is applied at **O1 Hz** = the spectral window midpoint.

CW presaturation on **F2** at **O2 Hz** can be applied at any frequency within the spectral window range.

ES is applied on **F1** at **O1 Hz** = the spectral window point, or it can *optionally be offset* at **O1* Hz** where **SPOFFS1** (or **SPOFFS10** in some pp's) = **O1*-O1 Hz.**
Three solvent or other peaks can be suppressed if **ES** is **offset** in an **ESPRF1PRF2** experiment.

1.3 CW Presaturation (PR) Power Levels

CW presaturation is applied at power levels **PL9** and **PL21** via F1 and F2 respectively. If required presaturation power levels can be *decreased or increased* by *adding or subtracting* 3-12 db *respectively to their prosol Table linked values. 6 db = a factor 2.*

1.4 Processing

The COSY experiment is an absolute value experiment – no phasing is required.

TOCSY, CLEAN-TOCSY, DIPSI2, NOESY, ROESY and ROESY2 experiments are phase sensitive experiments. These spectra should be phased **before** using the **abs1** and **abs2** commands.

2.0 COSY Experiments and Parameter Sets

2.1 COSYPR with PR presaturation on F1

parameter set: **awcosypr (+ getprosol)**
pulse programme: **cosygpprqf**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
    O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (any number is OK), **DS** = 2, 4 or 8.
P0 = θ degree excitation pulse time, typically use a 45° or 90° pulse.
D1 = presaturation time = **2 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job. Check **gradients** are OK.
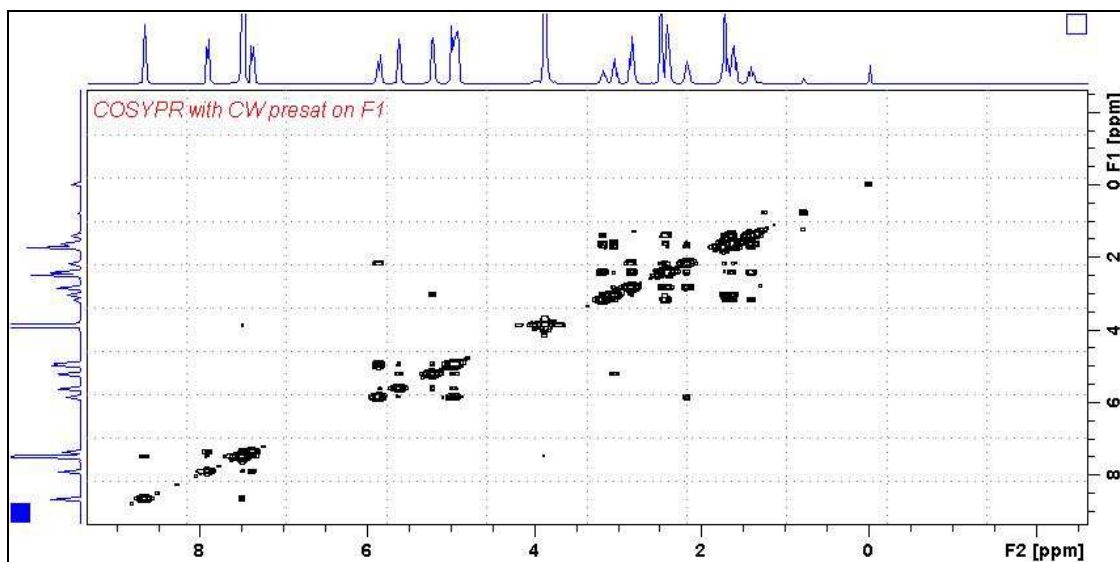The **PL9** prosol linked presaturation power level can be adjusted if required.
Set **receiver gain** using **RGA** *(important!).*

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

COSYPR spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm suppressed.
The spectrum is centered at the O1 frequency of the HOD line.

2.2 COSYPRF1PRF2 with PR presaturation on F1 and F2

parameter set: **awcosyprf1prf2 (+ getprosol)**
pulse programme: **awcosyprf1prf2**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be presaturated.
      O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (any number is OK), **DS** = 2, 4 or 8.
P0 = θ degree excitation pulse time, typically use a 45º or 90º pulse.
D1 = presaturation time = **2 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job. Check **gradients** are OK.
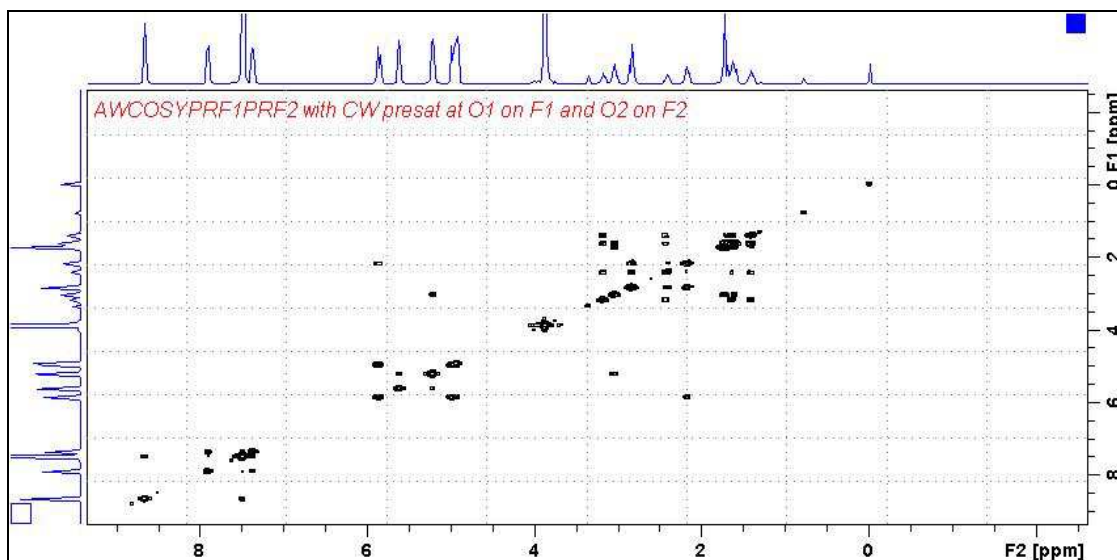The **PL9** and **PL21** presaturation power levels can be adjusted if required.
Set **receiver gain** using **RGA** *(important!).*

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

COSYPRF1PRF2 spectrum of quinine in D$_6$-DMSO with the HOD and DMSO lines at 3.38
ppm and 2.5 ppm suppressed. The spectrum is centered at the O1 frequency of the HOD line.

2.3 COSYPRF2ONLYwith PR presaturation on F2

parameter set: **awcosyprf2only (+ getprosol)**
pulse programme: **awcosyprf2only**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** in **Hz or ppm** = the spectral window midpoint
  and **O2 (Hz)** of the signal to be presaturated *in this order.*

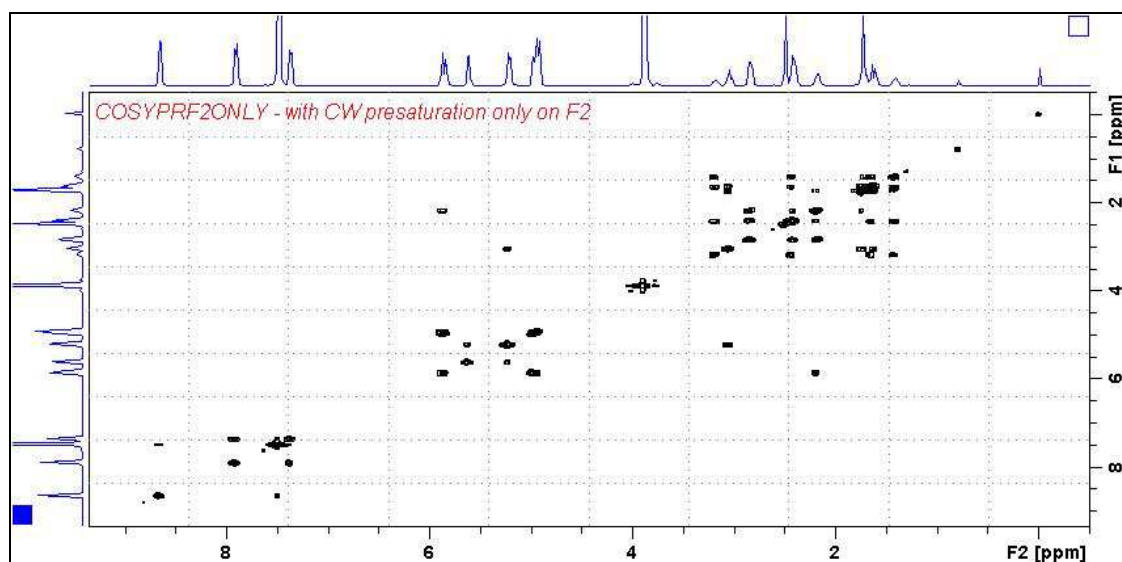**TD(F2)** = 1K or 2K, **TD(F1)** = 128 - 256 (your choice).
NS = 2, 4, 8 (any number is OK), **DS** = 2, 4 or 8.
P0 = θ degree excitation pulse time, typically use a 45º or 90º pulse.
D1 = presaturation time = **2 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job. Check **gradients** are OK. the **PL21** prosol linked presaturation power level can be adjusted if required. Set **receiver gain** using **RGA** *(Important!)*.

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

COSYPRF2ONLY spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm presaturated at O2 on F2.
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2.4 COSYES with Excitation Sculpting on F1

parameter set: **awcosyes (+ getprosol)**
pulse programme: **awcosyes**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
      O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (any number is OK), **DS** = 2, 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job.
Verify **gradients** are OK and that **a 2000 usec squa100.1000** shaped pulse is used.
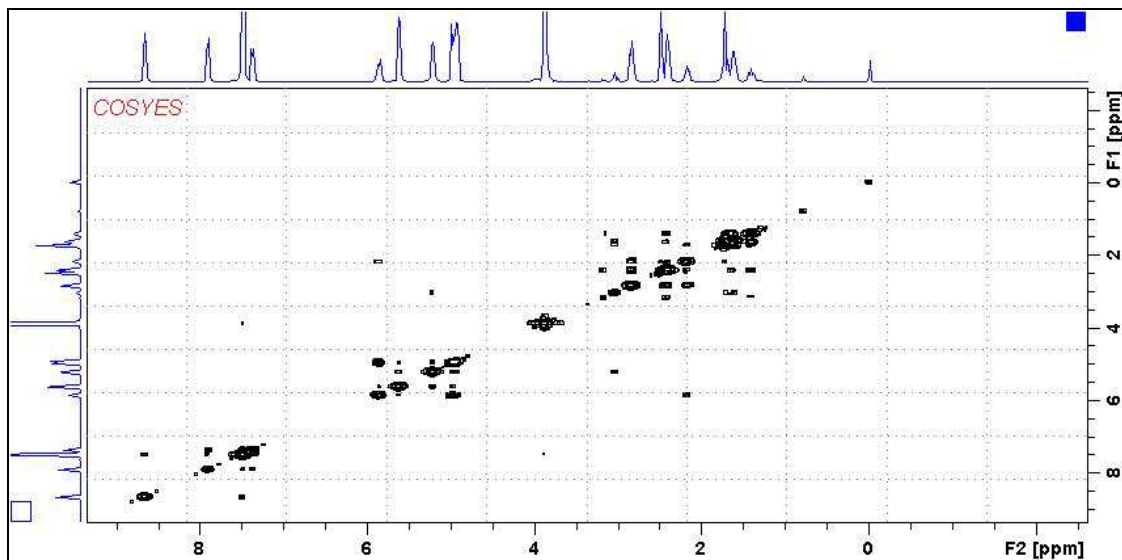Set **receiver gain** using **RGA** *(important!).*

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

COSYES spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES suppressed. The
spectrum is centered at the O1 frequency of the HOD line.

2.5 COSYESPR with Excitation Sculpting and CW presaturation on F1

parameter set: **awcosyespr (+ getprosol)**
pulse programme: **awcosyespr**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
    O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS =1, 2, 4, 8 (any number is OK), **DS** = 2, 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job.
The **PL9** presaturation power level can be adjusted if required.
Verify **gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
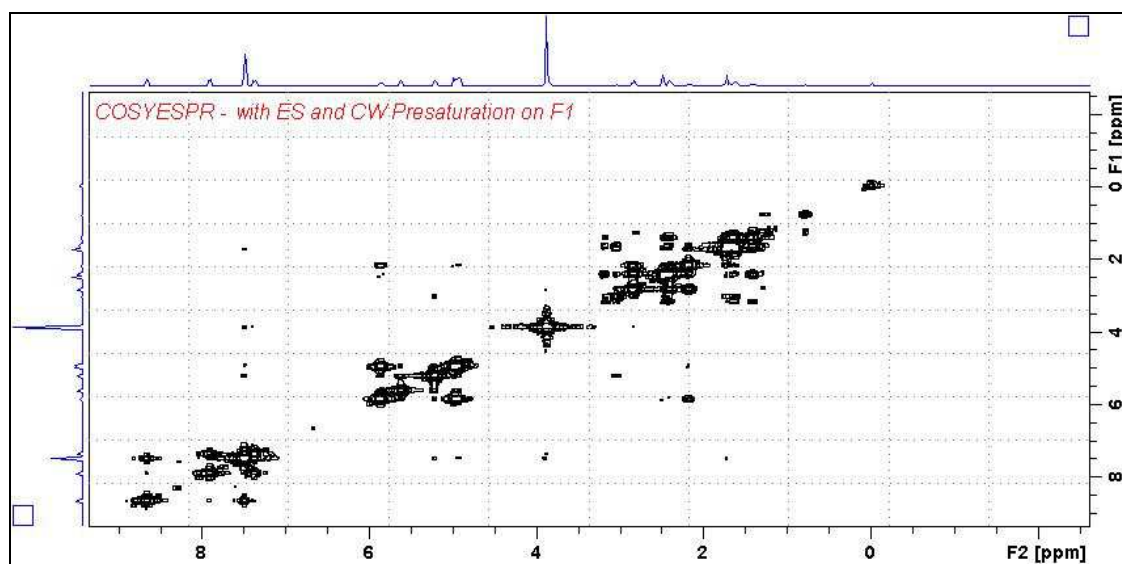Set **receiver gain** using **RGA** *(important!).*

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

COSYESPR spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES and PR suppressed. The spectrum is centered at the O1 frequency of the HOD line.

