



KJM 9250

**AVII-600 COSY, TOCSY, CLEAN-TOCSY, DIPSI2, NOESY,  
ROESY, ROESY2 spectra with CW presaturation (PR) and/or  
Excitation Sculpturing (ES) peak suppression**

Version 7.3

Topspin 3.2 Windows 7 AVII600



© Professor Emeritus Alistair Lawrence Wilkins,  
University of Waikato, New Zealand.  
January 2020

# AVII-600 COSY, TOCSY, CLEAN-TOCSY, DIPSI2, NOESY, ROESY, ROESY2 spectra 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  $^1\text{H}$  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  $^1\text{H}$  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 awcosypr**

**2.2 awcosyprf1prf2**

**2.3 awcosyprf2only**

**2.4 awcosyes**

**2.5 awcosyespr**

**2.6 awcosyesprf1prf2**

## 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** =  $\theta$  degree excitation pulse time, typically use a  $45^\circ$  or  $90^\circ$  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.

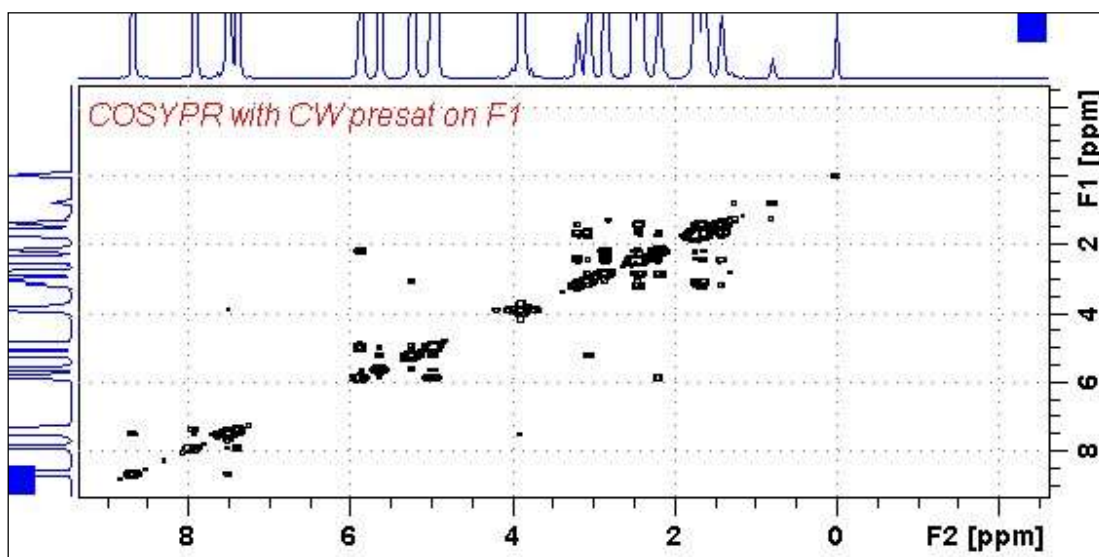
Set **receiver gain** using **RGA** (*important!*).

Process with: **SI(F2) = SI(F1) = 1K or 2K**

**WDW(F1) = WDW(F2) = SINE**

**SSB(F2) = SSB(F1) = 0**

**xfb, abs1, abs2 sym**



600 MHz **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** =  $\theta$  degree excitation pulse time, typically use a  $45^\circ$  or  $90^\circ$  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.

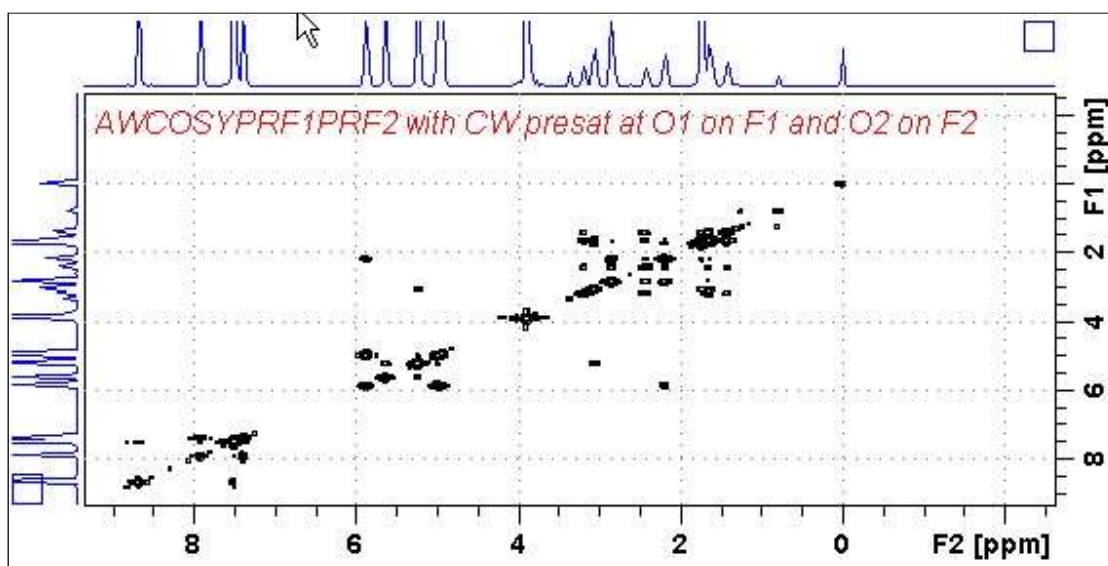
Set **receiver gain** using **RGA** (*important!*).

Process with: **SI(F2) = SI(F1) = 1K** or **2K**

**WDW(F1) = WDW(F2) = SINE**

**SSB(F2) = SSB(F1) = 0**

**xfb, abs1, abs2 sym**



600 MHz **COSYPRF1PRF2** spectrum of quinine in D<sub>6</sub>-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).

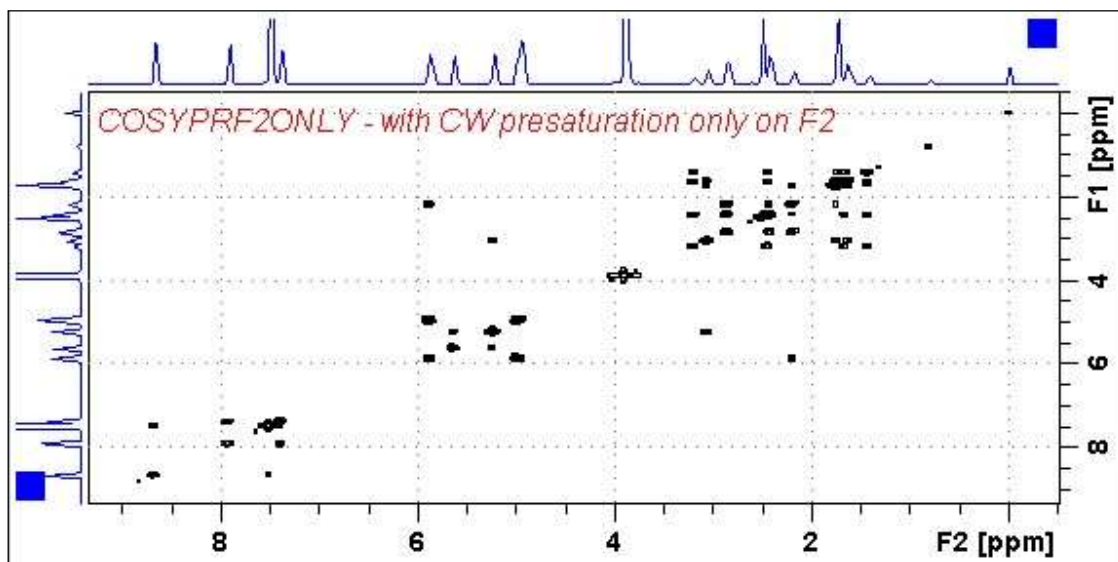
**NS** = 2, 4, 8 (any number is OK), **DS** = 2, 4 or 8.

**P0** =  $\theta$  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 **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**



600 MHz **COSYPRF2ONLY** spectrum of quinine in D<sub>6</sub>-DMSO with the HOD line at 3.38 ppm presaturated at O2 on F2.

## 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.

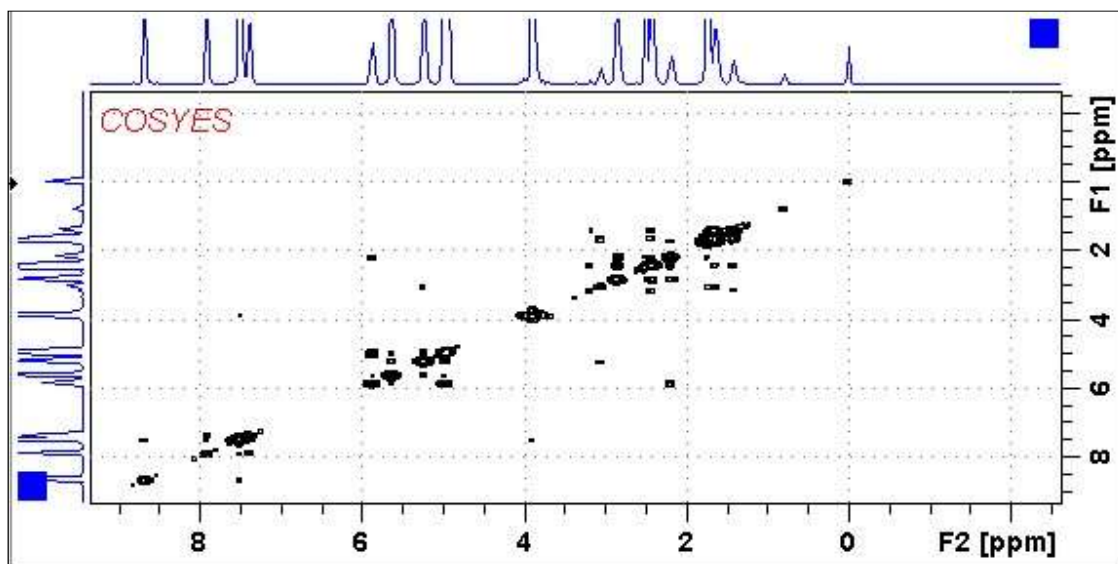
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz COSYES spectrum of quinine in D<sub>6</sub>-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 **ES + PR** 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.

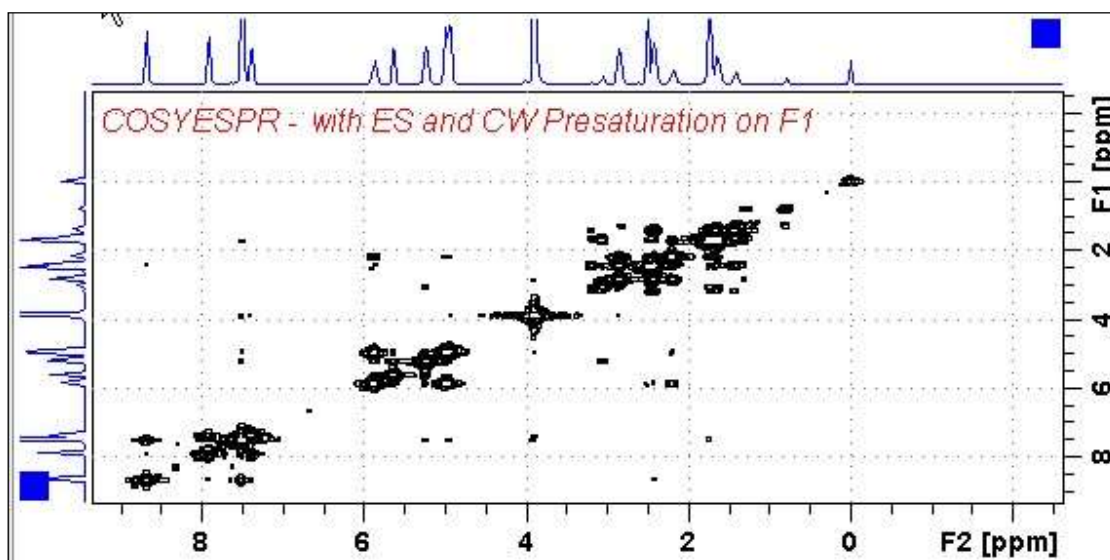
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz COSYESPR spectrum of quinine in D<sub>6</sub>-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.

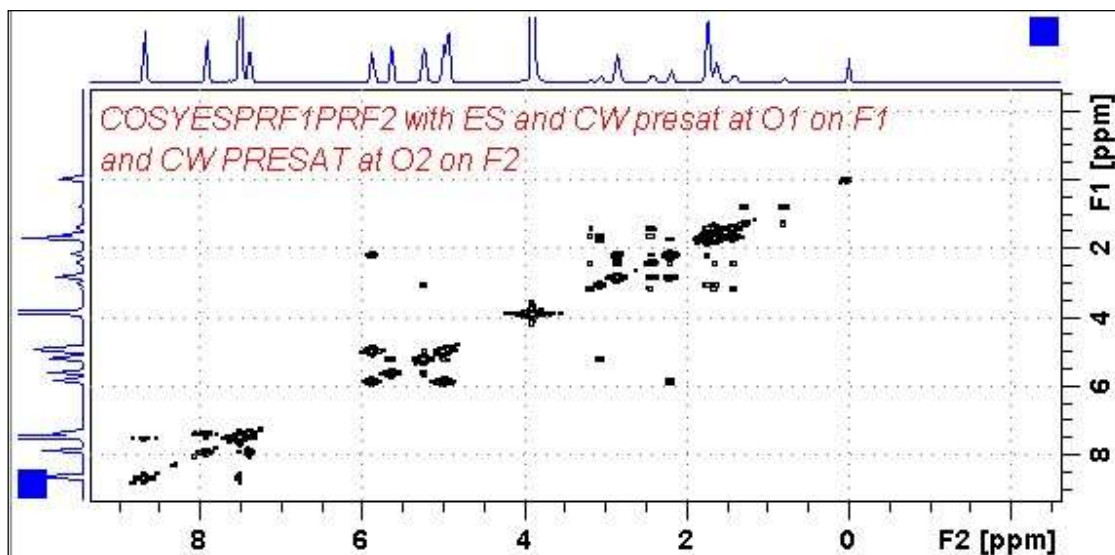
Enter **O1** and **O2 in Hz** (*in this order!*) of the signals to be **ES + PR** presaturated at **O1 on F1** and **PR** presaturated at **O2 on F2**.

**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**



600 MHz **COSYESPRF1PRF2** spectrum of quinine in D<sub>6</sub>-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 awtocsypr**

**3.2 awtocsyprf1prf2**

**3.3 awtocsyprf2only**

**3.4 awtocsyes**

**3.5 awtocsyespr**

**3.6 awtocsyesprf1prf2**

### 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.

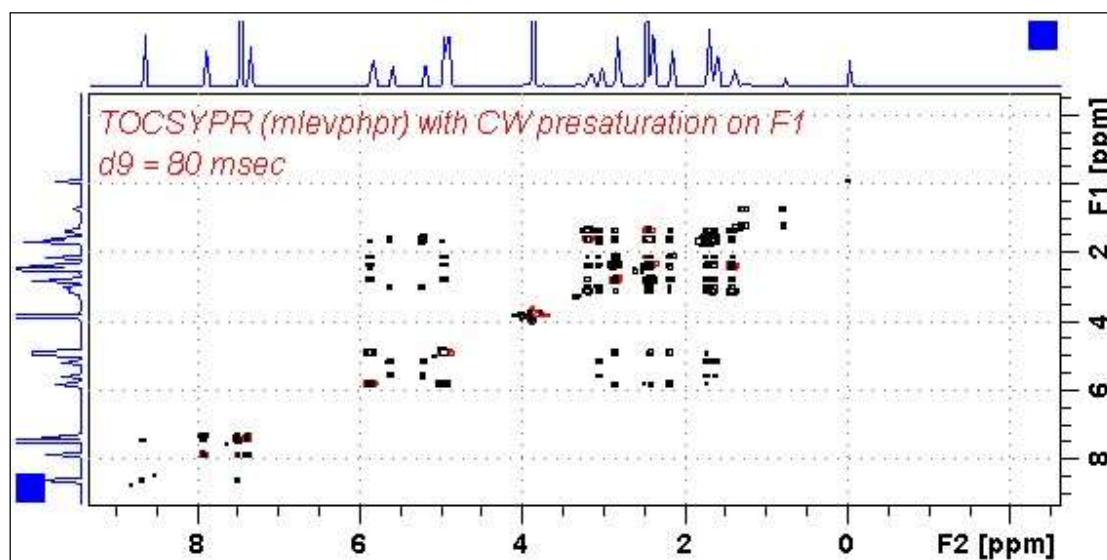
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **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.

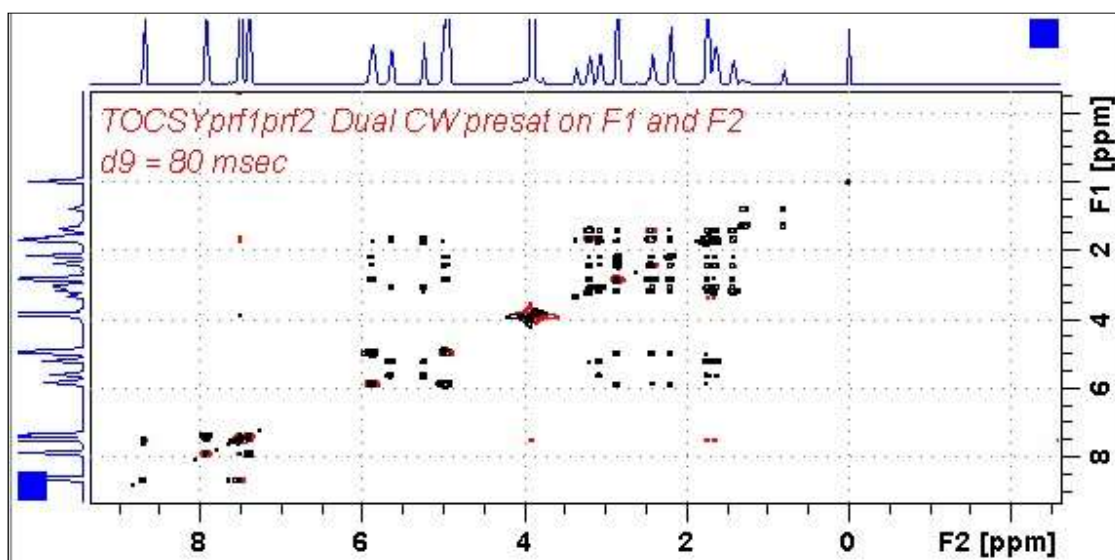
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **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 TOCSYPRF2ONLYwith PR presaturation on F2

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

pulse programme: **awtocsypr2only**

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.

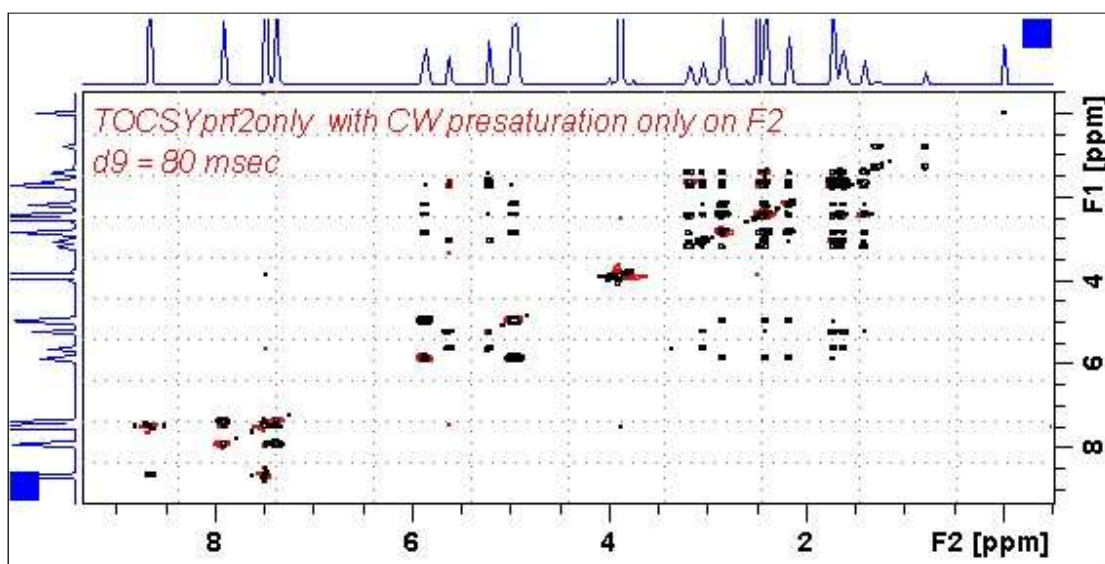
**D9** = correlation time = **80 msec** or other time of your choice (6-240 msec).

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**



600 MHz **TOCSYPRF2ONLY** spectrum of quinine in D<sub>6</sub>-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: **mlevesgpqh** (or **awtocsyes**)

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.

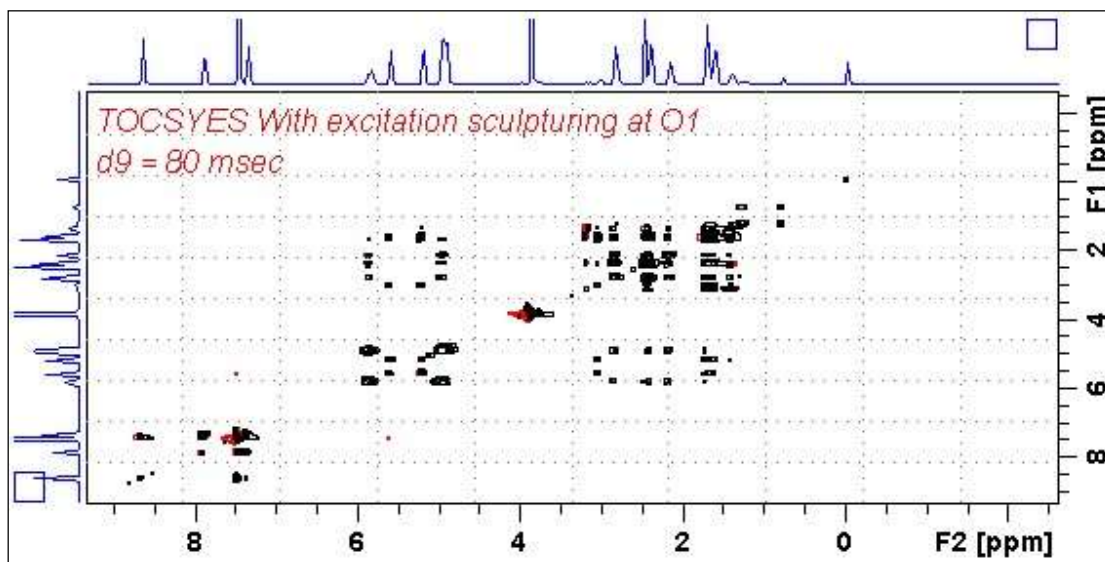
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **TOCSYES** spectrum of quinine in D<sub>6</sub>-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 **ES + PR** 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.