2.6 COSYESPRF1PRF2 with ES and PR presaturation on F1 and PR presaturation on F2

parameter set: **awcosyesprf1prf2 (+ getprosol)**
pulse programme: **awcosyesprf1prf2**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be **ES** + **PR** presaturated.
  O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (any number is OK), **DS** = 2, 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job.
The **PL9** and **PL21** presaturation power levels can be adjusted if required.
Verify **gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
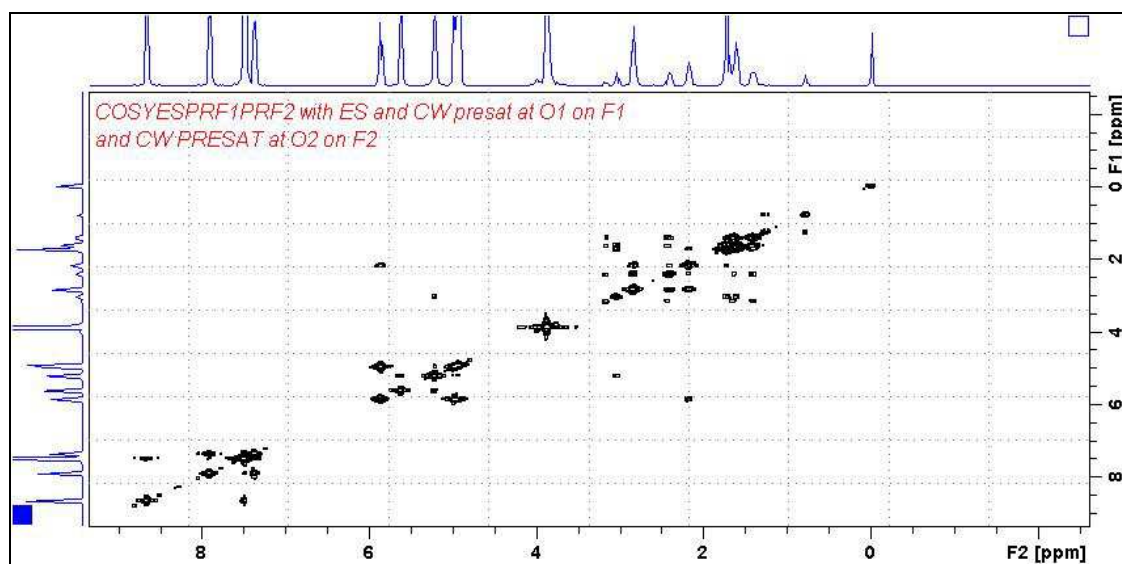Set **receiver gain** using **RGA** *(important!).*

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

COSYESPRF1PRF2 spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES and PR suppressed and the DMSO line at 2.5 ppm PR presaturated. The spectrum is centered at the O1 frequency of the HOD line.

3.0 TOCSY Experiments and Parameter Sets

3.1 TOCSYPR with PR presaturation on F1

parameter set: **awtocsypr (+ getprosol)**
pulse programme: **mlevphpr**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
    O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
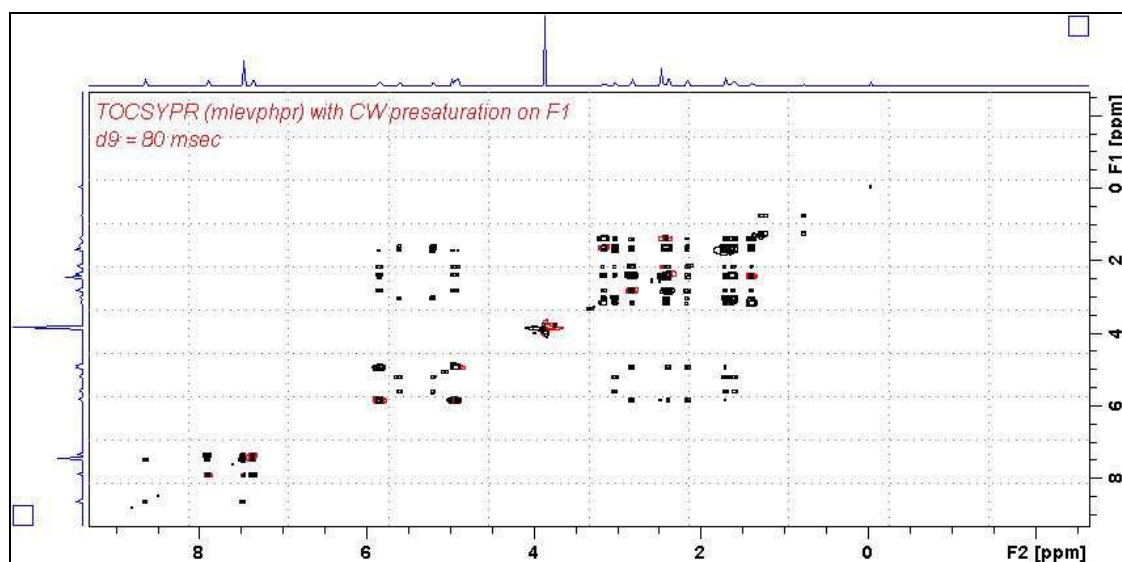The **PL9** presaturation power level can be adjusted if required.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
          WDW(F1) = WDW(F2) = QSINE
          SSB(F2) = SSB(F1) = 2
          xfb, abs1, abs2 and optionally **syma**

TOCSYPR spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm suppressed.
The spectrum is centered at the O1 frequency of the HOD line.

3.2 TOCSYPRF1PRF2 with PR presaturation on F1 and F2

parameter set: **awtocsyprf1prf2 (+ getprosol)**
pulse programme: **awtocsyprf1prf2**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be presaturated.
 O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
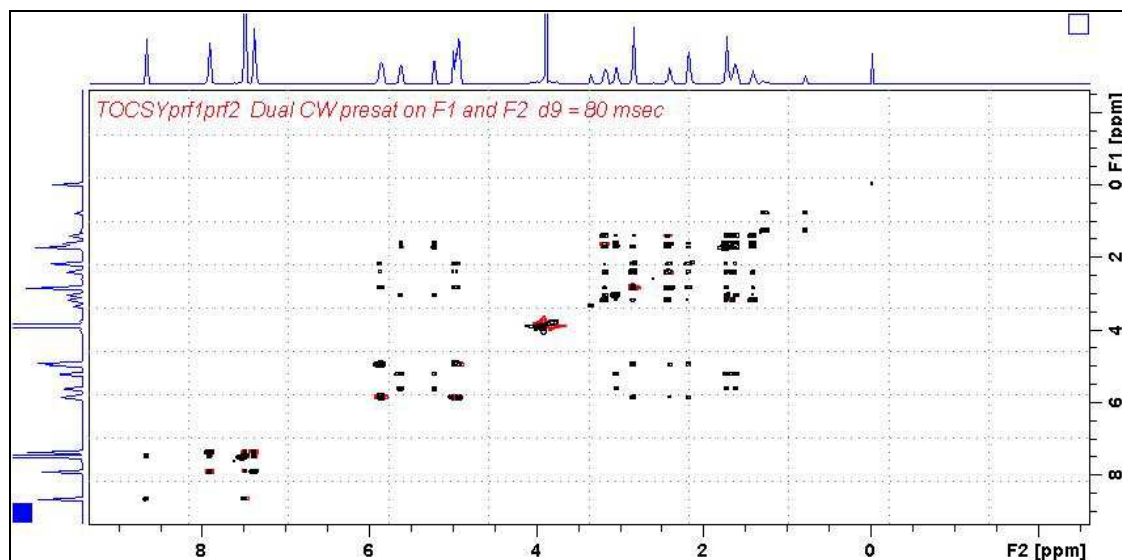The **PL9** and **PL21** presaturation power levels can be adjusted if required.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
 WDW(F1) = WDW(F2) = QSINE
 SSB(F2) = SSB(F1) = 2
 xfb, abs1, abs2 and optionally **syma**

TOCSYPRF1PRF2 spectrum of quinine in D_6-DMSO with the HOD and DMSO lines at 3.38
ppm and 2.5 ppm suppressed. The spectrum is centered at the O1 frequency of the HOD line.

3.3 TOCSYPRF2ONLY with PR presaturation on F2

parameter set: **awtocsyprf2only (+ getprosol)**
pulse programme: **awtocsyprf2only**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** in **Hz or ppm** = the spectral window midpoint
  and **O2 (Hz)** of the signal to be presaturated *in this order.*

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
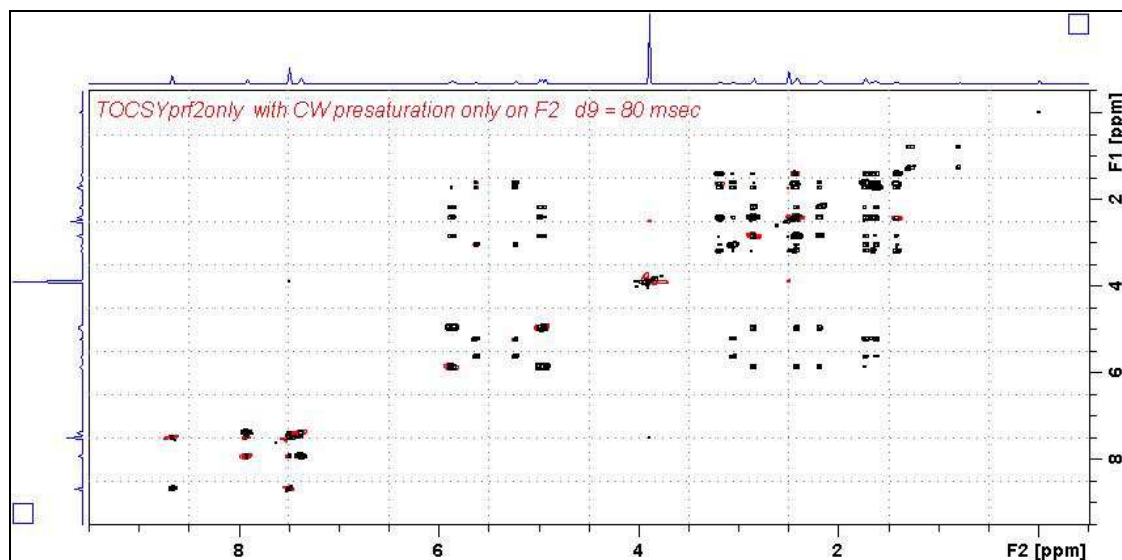**D1** = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job and **gradients** are OK.
The **PL21** presaturation power level can be adjusted if required.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

TOCSYPRF2ONLY spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm presaturated at O2 on F2.

3.4 TOCSYES with Excitation Sculpting on F1

parameter set: **awtocsyes (+ getprosol)**
pulse programme: **mlevesgpph**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
    O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = repetition time = **1.5 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
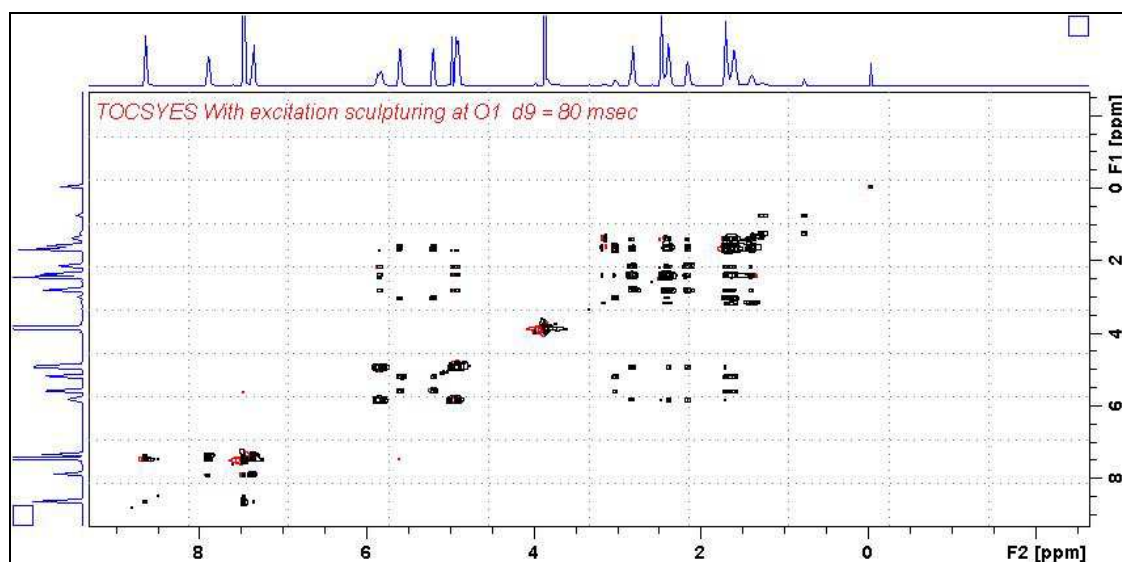Verify **ES gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
                   WDW(F1) = WDW(F2) = QSINE
                   SSB(F2) = SSB(F1) = 2
                   xfb, abs1, abs2 and optionally **syma**

TOCSYES spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES suppressed. The spectrum is centered at the O1 frequency of the HOD line.

3.5 TOCSYESPR with ES and PR presaturation on F1

parameter set: **awtocsyespr (+ getprosol)**
pulse programme: **awtocsyespr**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
       O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
The **PL9** presaturation power level can be adjusted if required.
Verify **ES gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
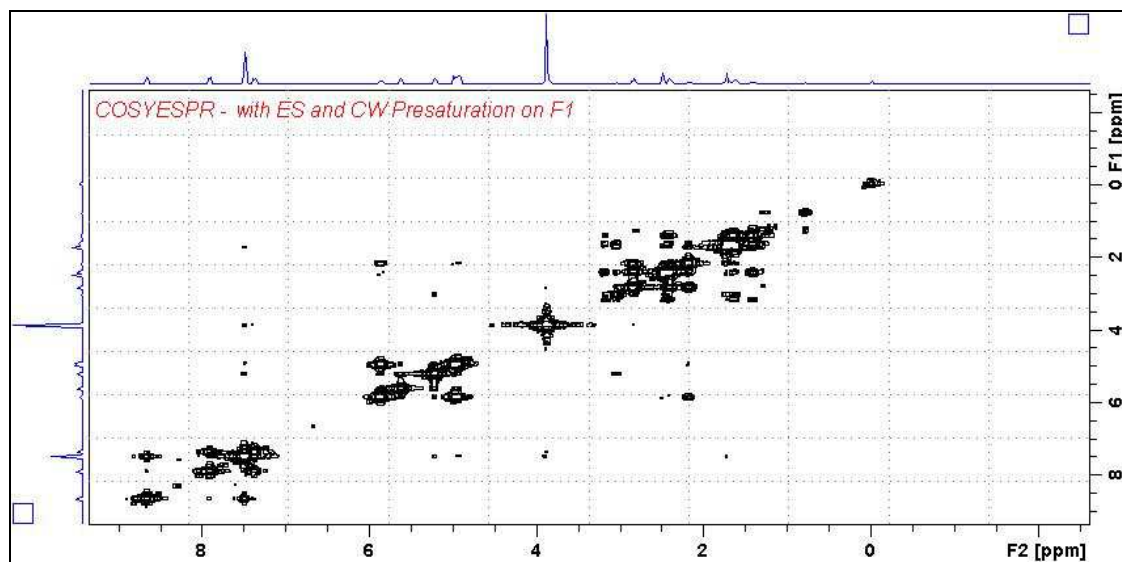Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

TOCSYESPR spectrum of quinine in D$_6$-DMSO with the HOD line at 3.38 ppm ES and PR
suppressed. The spectrum is centered at the O1 frequency of the HOD line.