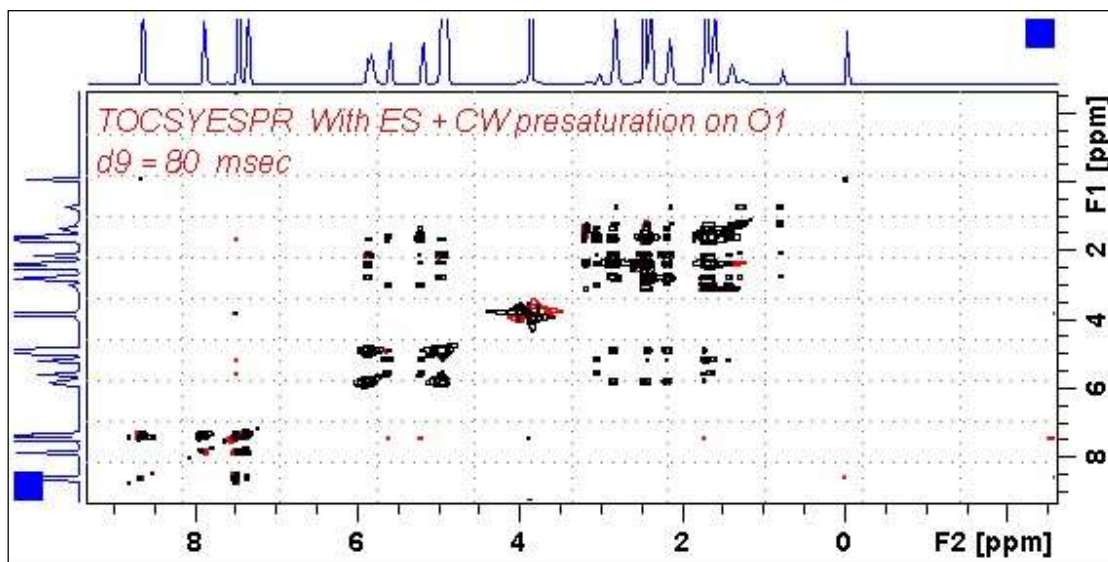
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **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: **awtocsyesprf1prf2**

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 at **O1 on F1** and **PR** presaturated at **O2 on F2**.

**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).

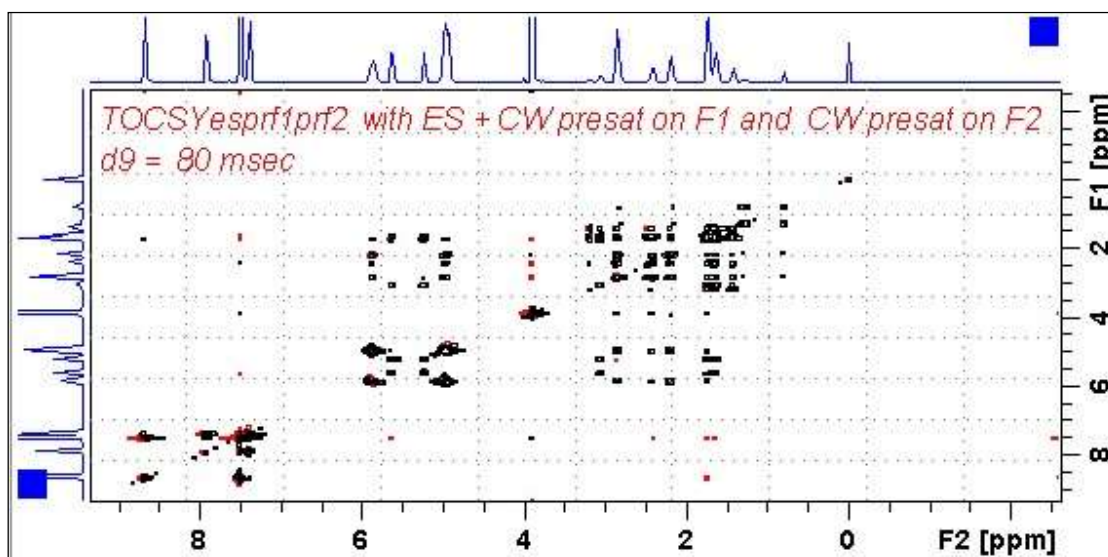
Type **ased** (enter) and review parameters used in the job.

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**



600 MHz **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 **clmlevpr** 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.

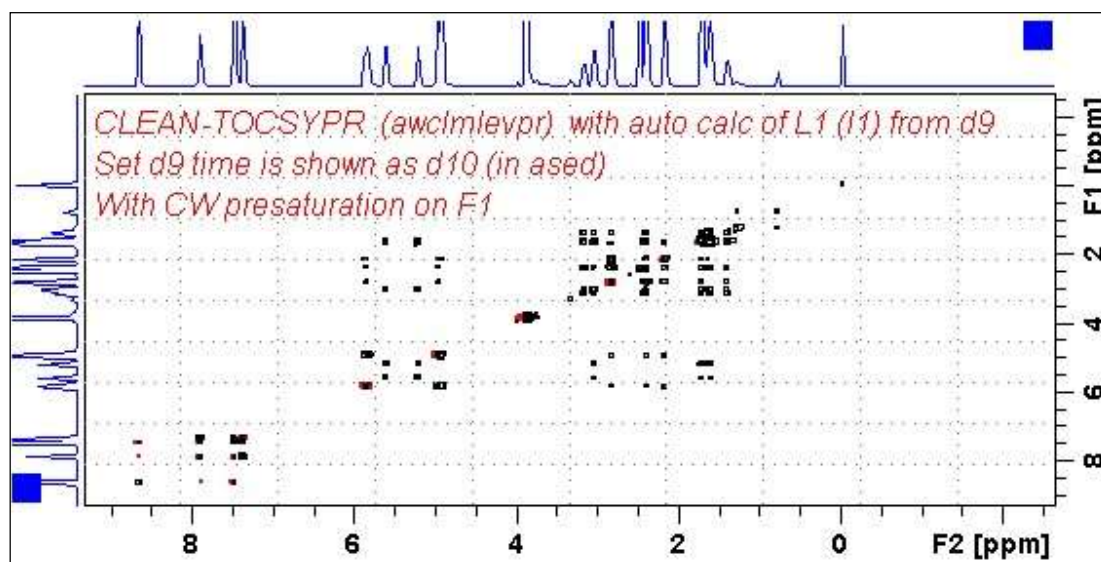
Set **receiver gain** using **RGA** (*Important!*).

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**



600 MHz **CLEAN-TOCSYPR** spectrum of quinine in D<sub>6</sub>-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.

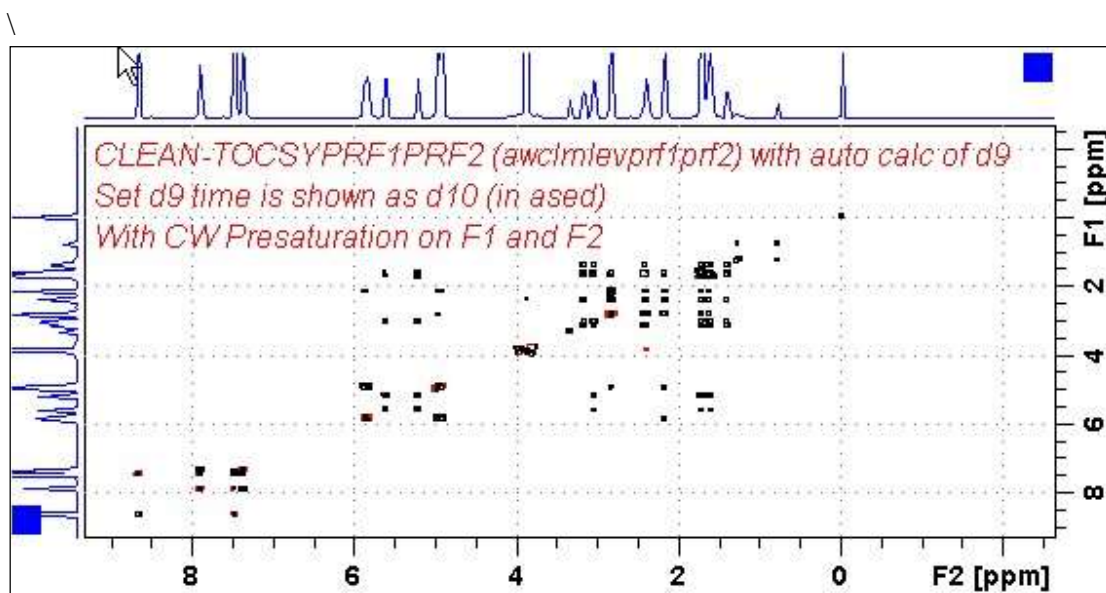
Set **receiver gain** using **RGA** (*Important!*).

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**



600 MHz CLEAN-TOCSYPRF1PRF2 spectrum of quinine in D<sub>6</sub>-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.

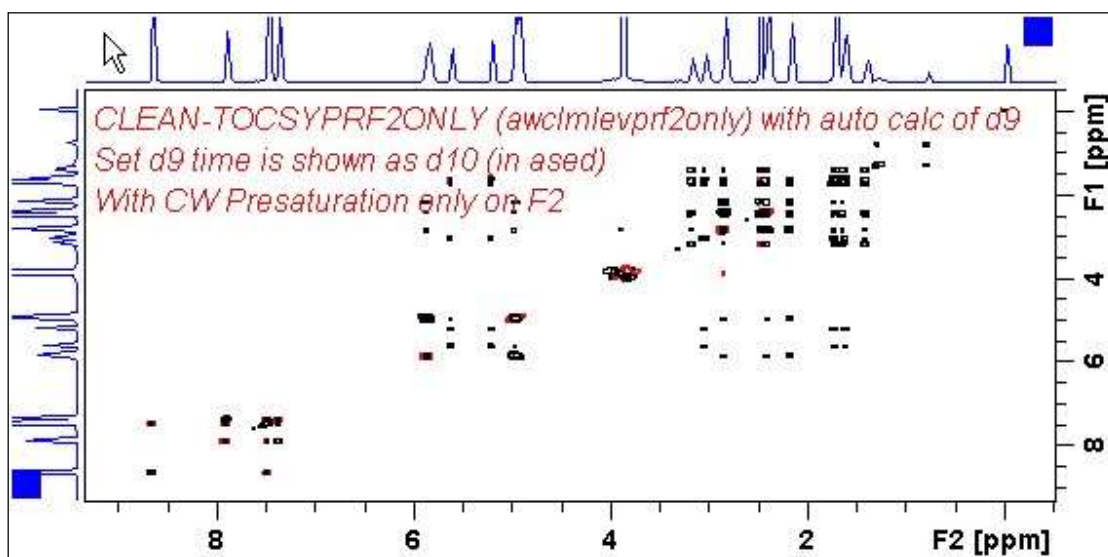
Set **receiver gain** using **RGA** (*Important!*).

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**



600 MHz **CLEAN-TOCSYPRF2ONLY** spectrum of quinine in D<sub>6</sub>-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** 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.

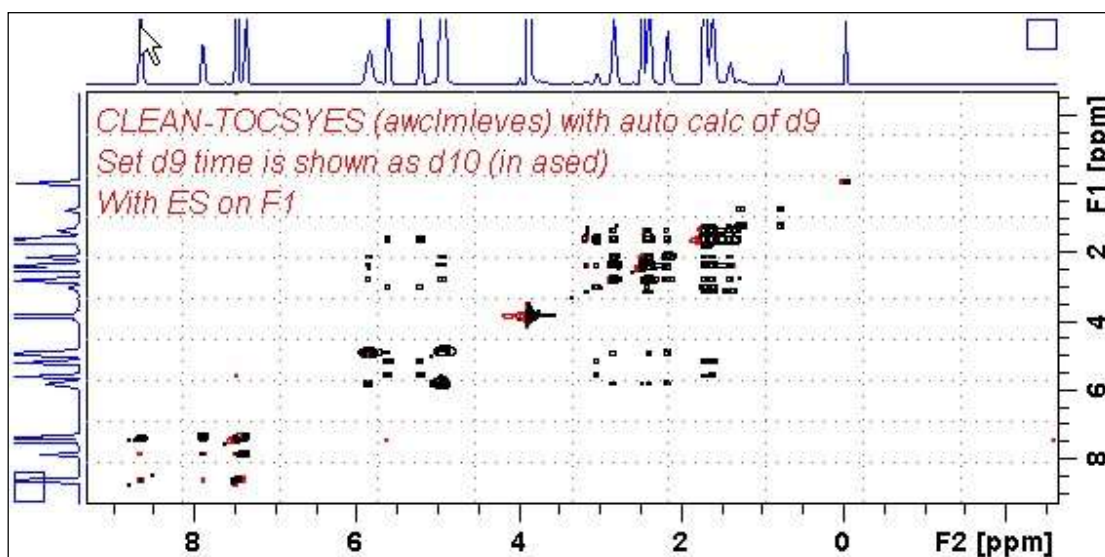
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz CLEAN-TOCSYES spectrum of quinine in D<sub>6</sub>-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 **ES + PR** 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.

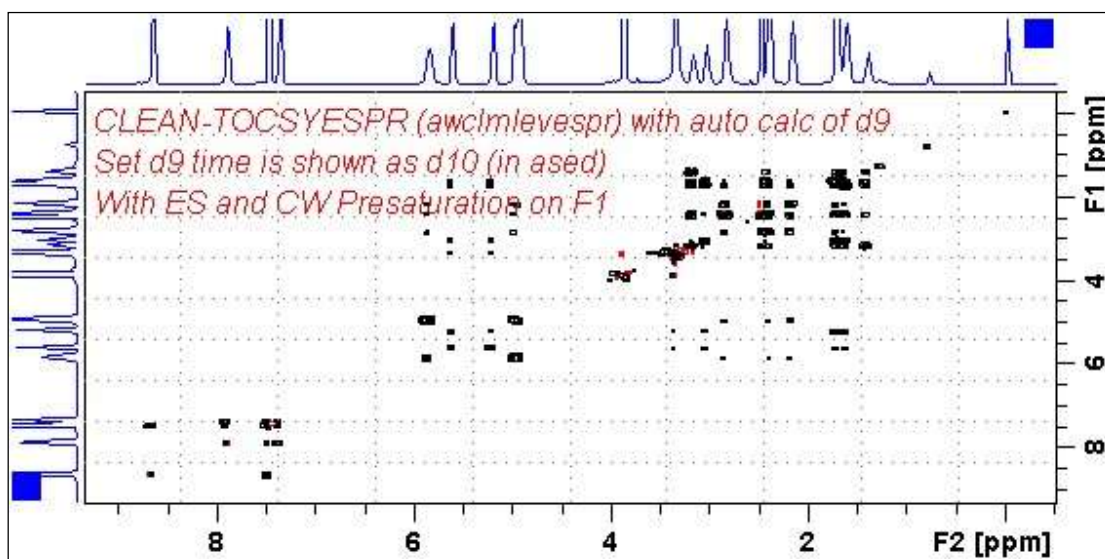
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz CLEAN-TOCSYESPR spectrum of quinine in D<sub>6</sub>-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: **aw cleantocsyesprf1prf2 (+ 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 at **O1 on F1** and **PR** presaturated at **O2 on F2**.

**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.

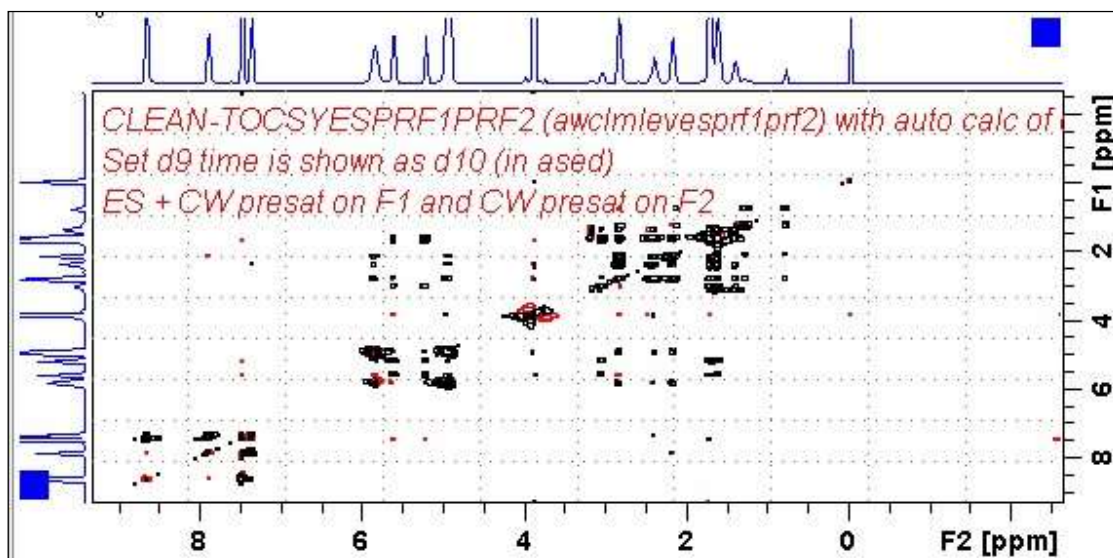
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz CLEAN-TOCSYESPRF1PRF2 spectrum of quinine in D<sub>6</sub>-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 DIPS12 Experiments and Parameter Sets**

**5.1 awdipsi2pr**

**5.2 awdipsi2prf1prf2**

**5.3 awdipsi2prf2only**

**5.4 awdipsi2es**

**5.5 awdipsi2espr**

**5.6 awdipsi2esprf1prf2**

## 5.1 DIPS12PR 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.

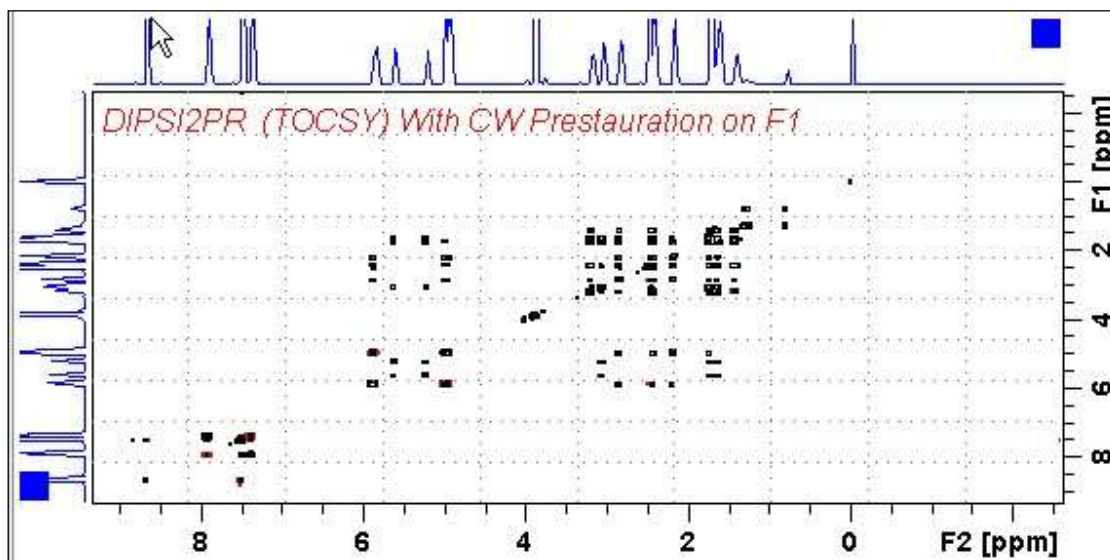
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **DIPS12PR** spectrum of quinine in D<sub>6</sub>-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.

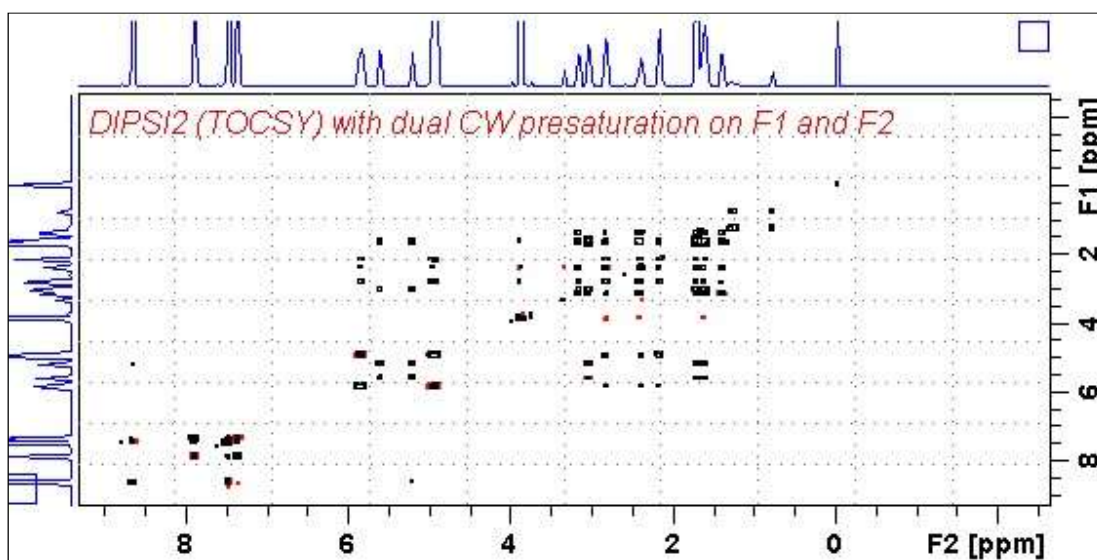
Set **receiver gain** using **RGA** (*important!*).

Process with: **SI(F2) = SI(F1) = 1K** or **2K**

**WDW(F1) = WDW(F2) = QSINE**

**SSB(F2) = SSB(F1) = 2**

**xfb, abs1, abs2** and optionally **syma**



600 MHz **DIPSI2PRF1PRF2** spectrum of quinine in D<sub>6</sub>-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.

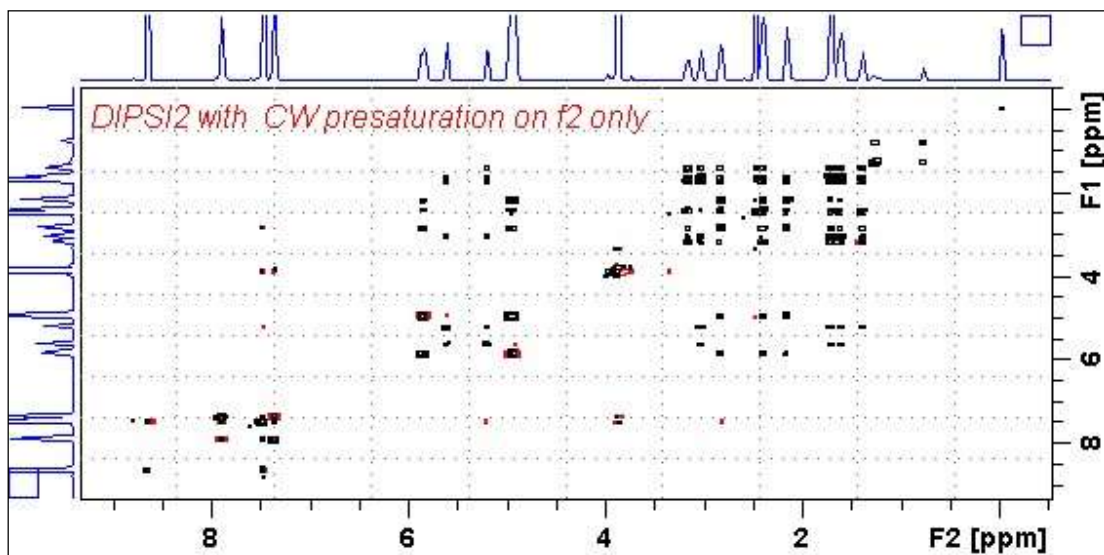
**D1** = presaturation time = **2 sec** or other time of your choice.