3.6 TOCSYESPRF1PRF2 with ES and PR presaturation on F1 and PR presaturation on F2

parameter set: **awtocsyesprf1prf2 (+ getprosol)**
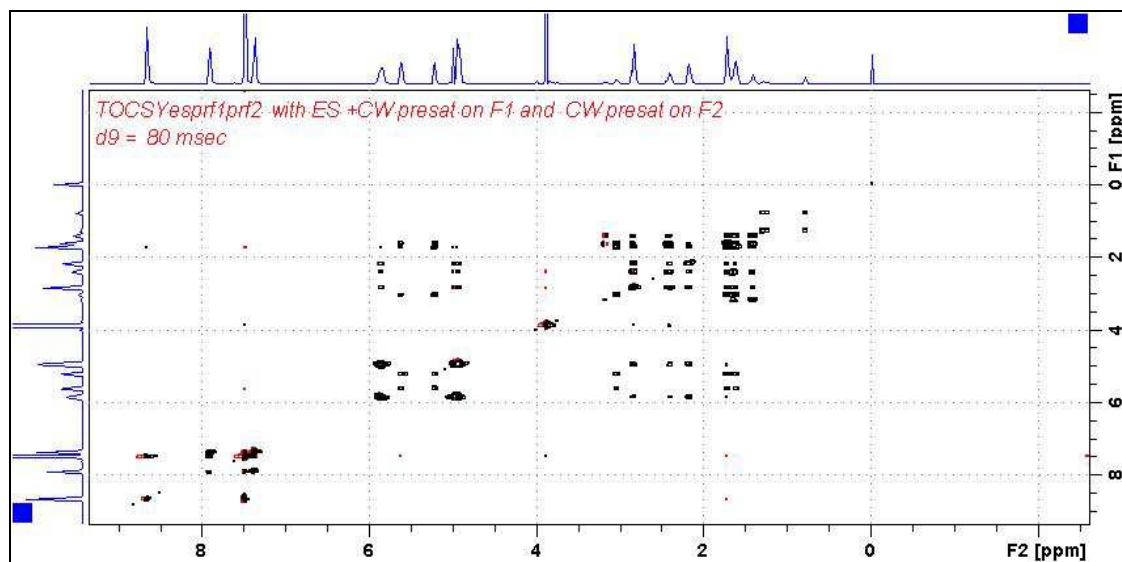pulse programme: aw**tocsyesprf1prf2**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be **ES + PR** presaturated.
   O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
The **PL9** and **PL21** presaturation power levels can be adjusted if required.
Verify **ES gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
   WDW(F1) = WDW(F2) = QSINE
   SSB(F2) = SSB(F1) = 2
   xfb, abs1, abs2 and optionally **syma**

TOCSYESPRF1PRF2 spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES and PR suppressed and the DMSO line at 2.5 ppm PR presaturated. The spectrum is centered at the O1 frequency of the HOD line.

4.0 CLEAN-TOCSY Experiments and Parameter Sets

4.1 awcleantocsypr

4.2 awcleantocsyprf1prf2

4.3 awcleantocsyprf2only

4.4 awcleantocsyes

4.5 awcleantocsyespr

4.6 awcleantocsyesprf1prf2

aw coded variants of Bruker's **clmlevp**r experiment are prosol compatible and include:

(i) **auto-calculation of d20** from the prosol table linked **p6** pulse time

(ii) **auto-calculation of L1** rounded off to the nearest whole number from a requested **d9** spin lock time input as per a standard TOCSY experiment

(iii) the set **d9** time is displayed as **d10** in the experiment's ___ased___ display immediately below the requested **d9** time.

Bruker's **clmlevpr** pp notes incorrectly include 2 x p17 pulses in their manual spin lock time calculation formula. While p17 appears twice in Bruker's **TOCSY** pp's it appears only once in their **clmlev** pp's.

4.1 CLEAN-TOCSYPR with PR presaturation on F1

parameter set: **awcleantocsypr (+ getprosol)**
pulse programme: **awclmlevpr**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
        O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
The **PL9** presaturation power level can be adjusted if required.
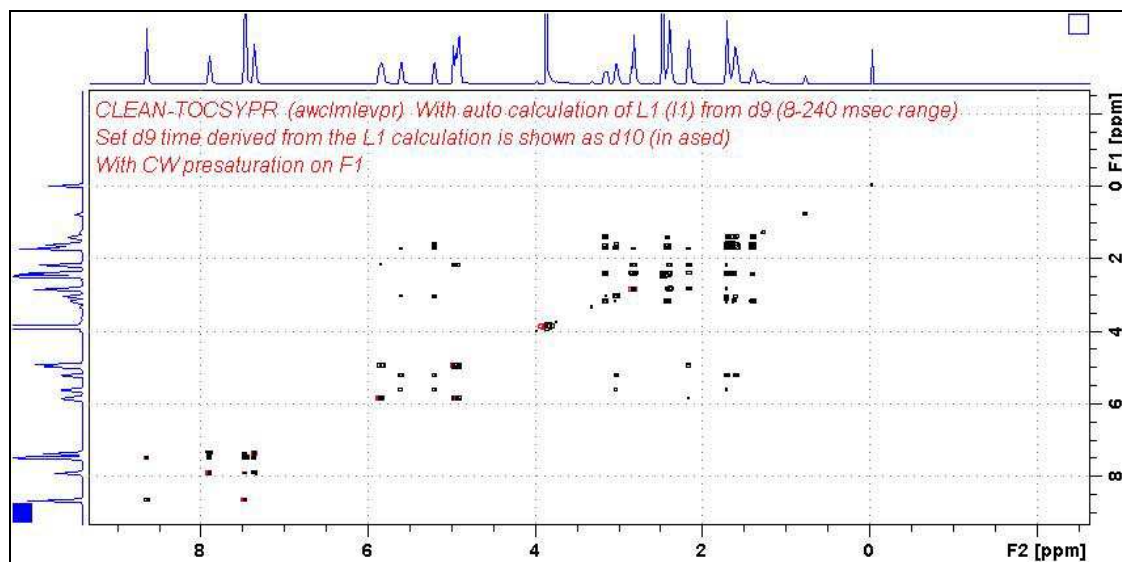Check the **D10** time derived from the requested **D9** time is OK.
Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

CLEAN-TOCSYPR (awclmlevpr) With auto calculation of L1 (l1) from d9 (8-240 msec range)
Set d9 time derived from the L1 calculation is shown as d10 (in ased)
With CW presaturation on F1

CLEANTOCSYPR spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm suppressed. The spectrum is centered at the O1 frequency of the HOD line.

4.2 CLEAN-TOCSYPRF1PRF2 with PR presaturation on F1 and F2

parameter set: **awcleantocsyprf1prf2 (+ getprosol)**
pulse programme: **awclmlevprf1prf2**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be presaturated.
    O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time **= 80** msec or other time of your choice (8-240 msec).

Type **ased** (enter) and review parameters used in the job.
The **PL9** and **PL21** presaturation power levels can be adjusted if required .
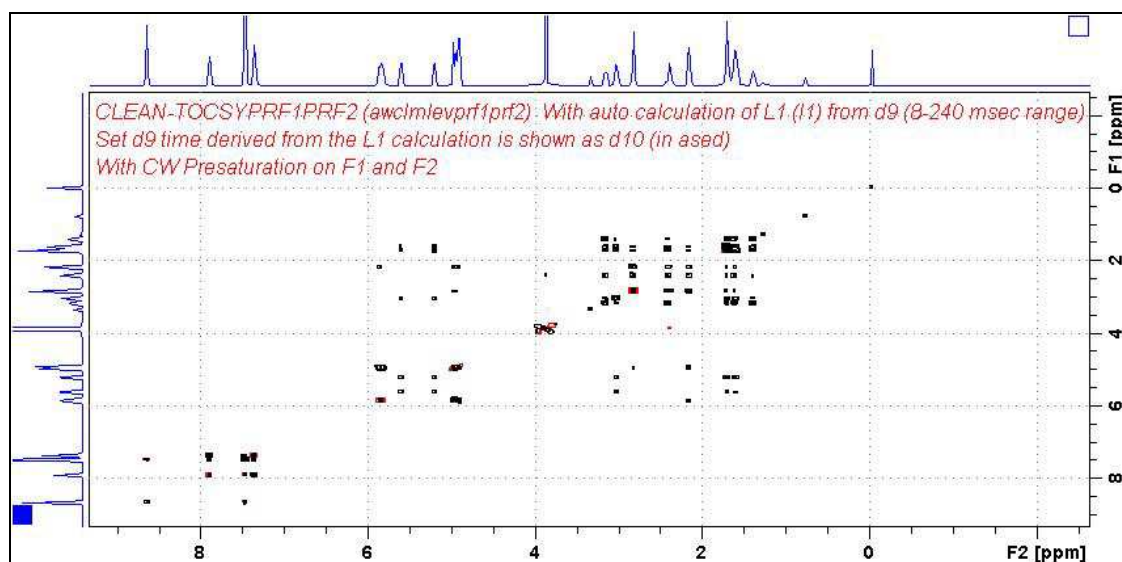Check the **D10** time derived from the requested **D9** time is OK.
Set **receiver gain** using **RGA** *(Important!)*.

Process with: **SI(F2) = SI(F1) = 1K or 2K**
            WDW(F1) = WDW(F2) = QSINE
            SSB(F2) = SSB(F1) = 2
            xfb, abs1, abs2 and optionally **syma**

CLEAN-TOCSYPRF1PRF2 spectrum of quinine in D_6-DMSO with the HOD and DMSO lines
at 3.38 ppm and 2.5 ppm suppressed. The spectrum is centered at the O1 frequency of the HOD
line.

4.3 CLEAN-TOCSYPRF2ONLY with PR presaturation on F2

parameter set: **awcleantocsyprf2only (+ getprosol)**
pulse programme: **awclmlevprf2only**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** in **Hz or ppm** = the spectral window midpoint
  and **O2 (Hz)** of the signal to be presaturated *in this order.*

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (8-240 msec).

Type **ased** (enter) and review parameters used in the job.
The **PL21** presaturation power level can be adjusted if required.
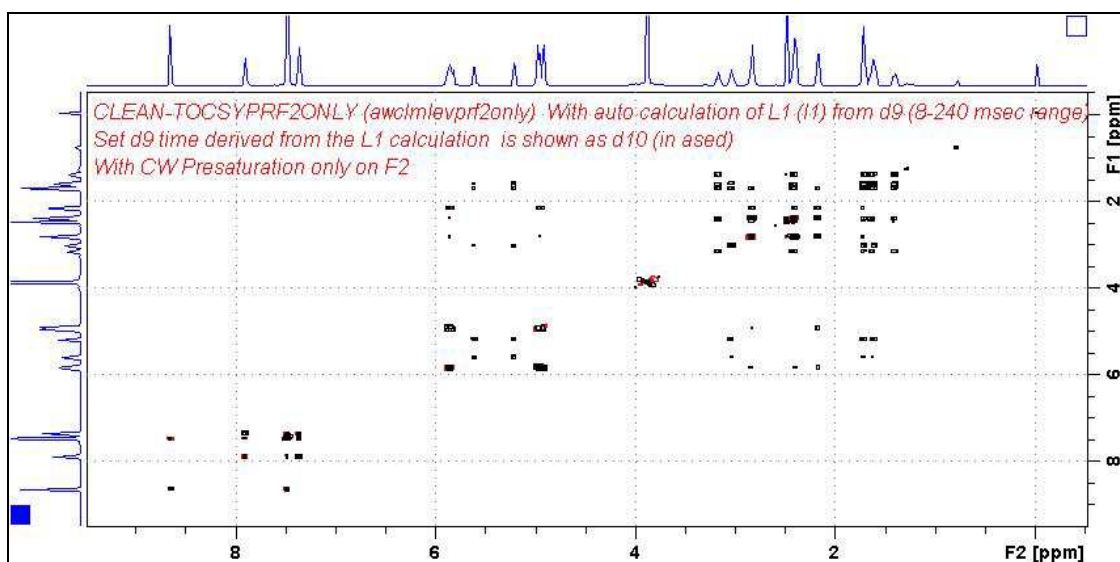Check the **D10** time derived from the requested **D9** time is OK.
Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
               WDW(F1) = WDW(F2) = QSINE
               SSB(F2) = SSB(F1) = 2
               xfb, abs1, abs2 and optionally **syma**

CLEAN-TOCSYPRF2ONLY spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm
presaturated at O2 on F2.

4.4 CLEAN-TOCSYES with Excitation Sculpting on F1

parameter set: **awcleantocsyes (+ getprosol)**
pulse programme: **awclmleves**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
    O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = repetition time =1.5 **sec** or other time of your choice.
D9 = correlation time = **80** msec msec or other time of your choice (8-240 msec).

Type **ased** (enter) and review parameters used in the job.
Check the **D10** time derived from the requested **D9** time is OK.
Verify **ES gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
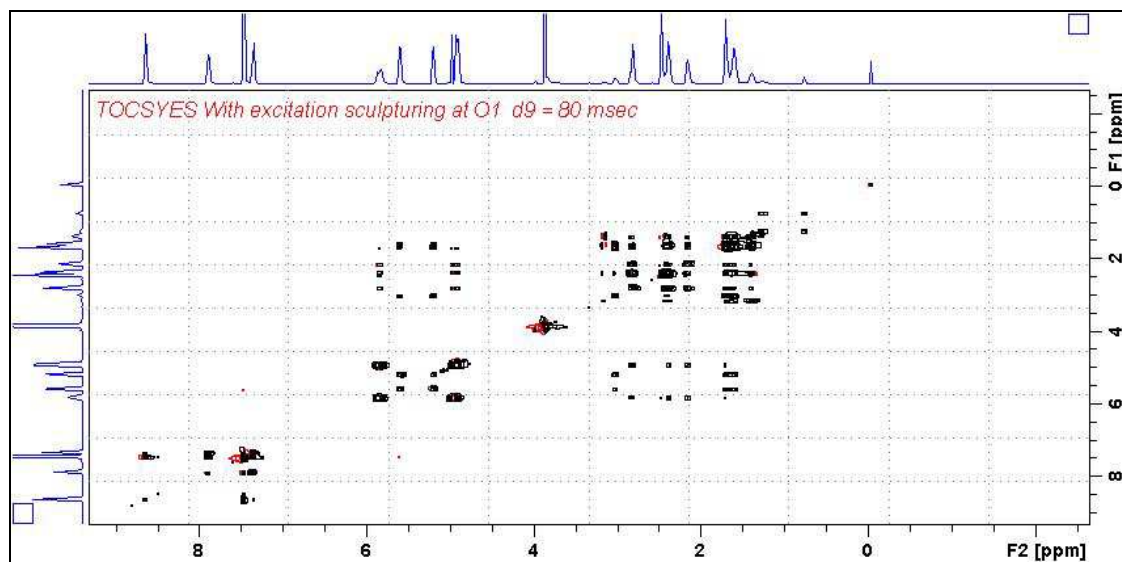Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
                 WDW(F1) = WDW(F2) = QSINE
                 SSB(F2) = SSB(F1) = 2
                 xfb, abs1, abs2 and optionally **syma**

CLEAN-TOCSYES spectrum of quinine in D$_6$-DMSO with the HOD line at 3.38 ppm ES suppressed. The spectrum is centered at the O1 frequency of the HOD line.

4.5 CLEAN-TOCSYESPR with ES and PR presaturation on F1

parameter set: **awcleantocsyespr (+ getprosol)**
pulse programme: **awclmlevespr**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
      O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (8-240 msec).

Type **ased** (enter) and review parameters used in the job.
Check the **D10** time derived from the requested **D9** time is OK.
The **PL9** presaturation power level can be adjusted if required.
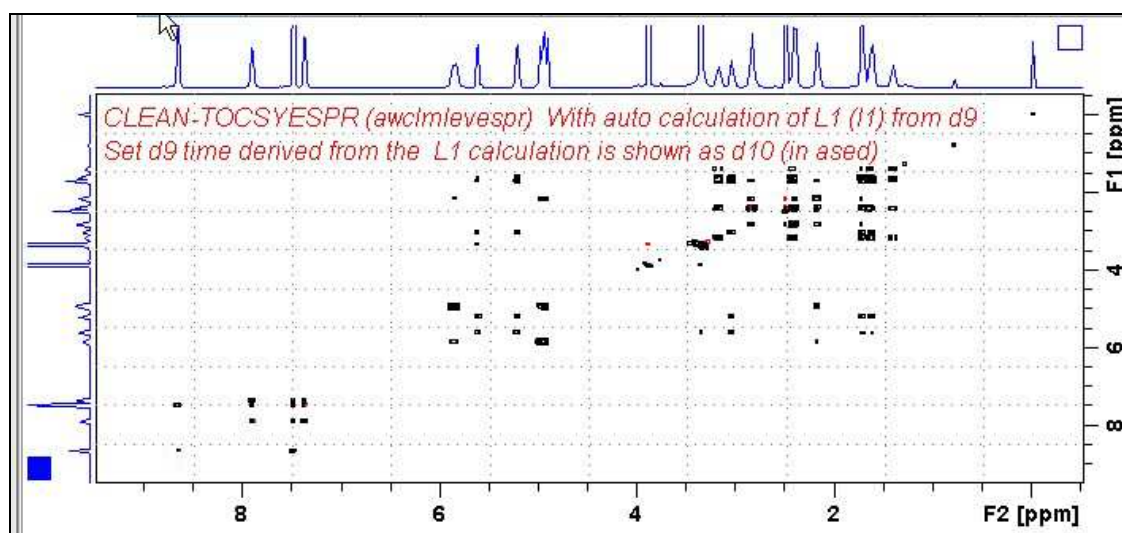Verify **ES gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!)*.

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
              WDW(F1) = WDW(F2) = QSINE
              SSB(F2) = SSB(F1) = 2
              xfb, abs1, abs2 and optionally **syma**

CLEAN-TOCSYESPR spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES and PR suppressed. The spectrum is centered at the O1 frequency of the HOD line.

4.6 CLEAN-TOCSYESPRF1PRF2 with ES and PR presaturation on F1 and PR presaturation on F2

parameter set: **awcleantocsyesprf1prf2 (+ getprosol)**
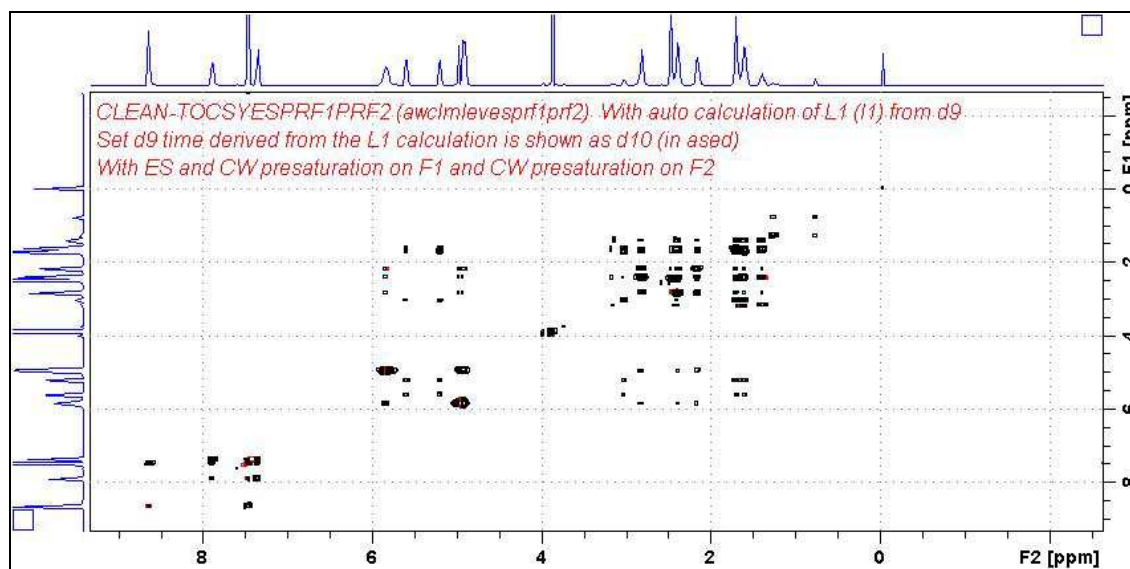pulse programme: **awmlevesprf1prf2**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be **ES** + **PR** presaturated.
    O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 2, 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (8-240 msec).

Type **ased** (enter) and review parameters used in the job.
Check the **D10** time derived from the requested **D9** time is OK.
The **PL9** and **PL21** presaturation power levels can be adjusted if required.
Verify **ES gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!)*.

Process with: **SI(F2) = SI(F1) = 1K or 2K**
             WDW(F1) = WDW(F2) = QSINE
             SSB(F2) = SSB(F1) = 2
             xfb, abs1, abs2 and optionally **syma**

CLEAN-TOCSYESPRF1PRF2 spectrum of quinine in D$_6$-DMSO with the HOD line at 3.38 ppm ES and PR suppressed and the DMSO line at 2.5 ppm PR presaturated. The spectrum is centered at the O1 frequency of the HOD line.

5.0 DIPSI2 Experiments and Parameter Sets

5.1 DIPSI2PR with PR presaturation on F1

parameter set: **awdipsi2pr (+ getprosol)**
pulse programme**: dipsi2phpr**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
    O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
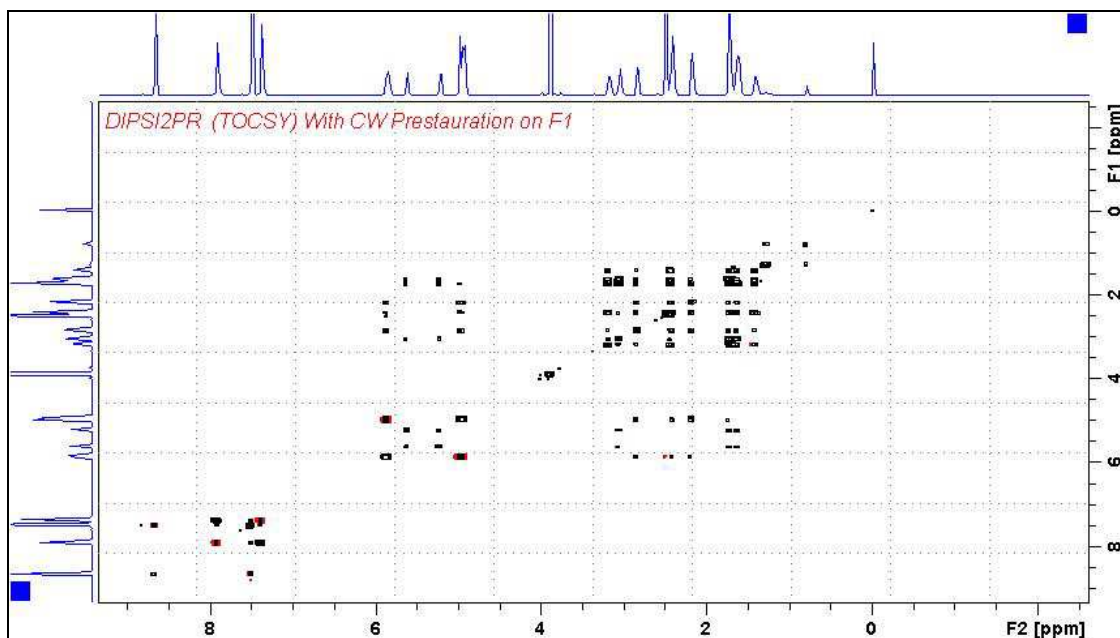The **PL9** presaturation power level can be adjusted if required.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
            WDW(F1) = WDW(F2) = QSINE
            SSB(F2) = SSB(F1) = 2
            xfb, abs1, abs2 and optionally **syma**

DIPSI2PR spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm suppressed.
The spectrum is centered at the O1 frequency of the HOD line.

5.2 DIPSI2PRF1PRF2 with PR presaturation on F1 and F2

parameter set: **awdipsi2prf1prf2 (+ getprosol)**
pulse programme: **awdipsi2prf1prf2**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be presaturated.
    O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80** msec or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
The **PL9** and **PL21** presaturation power levels can be adjusted if required.
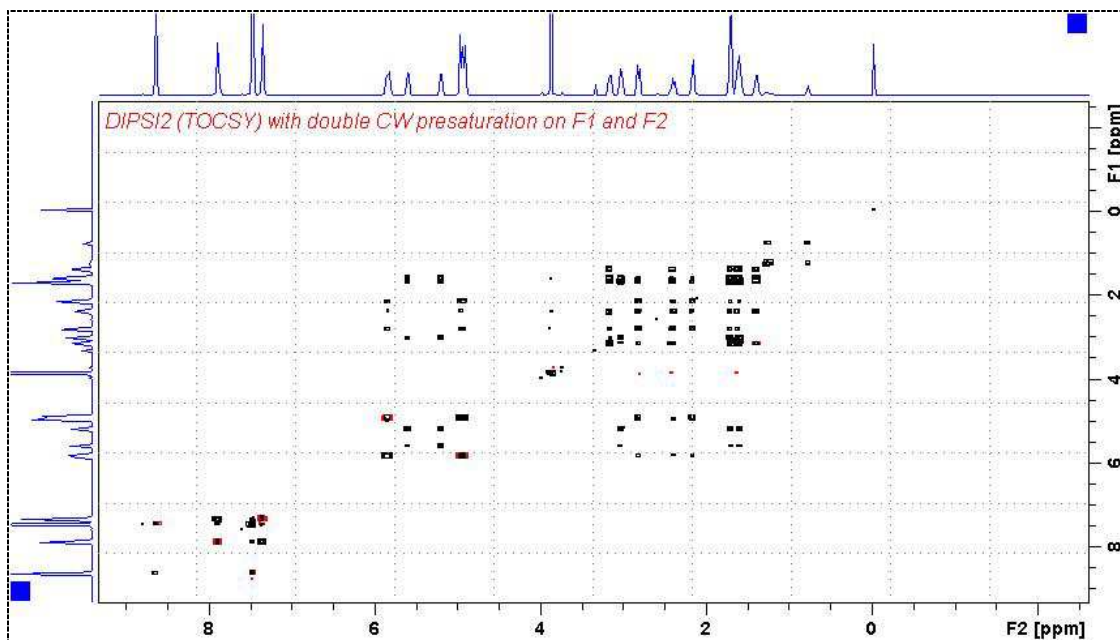Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or 2**K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

DIPSI2PRF1PRF2 spectrum of quinine in D$_6$-DMSO with the HOD and DMSO lines at 3.38
ppm and 2.5 ppm suppressed. The spectrum is centered at the O1 frequency of the HOD line.

5.3 DIPSI2PRF2ONLY with PR presaturation on F2

parameter set: **awdipsi2prf2only (+ getprosol**)
pulse programme: **awdipsi2pr2only**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** in **Hz or ppm** = the spectral window midpoint
  and **O2 (Hz)** of the signal to be presaturated *in this order.*

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
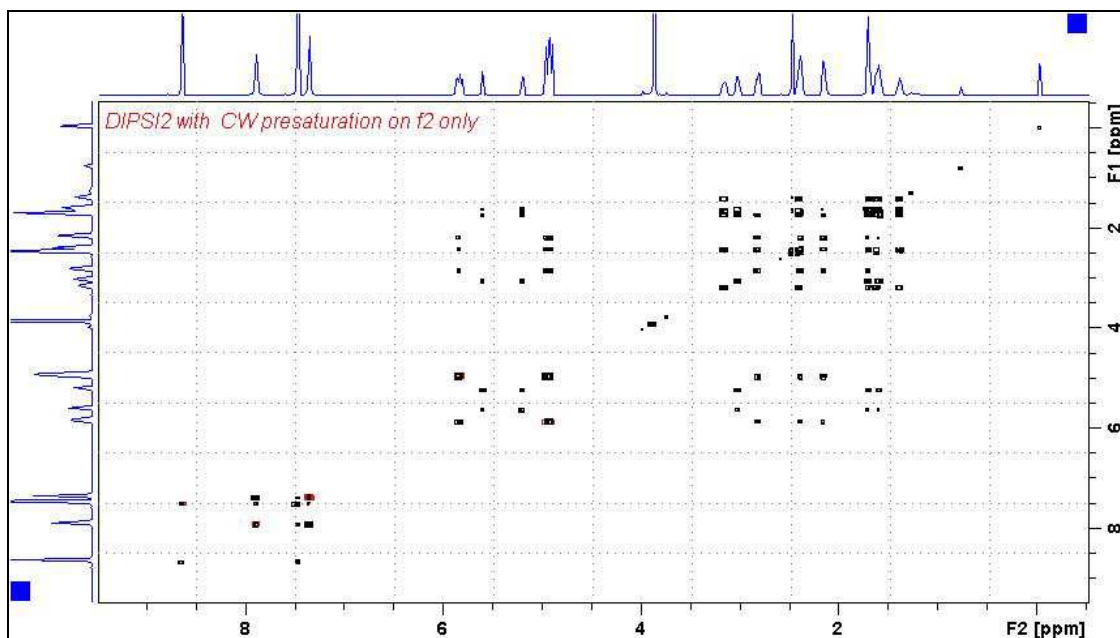**NS** = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time **= 80 msec** or other time of your choice (6-240 msec)

Type **ased** (enter) and review parameters used in the job. Verify **gradients** are OK.
The **PL21** presaturation power level can be adjusted if required.