**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**



600 MHz **DIPSI2PRF2ONLY** spectrum of quinine in D<sub>6</sub>-DMSO with the HOD line at 3.38 ppm presaturated at O2 on F2.

## 5.4 DIPSIES with Excitation Sculpting on F1

parameter set: **awdipsies (+ getprosol)**

pulse programme: **awdipsies**

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.

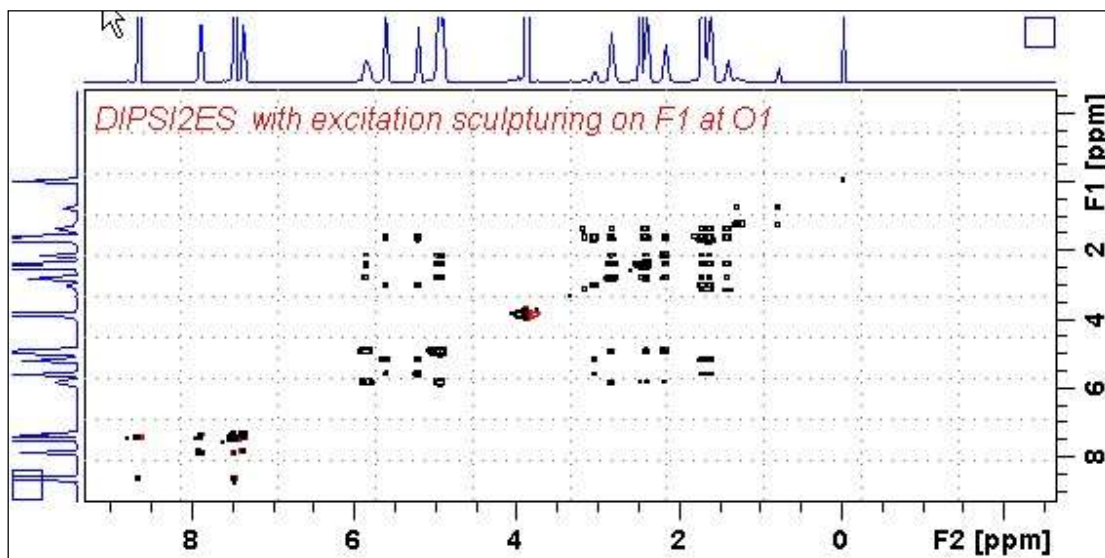
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **DIPSIES** spectrum of quinine in D<sub>6</sub>-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 **ES + PR** 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.

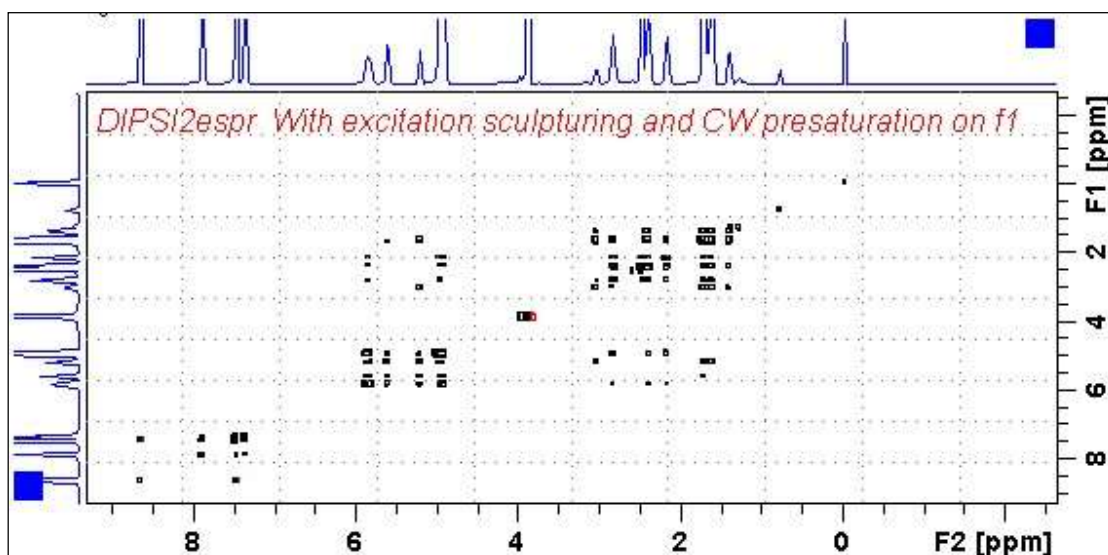
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **DIPSI2ESPR** spectrum of quinine in D<sub>6</sub>-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 DIPS12ESPRF1PRF2 with ES and PR presaturation on F1 and PR presaturation 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 at **O1 on F1** and **PR** presaturated at **O2 on F2**.

**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).

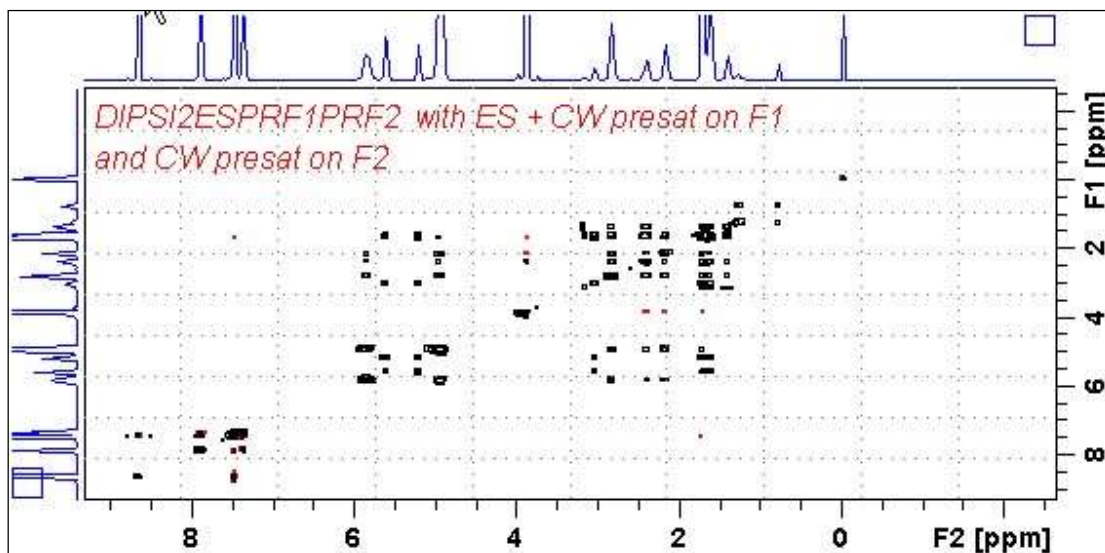
Type **ased** (enter) and review parameters used in the job.

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**



600 MHz **DIPS12ESPRF1PRF2** 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 awnoesypr**

**6.5 awnoesypr**

**6.6 awnoesyprf1prf2**

## 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.

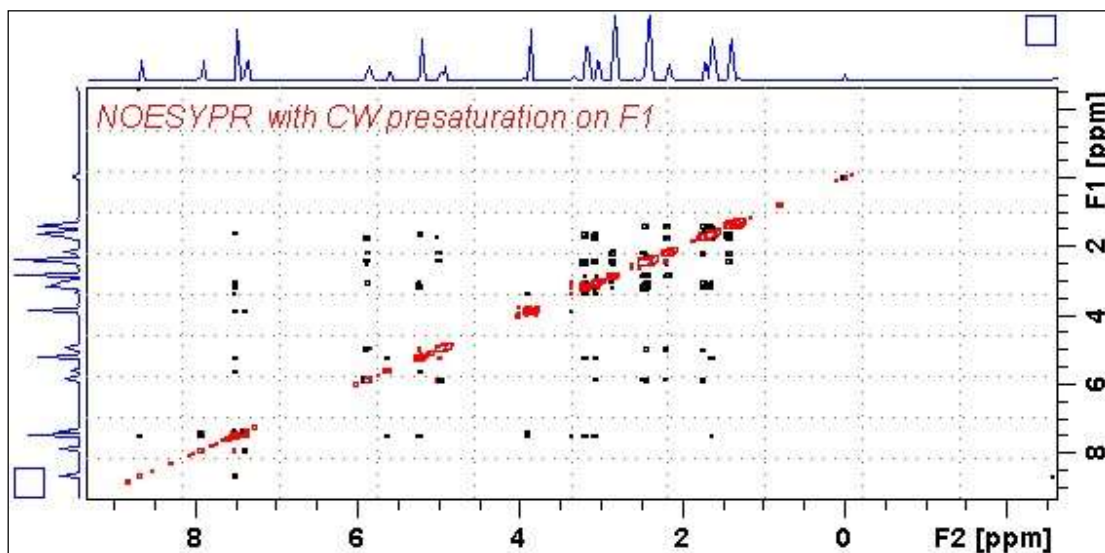
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz NOESYPR spectrum of quinine in D<sub>6</sub>-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: **awnoesyprf1prf2**

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.

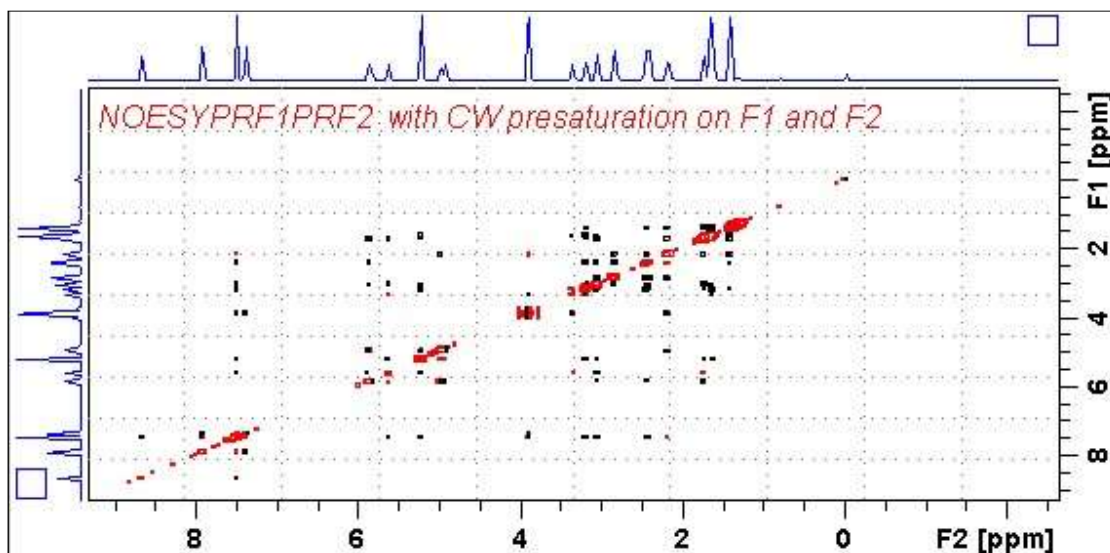
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz NOESYPRF1PRF2 spectrum of quinine in D<sub>6</sub>-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: **awnoesyprf2only**

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.