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

Process with: **SI(F2) = SI(F1) = 1K or 2K**
          WDW(F1) = WDW(F2) = QSINE
          SSB(F2) = SSB(F1) = 2
          xfb, abs1, abs2 and optionally **syma**

DIPSI2PRF2ONLY spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm
presaturated at O2 on F2.

5.4 DIPSI2ES with Excitation Sculpting on F1

parameter set: **awdipsi2es (+ getprosol)**
pulse programme: **awdipsi2es**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
        O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = repetition time = **1.5 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
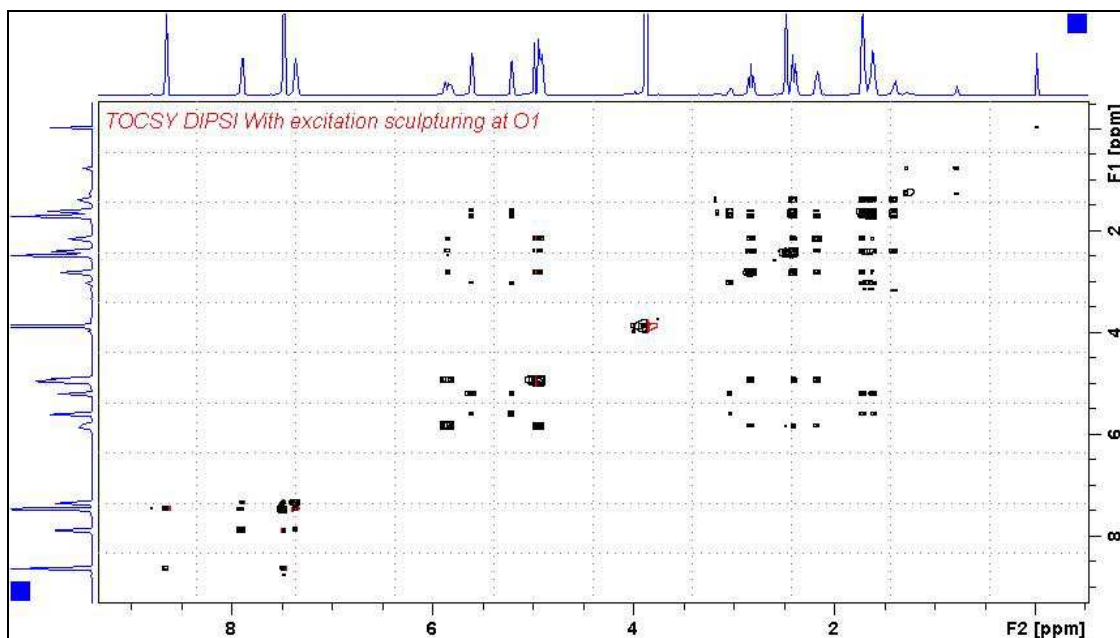Verify **ES gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!)*.

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
              WDW(F1) = WDW(F2) = QSINE
              SSB(F2) = SSB(F1) = 2
              xfb, abs1, abs2 and optionally **syma**

DIPSI2ES spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES suppressed.
The spectrum is centered at the O1 frequency of the HOD line.

5.5 DIPSI2ESPR with ES and PR presaturation on F1

parameter set: **awdipsi2espr (+ getprosol)**
pulse programme: **awdipsi2espr**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
        O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
The **PL9** presaturation power level can be adjusted if required.
Verify **ES gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
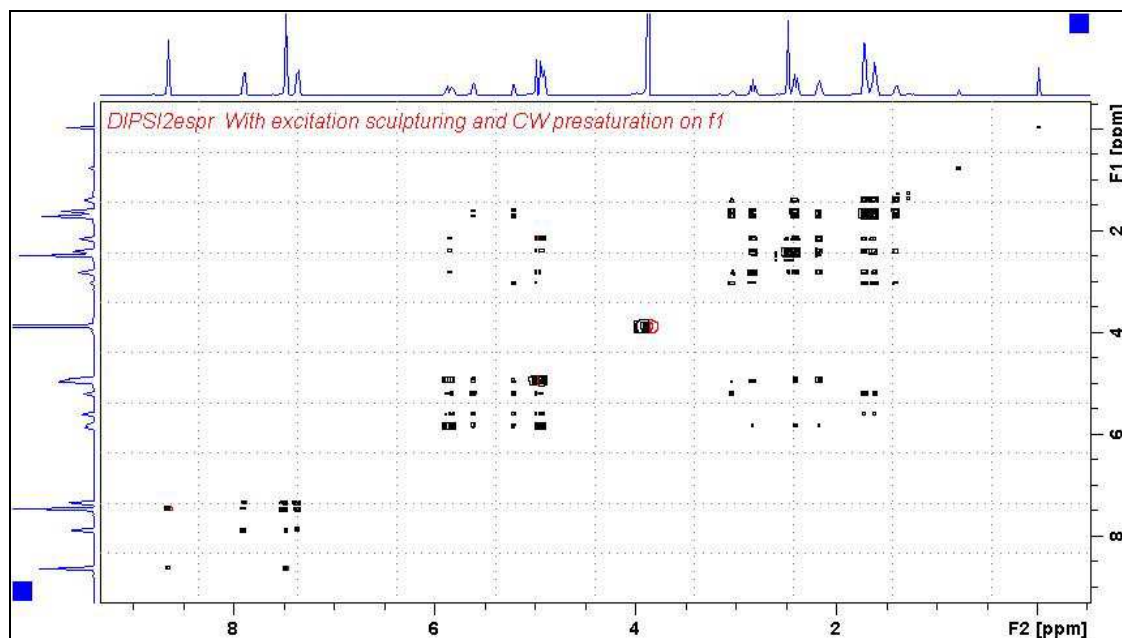Set **receiver gain** using **RGA** *(important!)*.

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

DIPSI2ESPR spectrum of quinine in D$_6$-DMSO with the HOD line at 3.38 ppm ES and PR suppressed. The spectrum is centered at the O1 frequency of the HOD line.

5.6 DIPSI2ESPRF1PRF2 with ES and PR presat on F1 and PR presat on F2

parameter set: **awdipsi2esprf1prf2 (+ getprosol)**
pulse programme: **awdipsi2esprf1prf2**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be **ES** + **PR** presaturated.
    O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
The **PL9** and **PL21** presaturation power levels can be adjusted if required.
Verify **ES gradients** are OK and that a **2000 usec squa100.1000** shaped pulse is used.
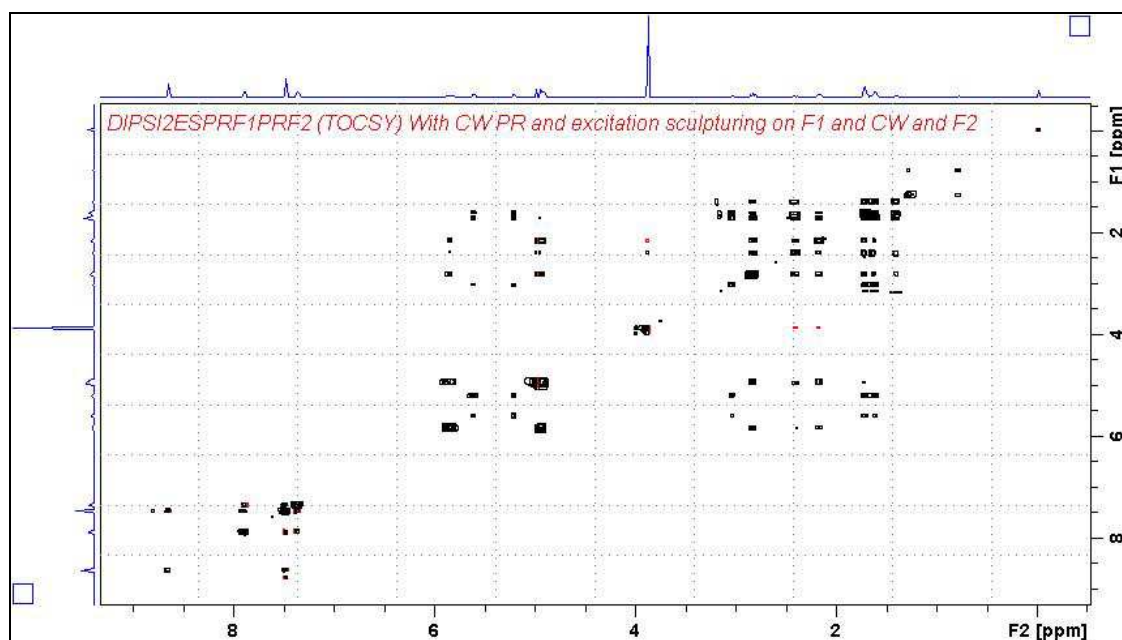Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
           WDW(F1) = WDW(F2) = QSINE
           SSB(F2) = SSB(F1) = 2
           xfb, abs1, abs2 and optionally **syma**

DIPSI2ESPRF1PRF2 spectrum of quinine in D$_6$-DMSO with the HOD line at 3.38 ppm ES
and PR suppressed and the DMSO line at 2.5 ppm PR presaturated. The spectrum is centered at
the O1 frequency of the HOD line.

6.0 NOESY Experiments and Parameter Sets

6.1 awnoesypr

6.2 awnoesyprf1prf2

6.3 awnoesyprf2only

6.4 awnoesyes

6.5 awnoesyespr

6.6 awnoesyesprf1prf2

6.1 NOESYPR with PR presaturation on F1

parameter set: **awnoesypr (+ getprosol)**
pulse programme: **awnoesygppr**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
     O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D8 = NOE mixing time **= 0.5 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
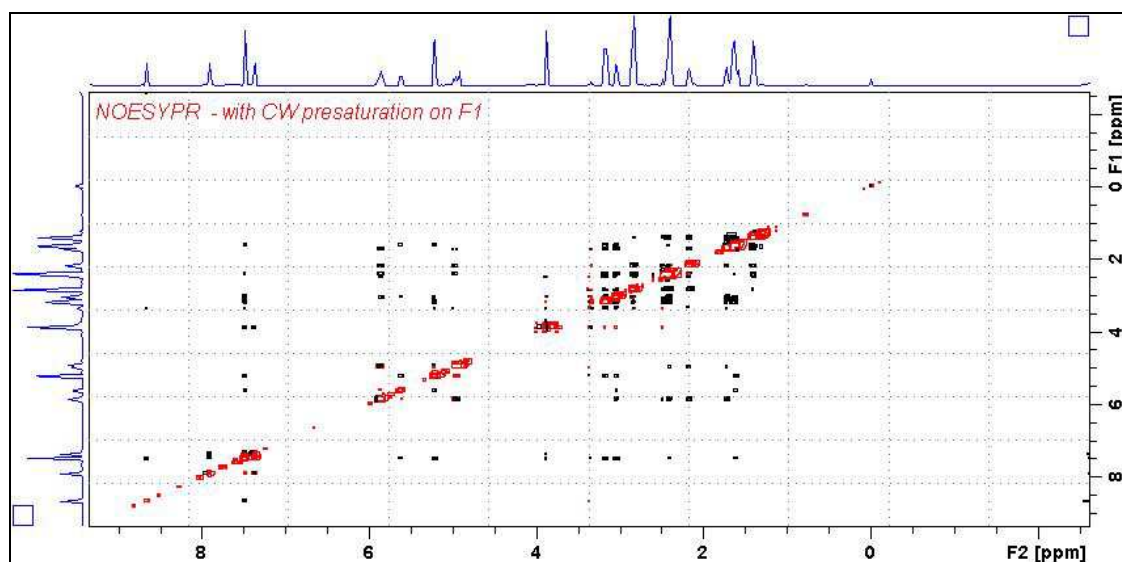The **PL9** presaturation power level can be adjusted if required.
Set **receiver gain** using **RGA** *(important!)*.

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
               WDW(F1) = WDW(F2) = QSINE
               SSB(F2) = SSB(F1) = 2
               xfb, abs1, abs2 and optionally **syma**

NOESYPR spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm suppressed.
The spectrum is centered at the O1 frequency of the HOD line.

6.2 NOESYPRF1PRF2 with PR presaturation on F1 and F2

parameter set: **awnoesyprf1prf2 (+ getprosol)**
pulse programme: **awnoesygpprf1prf2**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be presaturated.
      O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D8 = NOE mixing time = **0.5 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
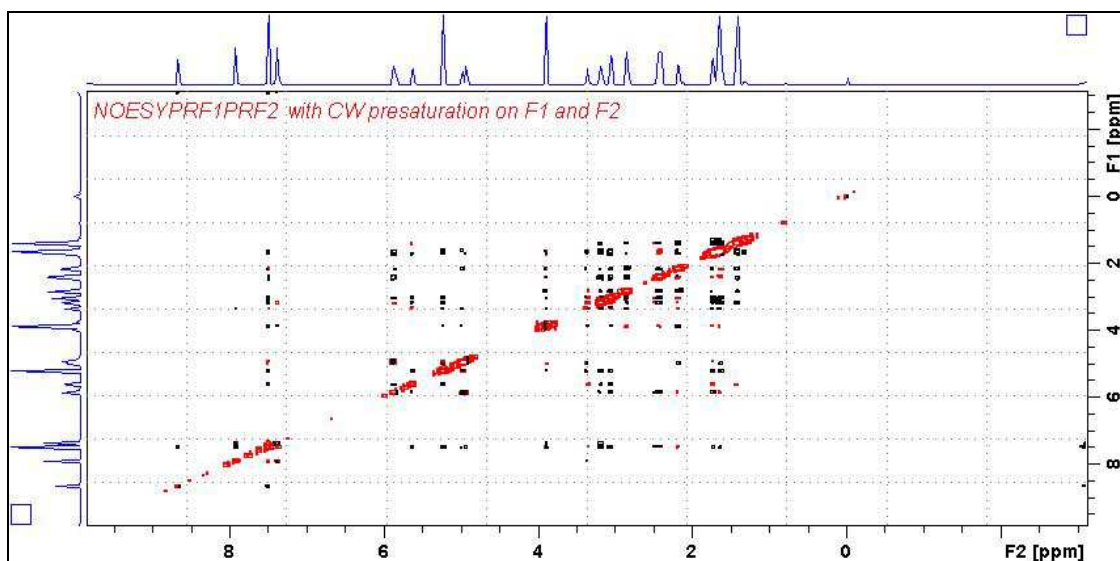The **PL9** and **PL21** presaturation power levels can be adjusted if required.
Set **receiver gain** using **RGA** *(important!)*.
Process with: **SI(F2) = SI(F1) = 1K** or **2K**
                    WDW(F1) = WDW(F2) = QSINE
                    SSB(F2) = SSB(F1) = 2
                    xfb, abs1, abs2 and optionally **syma**

NOESYPRF1PRF2 spectrum of quinine in D_6-DMSO with the HOD and DMSO lines at 3.38 ppm and 2.5 ppm suppressed. The spectrum is centered at the O1 frequency of the HOD line.