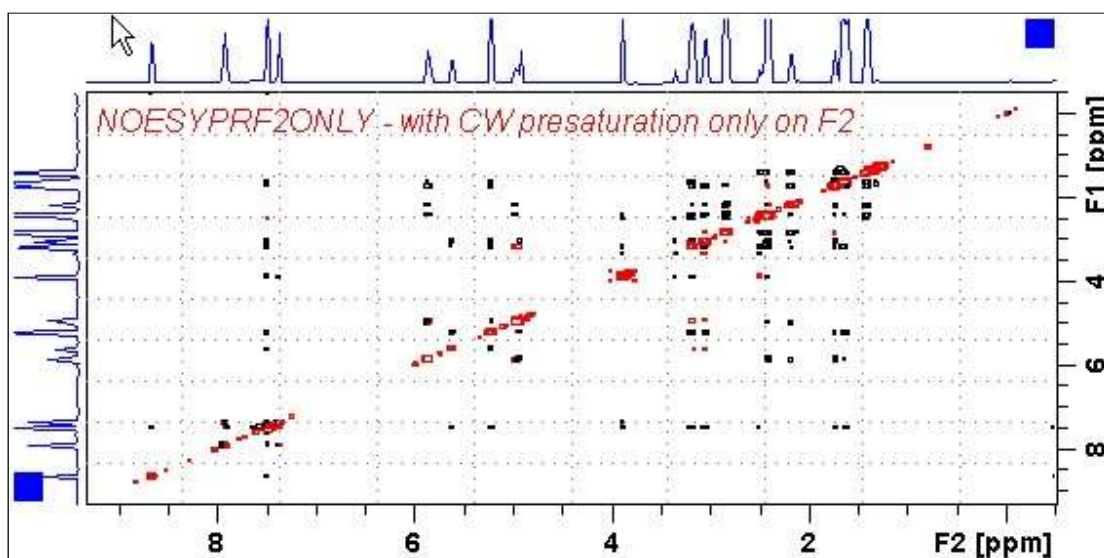
**D8** = NOE mixing time = **0.5 sec** or other time of your choice.

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**



600 MHz NOESYPRF2ONLY spectrum of quinine in D<sub>6</sub>-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: **awnoesy** (+ **getprosol**)

pulse programme: **noesyegpph**

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.

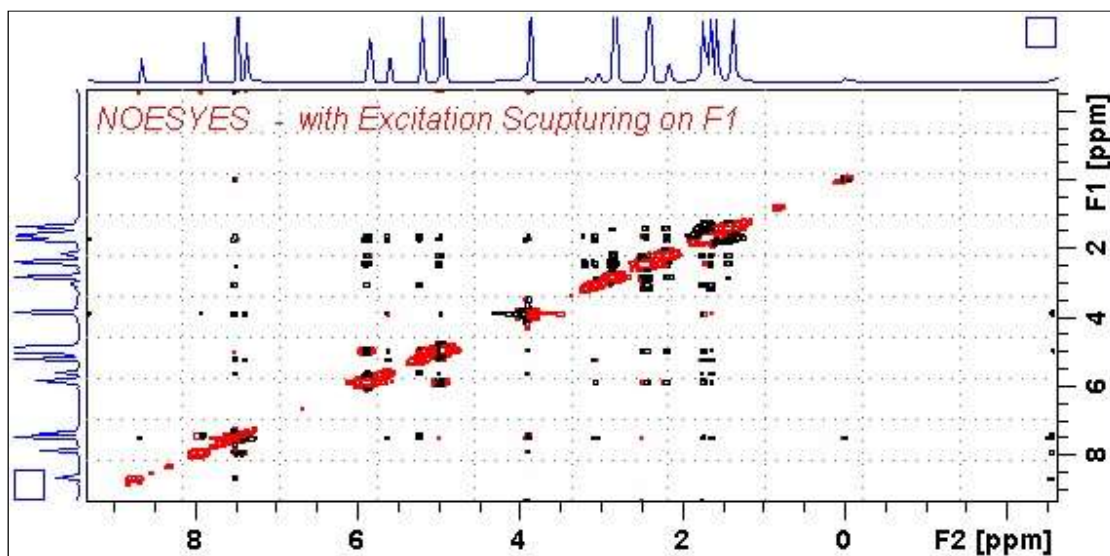
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz NOESYES spectrum of quinine in D<sub>6</sub>-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: **awnoesyespr**

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 **ES + PR** 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.

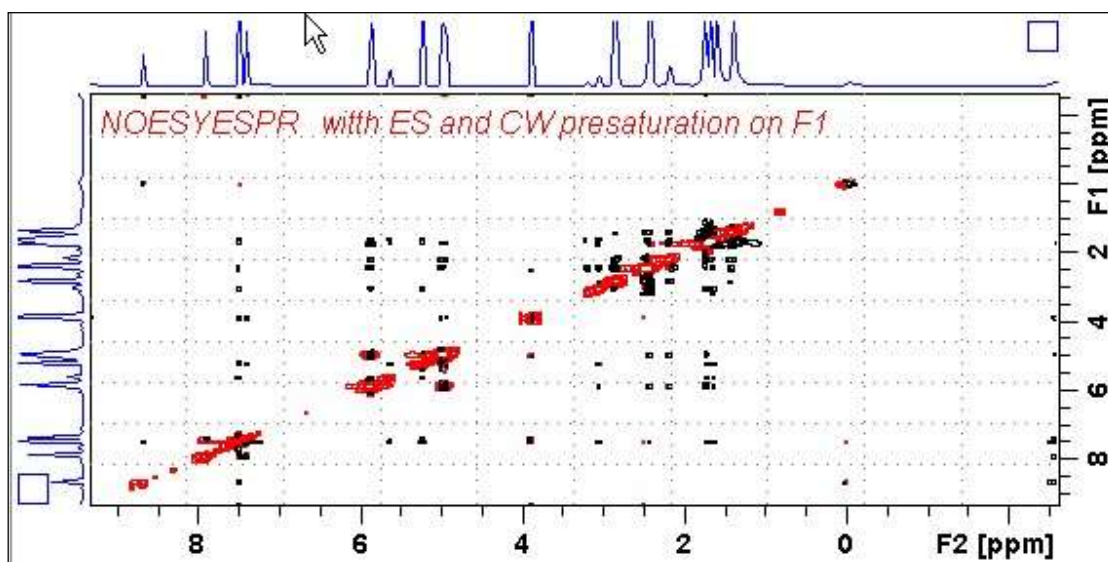
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz 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 NOESYSPRF1PRF2 with ES and PR presaturation on F1 and PR presaturation on F2

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

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.

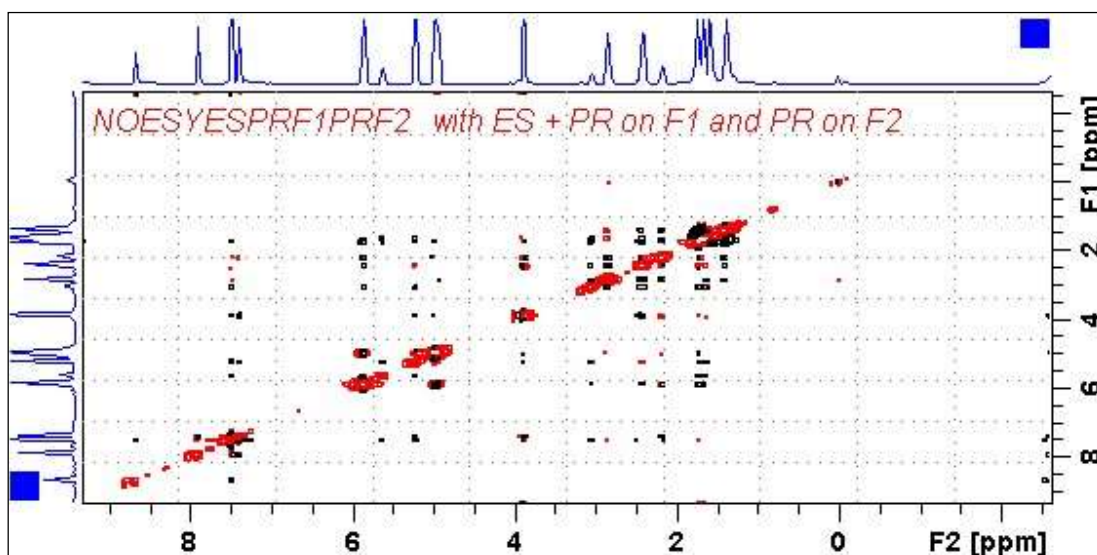
Enter **O1** and **O2 in Hz** (*in this order!*) of the signals to be **ES + PR** presaturated at **O1 on F1** and **PR** presaturated at **O2 on F2**.

**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**



600 MHz NOESYSPRF1PRF2 spectrum of quinine in D<sub>6</sub>-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 awroesypr**

**7.2 awroesyprf1prf2**

**7.3 awroesyprf2only**

**7.4 awroesypr**

**7.5 awroesypr**

**7.6 awroesyprf1prf2**



## 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.

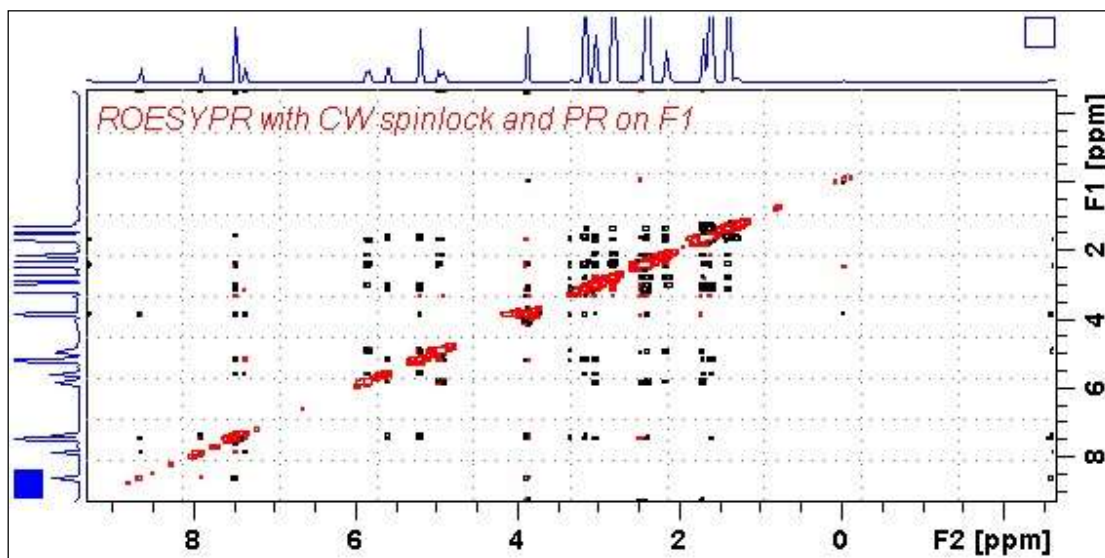
**P15** = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

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**



600 MHz **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.

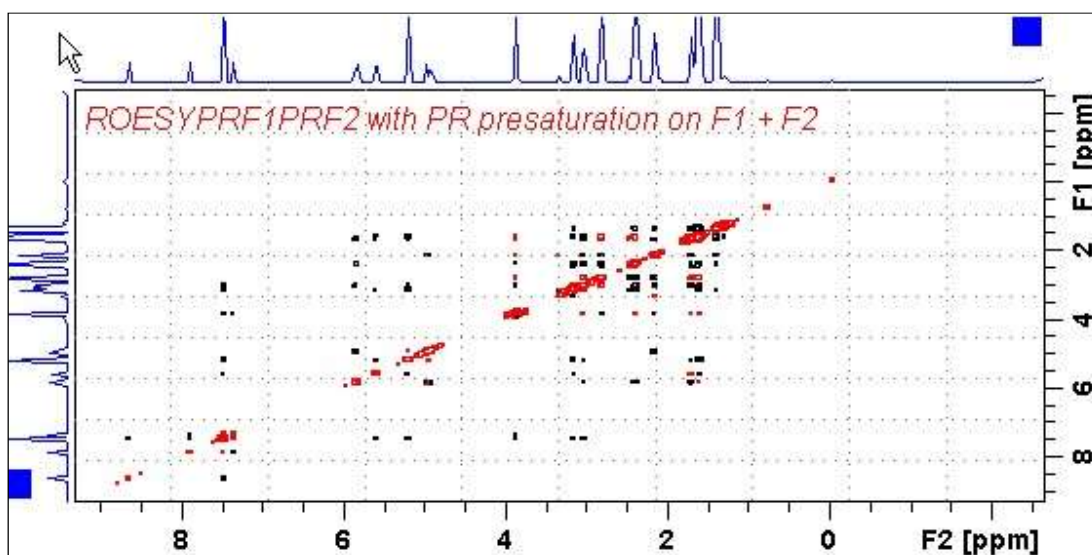
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **ROESYPRF1PRF2** spectrum of **quinine** in **D<sub>6</sub>-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.