6.3 NOESYPRF2ONLY with PR presaturation on F2

parameter set: **awnoesyprf2only (+ getprosol**)
pulse programme: **awnoesygpprf2only**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** in **Hz or ppm** = the spectral window midpoint
  and **O2 (Hz)** of the signal to be presaturated *in this order.*

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
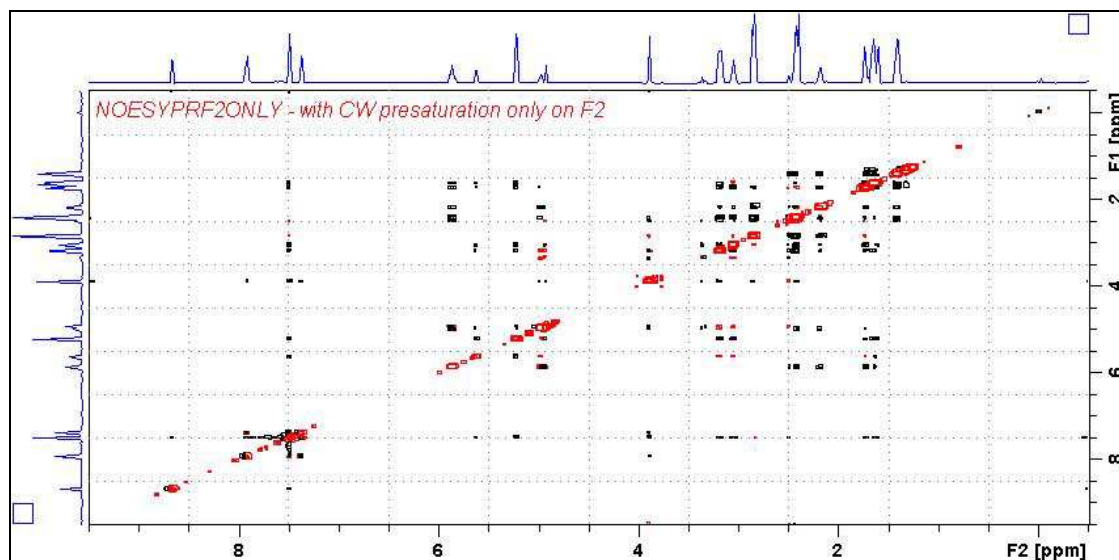**D1** = presaturation time = **2 sec** or other time of your choice.
D8 = NOE mixing time = **0.5 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
The **PL21** presaturation power level can be adjusted if required.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
               WDW(F1) = WDW(F2) = QSINE
               SSB(F2) = SSB(F1) = 2
               xfb, abs1, abs2 and optionally **syma**

NOESYPRF2ONLY spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm
presaturated at O2 on F2.

6.4 NOESYES with Excitation Sculpting presaturation on F1

parameter set: **awnoesyes (+ getprosol)**
pulse programme: **noesyesgpph**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
    O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = repetition time = **1.5 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
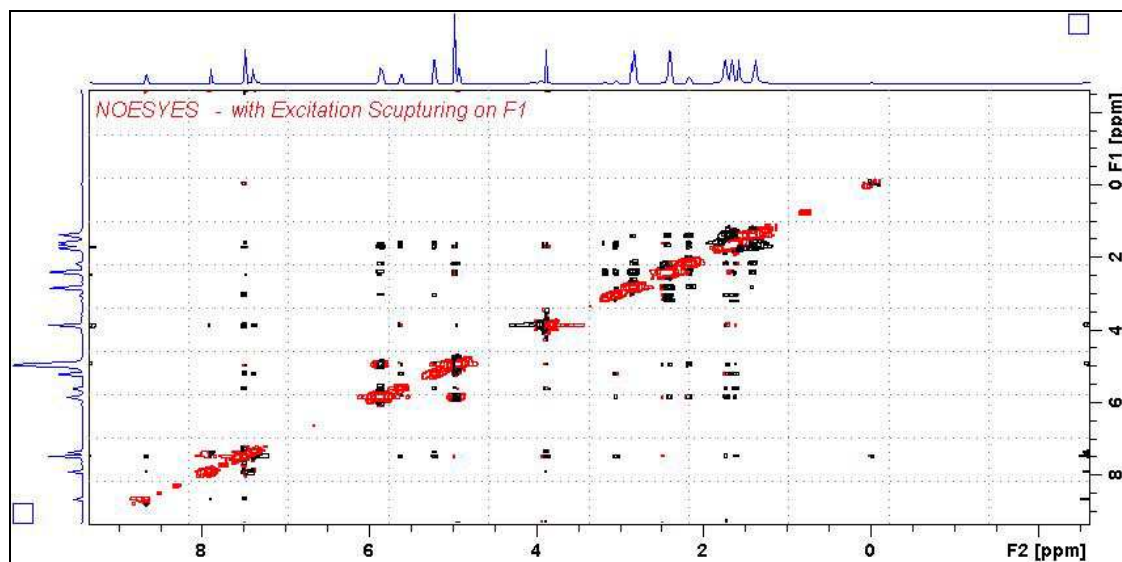Verify that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

NOESYES spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES suppressed.
The spectrum is centered at the O1 frequency of the HOD line.

6.5 NOESYESPR with ES and PR presaturation on F1

parameter set: **awnoesyespr (+ getprosol)**
pulse programme: **awnoesygpespr**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
        O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
D8 = NOE mixing time **= 0.5 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
The **PL9** presaturation power level can be adjusted if required.
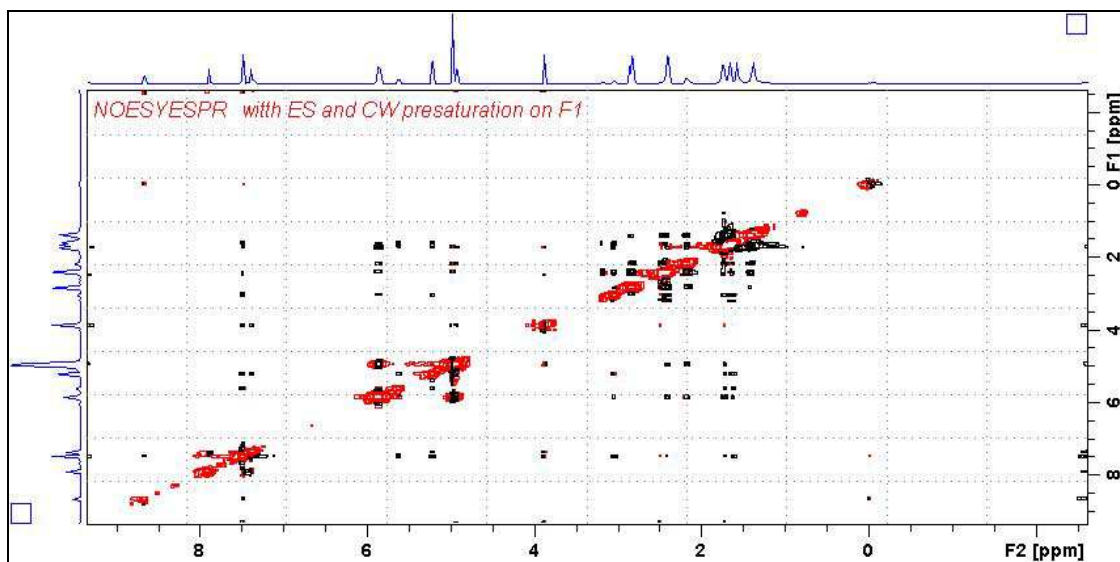Verify that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!)*.

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

NOESYESPR spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES and PR
suppressed. The spectrum is centered at the O1 frequency of the HOD line.

6.6 NOESYESPRF1PRF2 with ES and PR presat on F1 and PR presat on F2

parameter set: **awnoesyesprf1prf2 (+ getprosol)**
pulse programme: aw**noesygpesprf1prf2**

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be **ES** + **PR** presaturated **O1** = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
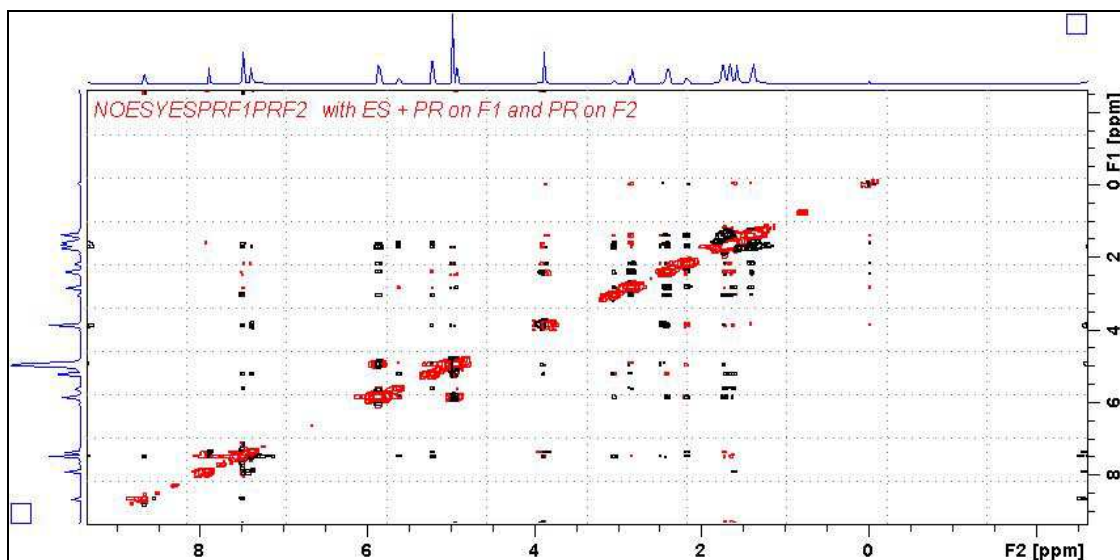**D8** (NOE mixing time) **= 0.5 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
The **PL9** and **PL21** presaturation power levels can be adjusted if required.
Verify that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
          WDW(F1) = WDW(F2) = QSINE
          SSB(F2) = SSB(F1) = 2
          xfb, abs1, abs2 and optionally **syma**

NOESYESPRF1PRF2 spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES and PR suppressed and the DMSO line at 2.5 ppm PR presaturated. The spectrum is centered at the O1 frequency of the HOD line.

7.0 ROESY Experiments and Parameter Sets

ROESY experiments with CW spin lock

7.1 ROESYPR with PR presaturation on F1 at O1

parameter set: **awroesypr (+ getprosol)**
pulse programme: **roesyphpr** (with CW spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
    O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job.
The **PL9** presaturation power level can be adjusted if required.
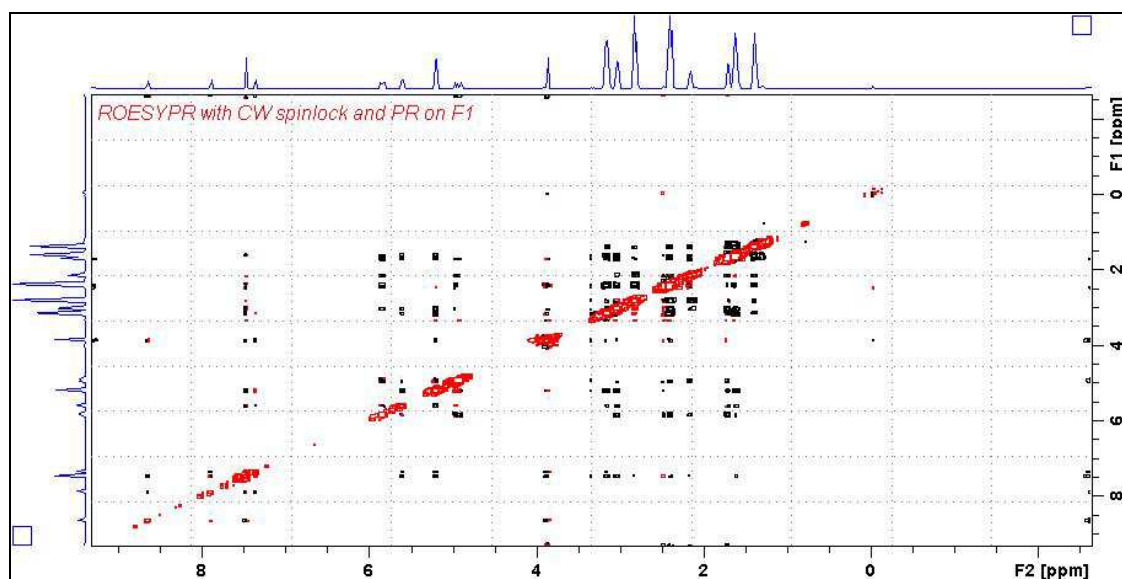Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
        WDW(F1) = WDW(F2) = QSINE
        SSB(F2) = SSB(F1) = 2
        xfb, abs1, abs2 and optionally **syma**

ROESYPR spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm suppressed.
The spectrum is centered at the O1 frequency of the HOD line.