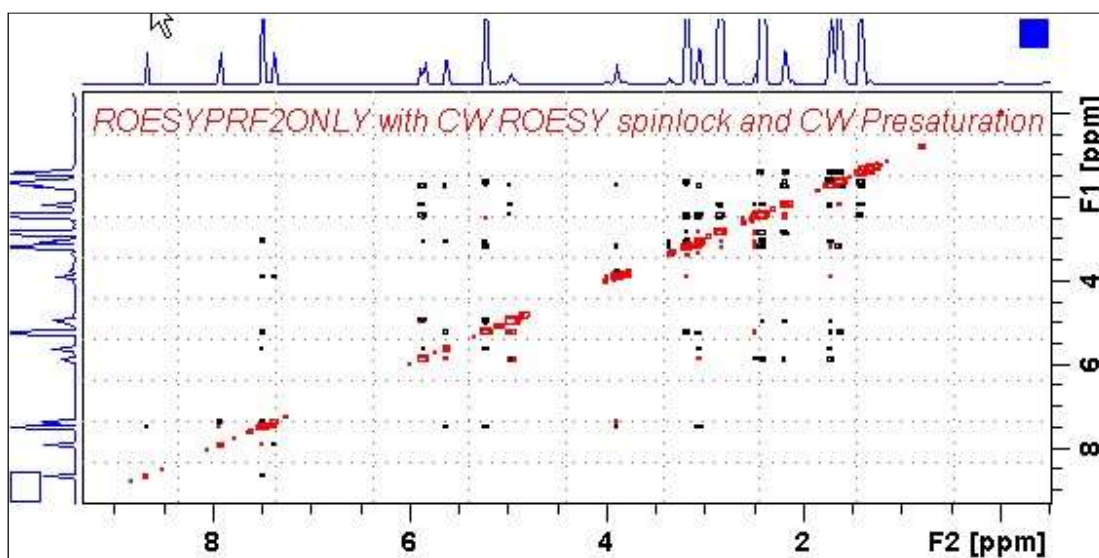
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz ROESYPRF2ONLY spectrum of quinine in D<sub>6</sub>-DMSO with the HOD line at 3.38 ppm presaturated at O2 on F2.

## 7.4 ROESYES with Excitation Sculpting on F1

parameter set: **awroesy** (+ **getprosol**)

pulse programme: **roesyegpph** (or **awroesy**) (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.

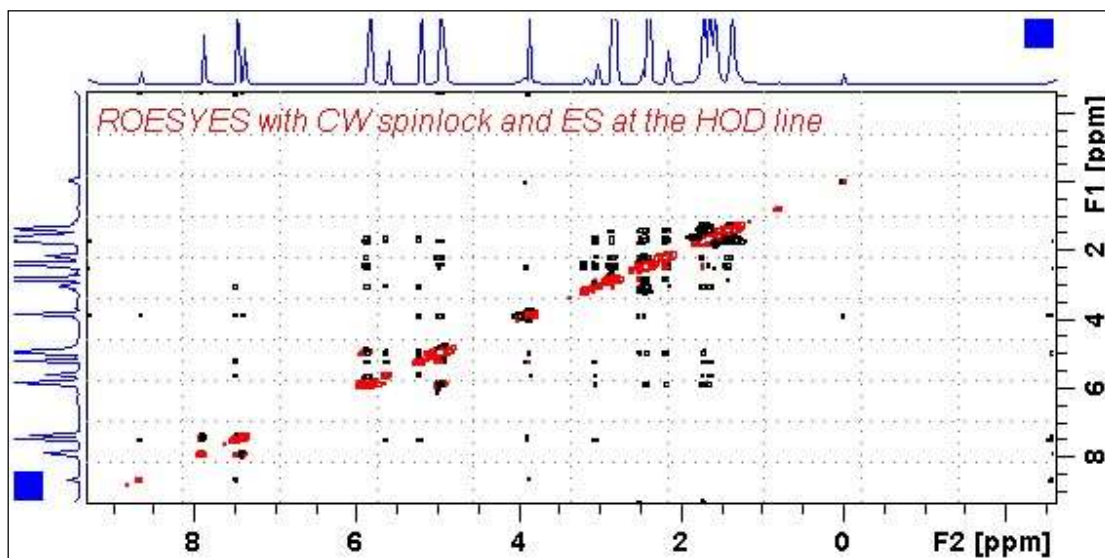
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz ROESYES spectrum of quinine in D<sub>6</sub>-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 **ES + PR** 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.

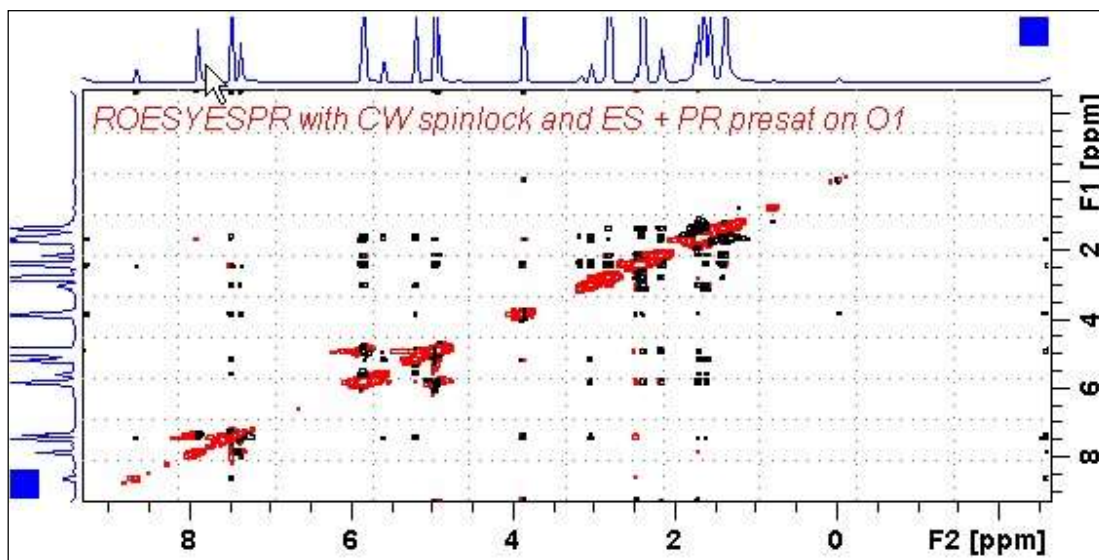
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **ROESYESPR** spectrum of quinine in D<sub>6</sub>-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 ROESYSPRF1PRF2 with ES and PR presaturation on F1 and PR presaturation on F2

parameter set: **awroesyprf1prf2 (+ getprosol)**

pulse programme: **awnoesyprf1prf2** (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 at **O1 on F1** and **PR** presaturated at **O2 on F2**.

**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).

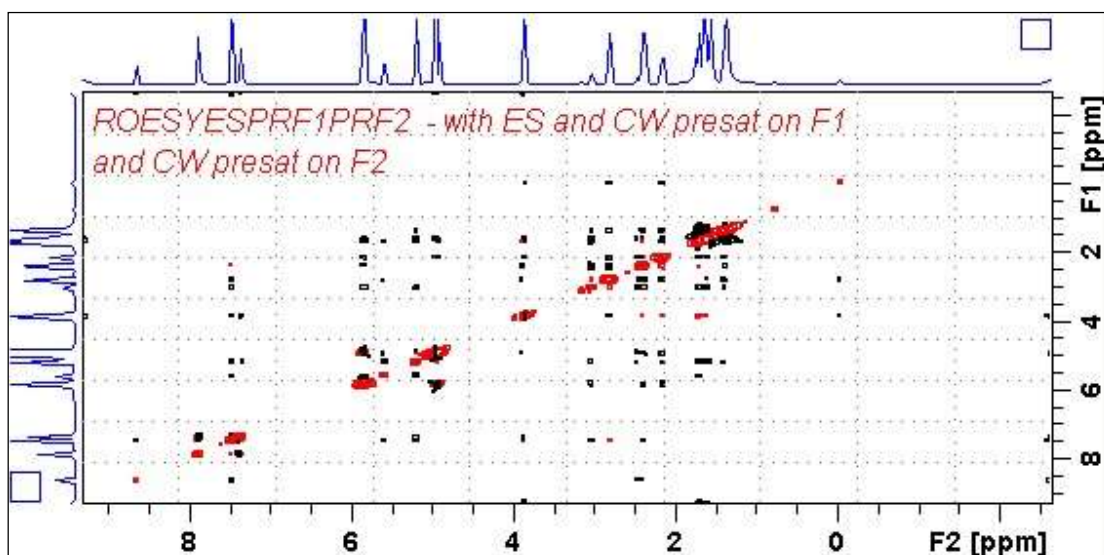
Type **ased** (enter) and review parameters used in the job and check gradients are OK.