7.2 ROESYPRF1PRF2 with PR presaturation on F1 and F2

parameter set: **awroesyprf1prf2 (+ getprosol)**
pulse programme: **awroesyprf1prf2** (with CW spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be presaturated.
        O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job.
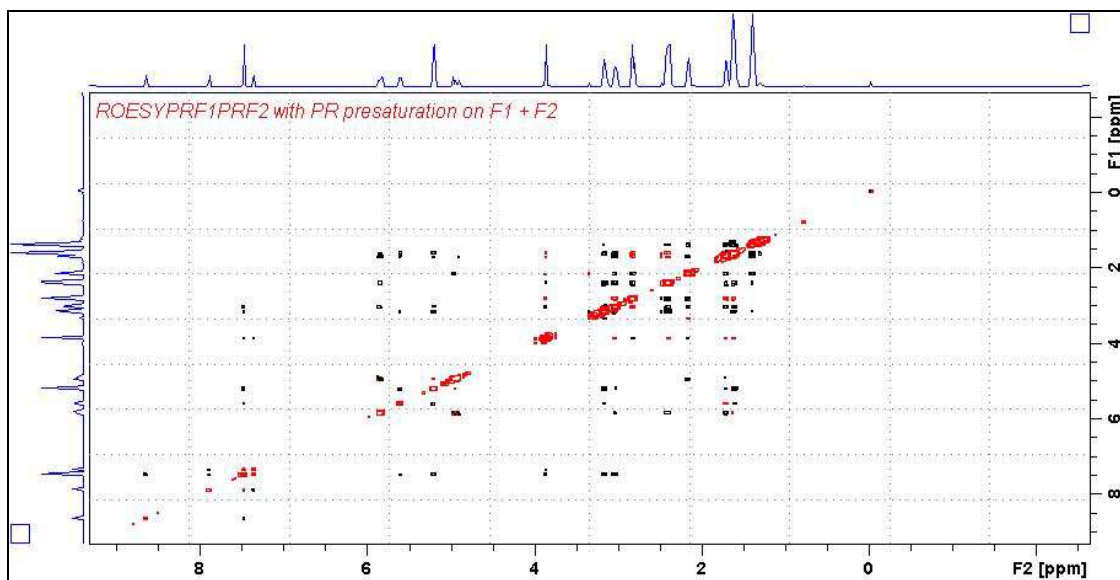The **PL9** and **PL21** presaturation power levels can be adjusted if required.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

ROESYPRF1PRF2 spectrum of quinine in D$_6$-DMSO with the HOD and DMSO lines at 3.38
ppm and 2.5 ppm suppressed. The spectrum is centered at the O1 frequency of the HOD line.

7.3 ROESYPRF2ONLY with PR presaturation on F2

parameter set: **awroesyprf2only (+ getprosol)**
pulse programme: **awroesyprf2only** (with CW spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** in **Hz or ppm** = the spectral window midpoint
   and **O2 (Hz)** of the signal to be presaturated *in this order.*

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

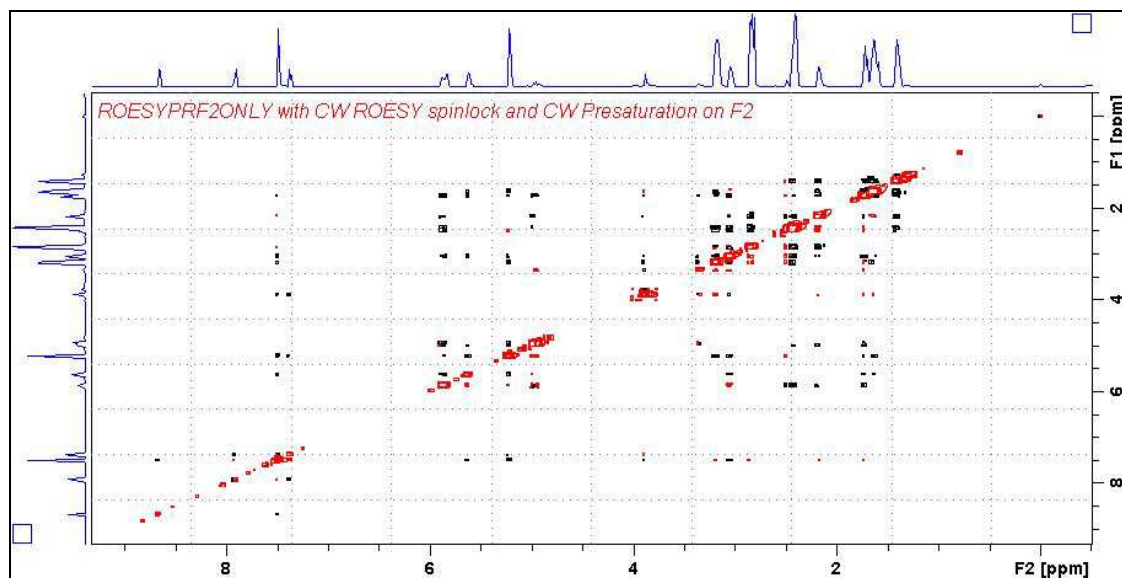Type **ased** (enter) and review parameters used in the job and check gradients are OK. The **PL21** presaturation power level can be adjusted if required. Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
              WDW(F1) = WDW(F2) = QSINE
              SSB(F2) = SSB(F1) = 2
              xfb, abs1, abs2 and optionally **syma**

ROESYPRF2ONLY spectrum of quinine in D$_6$-DMSO with the HOD line at 3.38 ppm presaturated at O2 on F2.

7.4 ROESYES with Excitation Sculpting on F1

parameter set: **awroesyes (+ getprosol)**
pulse programme: **roesyesgpph** (with CW spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
        O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = repetition time = **1.5 sec** or other time of your choice.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
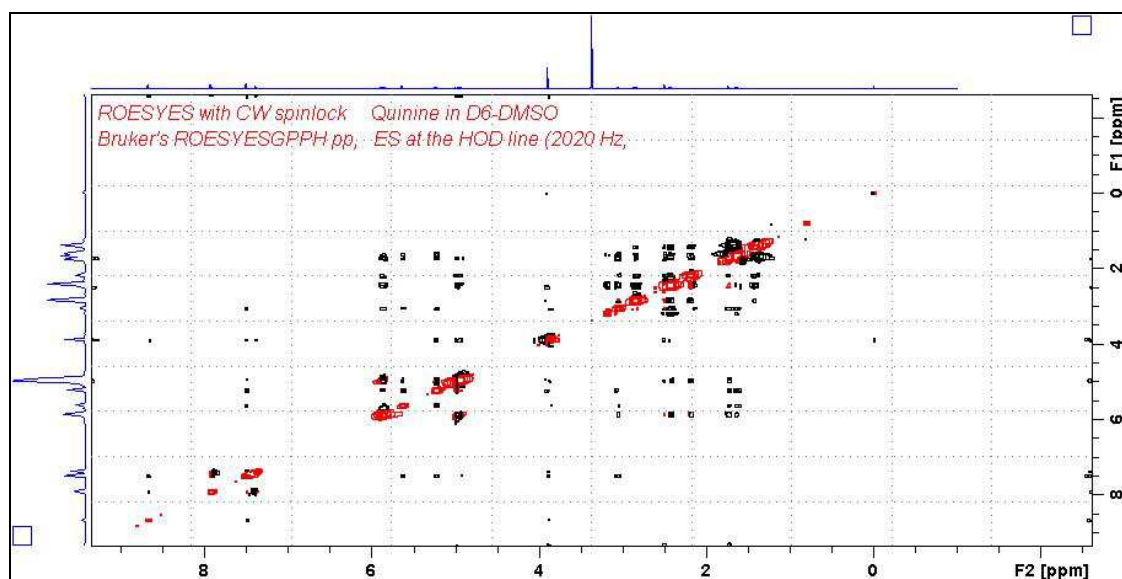Verify that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!)*.

Process with: **SI(F2) = SI(F1) = 1K or 2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

ROESYES spectrum of quinine in D$_6$-DMSO with the HOD line at 3.38 ppm ES suppressed.
The spectrum is centered at the O1 frequency of the HOD line.

7.5 ROESYESPR with ES and PR presaturation on F1

parameter set: **awroesyespr (+ getprosol)**
pulse programme: **awroesyespr** (with CW spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
      O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
P15 = CW spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
The **PL9** presaturation power level can be adjusted if required
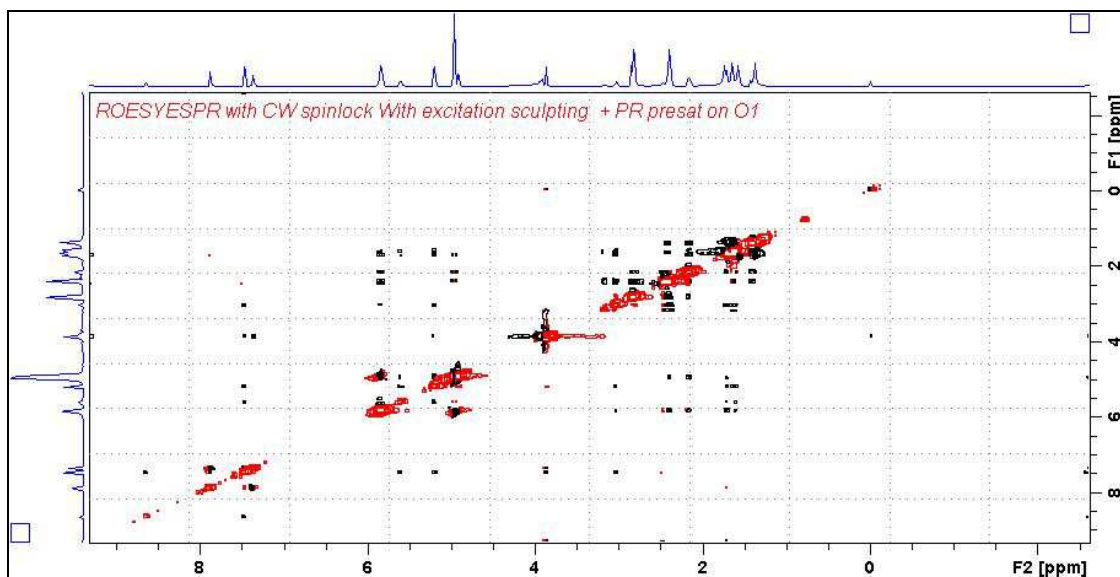Verify that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
              WDW(F1) = WDW(F2) = QSINE
              SSB(F2) = SSB(F1) = 2
              xfb, abs1, abs2 and optionally **syma**

ROESYESPR spectrum of quinine in D$_6$-DMSO with the HOD line at 3.38 ppm ES and PR suppressed. The spectrum is centered at the O1 frequency of the HOD line.

7.6 ROESYESPRF1PRF2 with ES and PR presat on F1 and PR presat on F2

parameter set: **awroesyesprf1prf2 (+ getprosol)**
pulse programme: **awroesyesprf1prf2** (with CW spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be **ES** + **PR** presaturated
        O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).
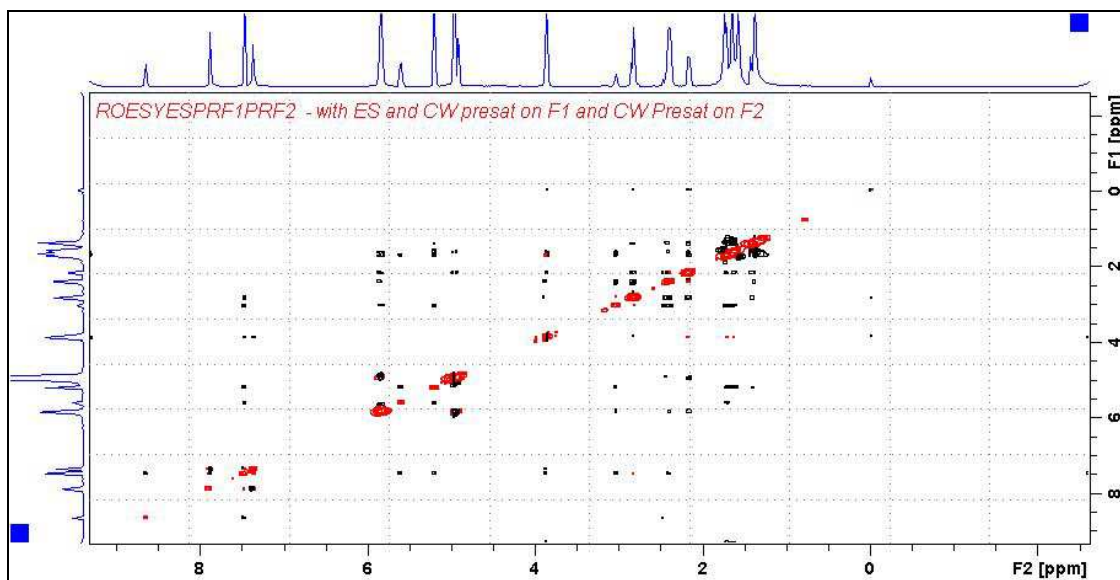
Type **ased** (enter) and review parameters used in the job and check gradients are OK.
The **PL9** and **PL21** presaturation power levels can be adjusted if required.
Verify that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

ROESYESPRF1PRF2 spectrum of quinine in D$_6$-DMSO with the HOD line at 3.38 ppm ES and PR suppressed and the DMSO line at 2.5 ppm is PR presaturated. The spectrum is centered at the O1 frequency of the HOD line.

8.0 ROESY2 Experiments and Parameter Sets

ROESY2 experiments with pulsed spin lock

8.1 ROESY2PR with PR presaturation on F1 at O1

parameter set: **awroesy2pr (+ getprosol)**
pulse programme: **roesyphpr.2** (with pulsed spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
        O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job.
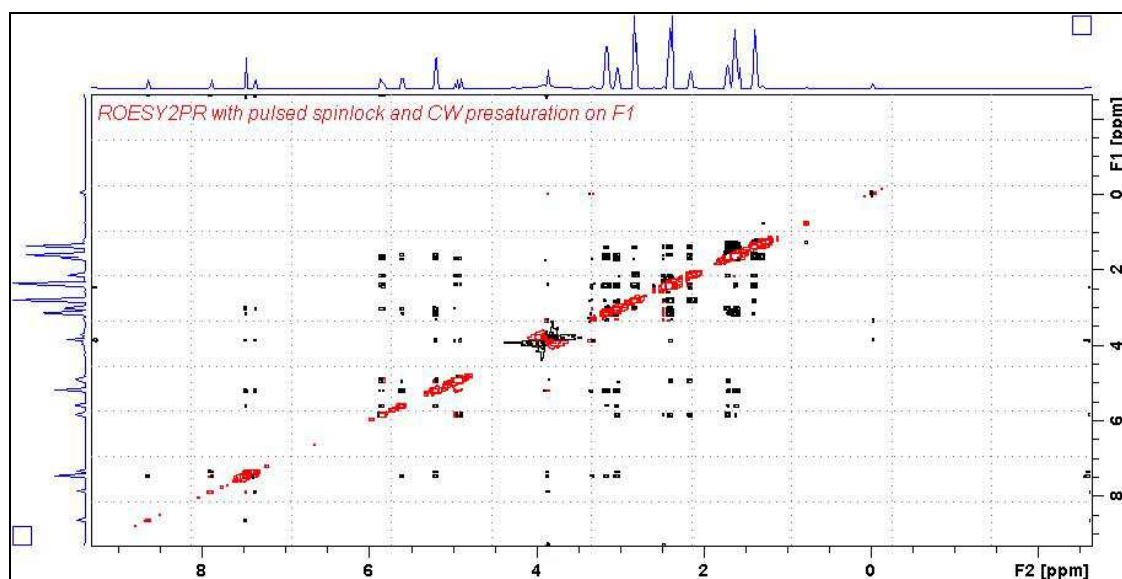The **PL9** presaturation power level can be adjusted if required
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K or 2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

ROESY2PR spectrum of quinine in D₆-DMSO with the HOD line at 3.38 ppm suppressed.
The spectrum is centered at the O1 frequency of the HOD line.

8.2 ROESY2PRF1PRF2 with PR presaturation on F1 and F2

parameter set: **awroesy2prf1prf2 (+ getprosol)**
pulse programme: **awroesy2prf1prf2** (with pulsed spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be presaturated.
    O1 = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job.
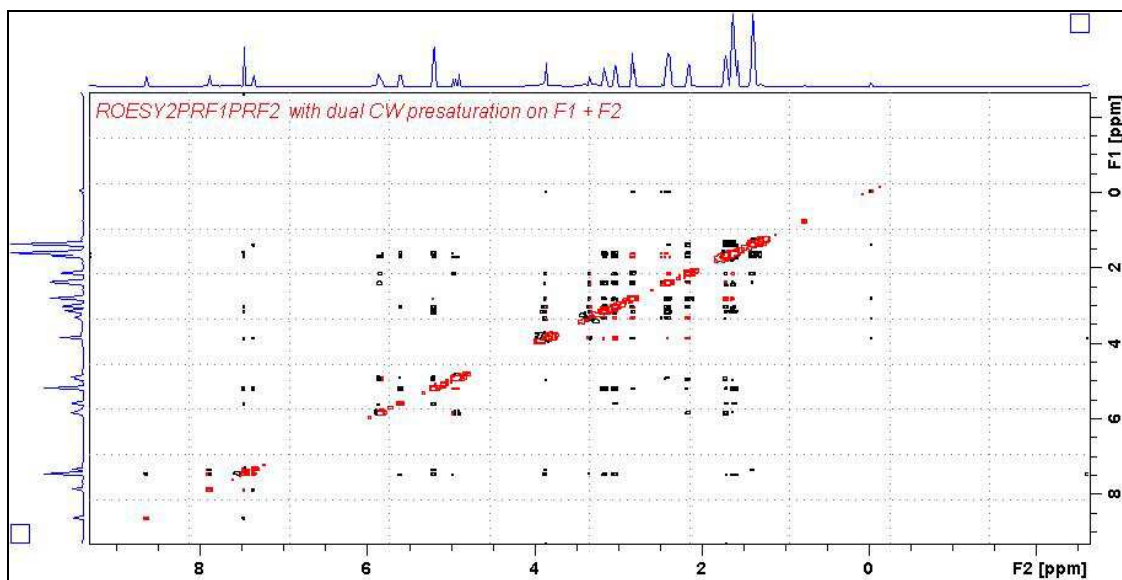The **PL9** and **PL21** presaturation power levels can be adjusted if required
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
              WDW(F1) = WDW(F2) = QSINE
              SSB(F2) = SSB(F1) = 2
              xfb, abs1, abs2 and optionally **syma**

ROESY2PRF1PRF2 spectrum of quinine in D$_6$-DMSO with the HOD and DMSO lines at 3.38
ppm and 2.5 ppm suppressed. The spectrum is centered at the O1 frequency of the HOD line.

8.3 ROESY2PRF2ONLY with PR presaturation on F2

parameter set: **awroesy2prf2only (+ getprosol)**
pulse programme: **awroesy2pr2only** (with pulsed spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that
appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box.
Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** in **Hz or ppm** = the spectral window midpoint
   and **O2 (Hz)** of the signal to be presaturated *in this order.*
.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
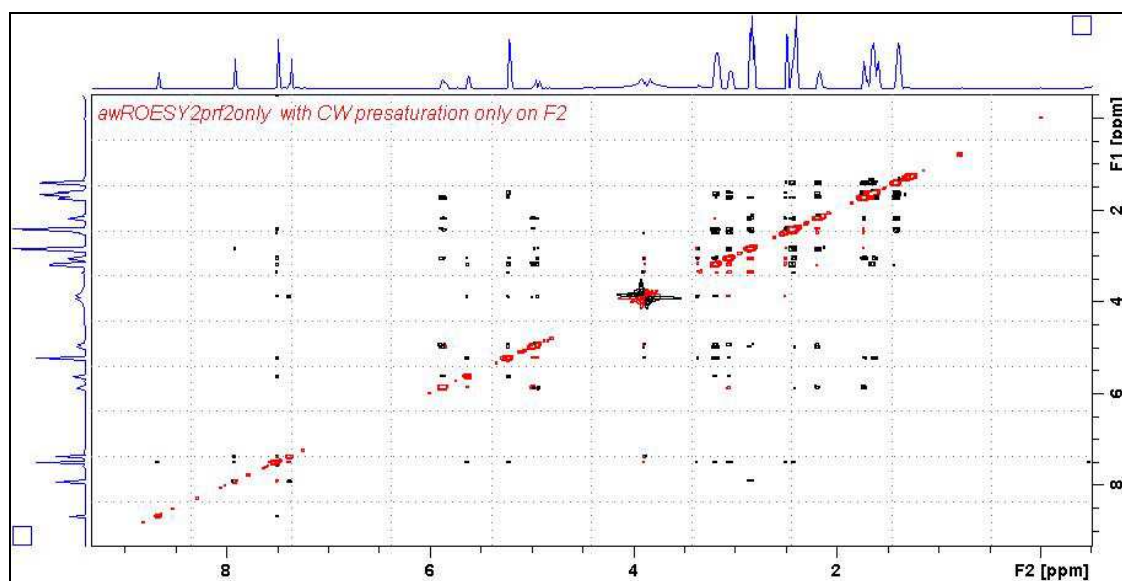The **PL21** presaturation power level can be adjusted if required.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1, abs2 and optionally **syma**

ROESY2PRF2ONLY spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm
presaturated at O2 on F2

8.4 ROESY2ES with Excitation Sculpting on F1

parameter set: **awroesy2es (+ getprosol)**
pulse programme: **roesyesgpph.2** (with pulsed spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
  O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = repetition time = **1.5 sec** or other time of your choice.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
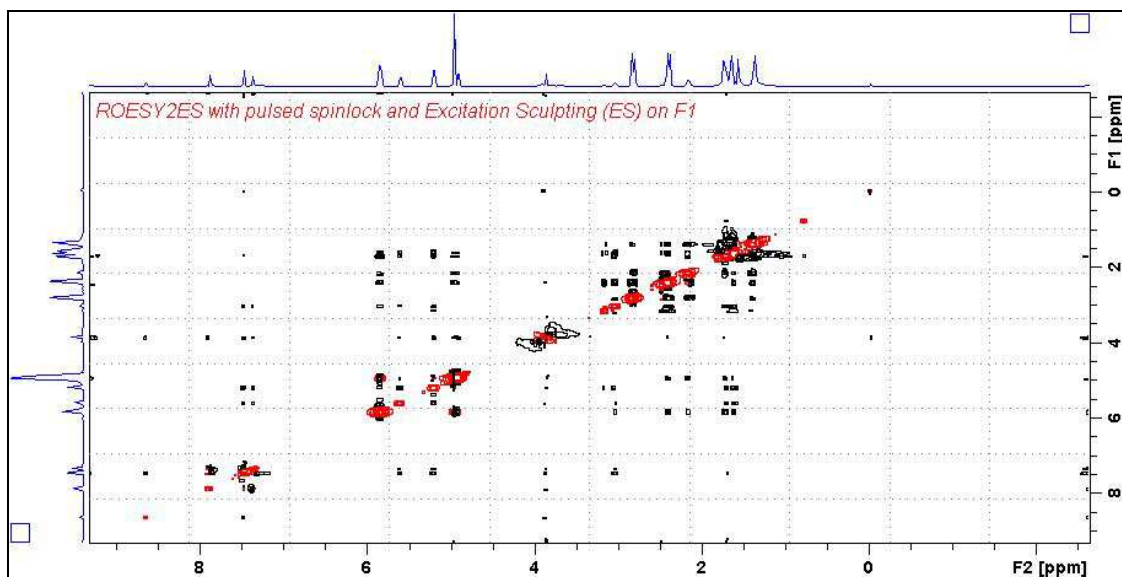Verify that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!).*

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
      WDW(F1) = WDW(F2) = QSINE
      SSB(F2) = SSB(F1) = 2
      xfb, abs1, abs2 and optionally **syma**

ROESY2ES spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES suppressed. The spectrum is centered at the O1 frequency of the HOD line.

8.5 ROESY2ESPR with ES and PR presaturation on F1

parameter set: **awroesy2espr (+ getprosol)**
pulse programme: **awroesy2espr** (with pulsed spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1 in Hz** of the signal to be presaturated.
　　　O1 = spectral window midpoint.
Type **O2** (return) and enter the **O1** frequency in Hz as the **O2** frequency.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
The **PL9** presaturation power level can be adjusted if required.
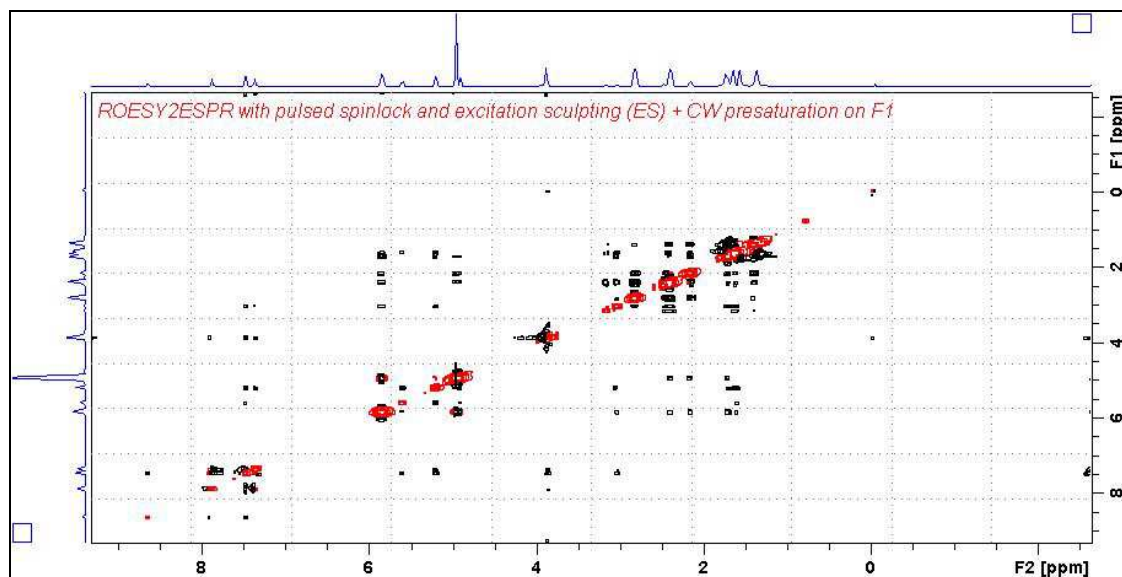Verify that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!)*.

Process with:　**SI(F2) = SI(F1) = 1K** or **2K**
　　　　　　　WDW(F1) = WDW(F2) = QSINE
　　　　　　　SSB(F2) = SSB(F1) = 2
　　　　　　　xfb, abs1, abs2 and optionally **syma**

ROESY2ESPR spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES and PR suppressed. The spectrum is centered at the O1 frequency of the HOD line.

8.6 ROESY2ESPRF1PRF2 with ES and PR presaturation on F1 and PR presaturation on F2

parameter set: **awroesy2esprf1prf2 (+ getprosol)**
pulse programme: **awroesy2esprf1prf2** (with pulsed spin lock)

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Type **eda** (enter) and enter **SW(F2) in ppm**, note the spectral window in **Hz** that appears in the **SWH(F2)** box and copy and paste this value into the **SWH(F1)** box. Check **SWH(F2) = SWH(F1)** in Hz including all dp's.

Enter **O1** and **O2 in Hz** *(in this order!)* of the signals to be **ES** + **PR** presaturated **O1** = spectral window midpoint.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 4, 8 (multiple of 4 or 8 recommended), **DS** = 4 or 8.
D1 = presaturation time = **2 sec** or other time of your choice.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
The **PL9** and **PL21** presaturation power levels can be adjusted if required.
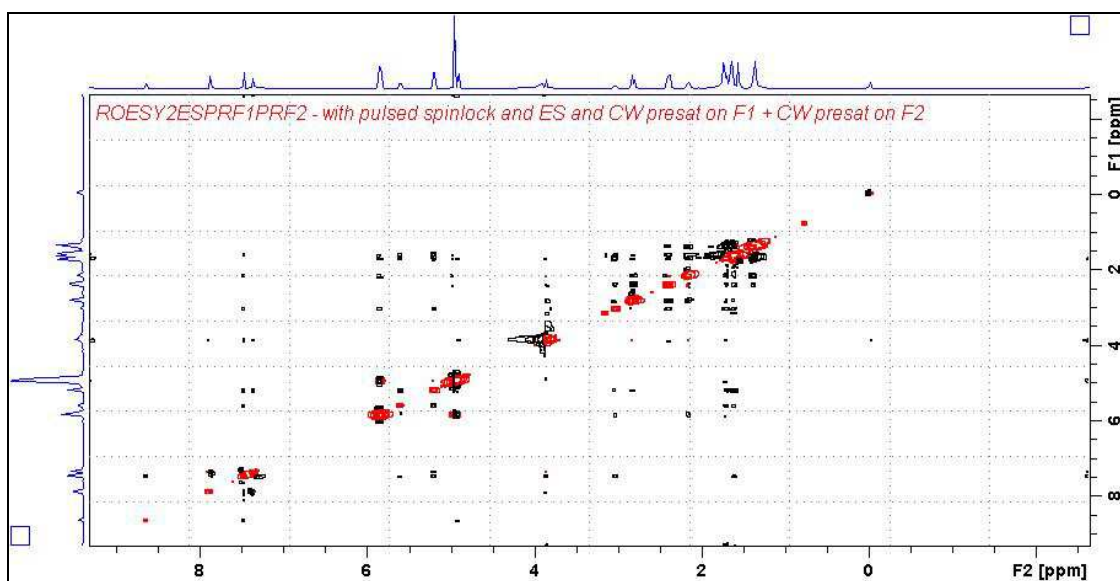Verify that a **2000 usec squa100.1000** shaped pulse is used.
Set **receiver gain** using **RGA** *(important!)*.

Process with: **SI(F2) = SI(F1) = 1K** or **2K**
            WDW(F1) = WDW(F2) = QSINE
            SSB(F2) = SSB(F1) = 2
            xfb, abs1, abs2 and optionally **syma**

ROESY2ESPRF1PRF2 spectrum of quinine in D_6-DMSO with the HOD line at 3.38 ppm ES and PR suppressed and the DMSO line at 2.5 ppm is PR presaturated. The spectrum is centered at the O1 frequency of the HOD line.