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**



600 MHz **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 awroesy2pr**

**8.2 awroesy2prf1prf2**

**8.3 awroesy2prf2only**

**8.4 awroesy2es**

**8.5 awroesy2espr**

**8.6 awroesy2esprf1prf2**

## 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

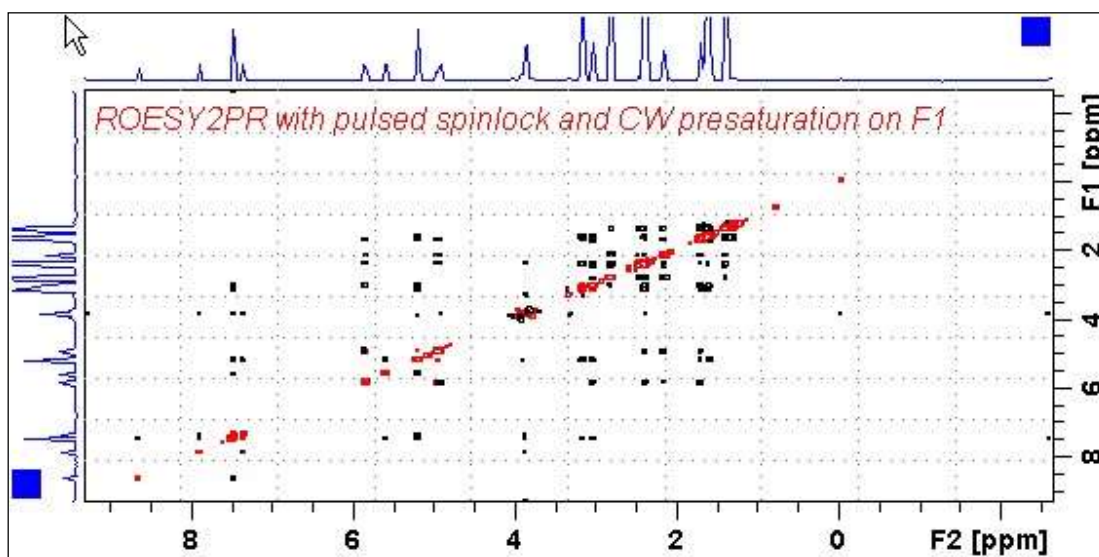
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **ROESY2PR** spectrum of quinine in D<sub>6</sub>-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

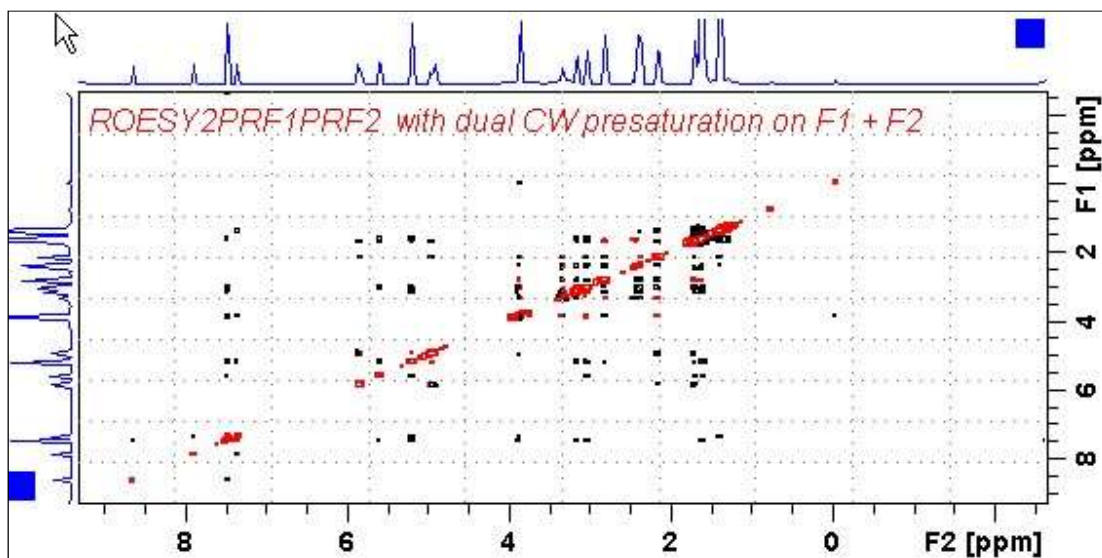
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **ROESY2PRF1PRF2** spectrum of quinine in **D<sub>6</sub>-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: **awroesy2prf2only** (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.

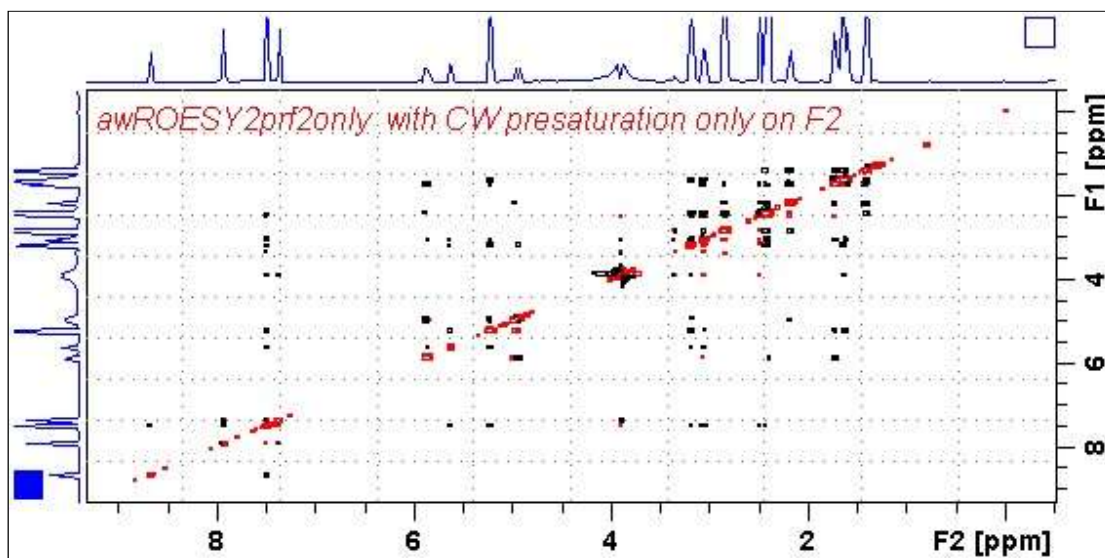
**P15** = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

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 **syms**



600 MHz **ROESY2PRF2ONLY** spectrum of quinine in D<sub>6</sub>-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: **awroesy2es** (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.

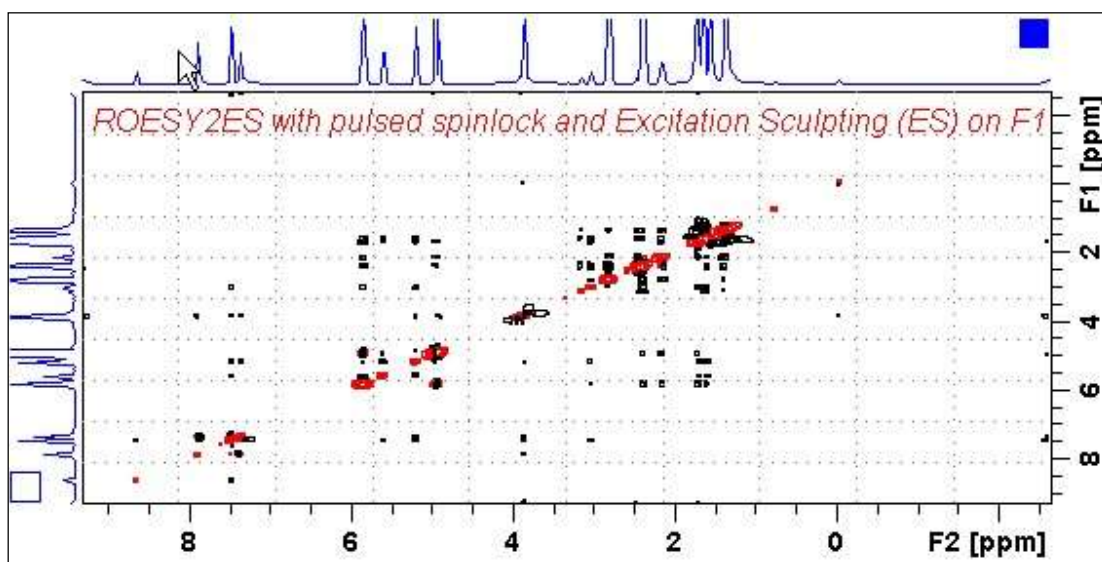
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **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 **ES + PR** 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.

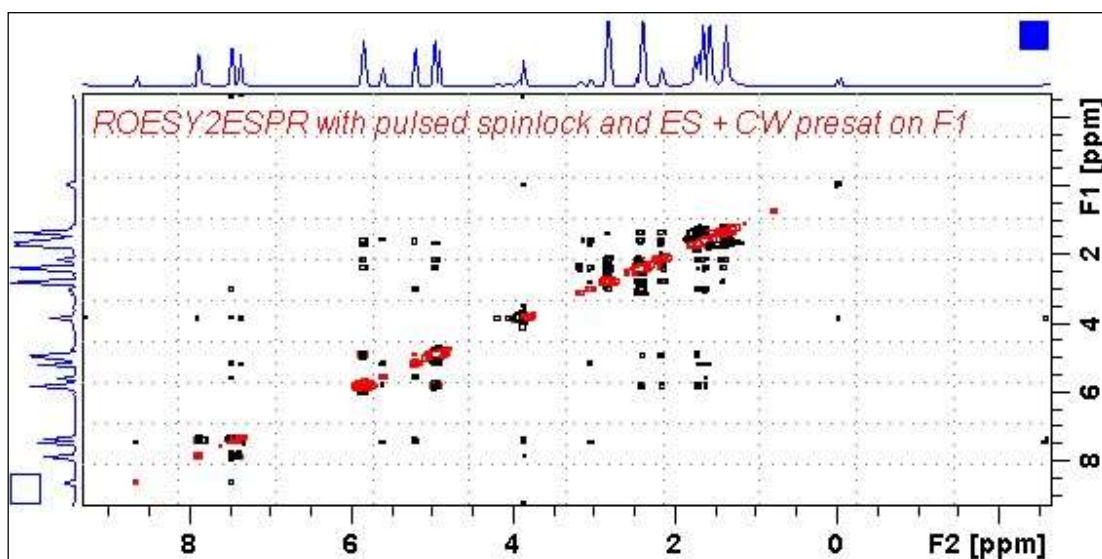
Set **receiver gain** using **RGA** (*important!*).

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: **awnoesy2esprf1prf2** (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 **ES + PR** presaturated at **O1 on F1** and **PR** presaturated at **O2 on F2**.

**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.

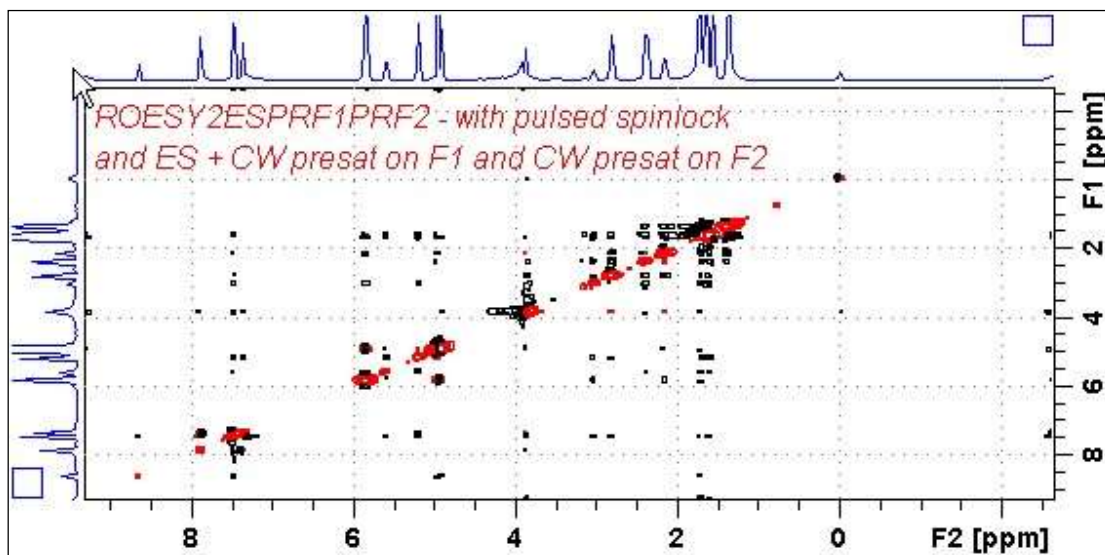
Set **receiver gain** using **RGA** (*important!*).

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**



600 MHz **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.