KJM 5250 and KJM 9250
COSY, TOCY, DIPSI, ROESY, NOESY NMR spectra with and without solvent suppression on the AVneo400 spectrometer.
Version 3.1
Topspin 4.3

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AVneo400 COSY, TOCSY, DIPSI2, NOESY, ROESY and ROESY2 Experiments - with and without CW Presatuartion

1.1 Spectral Window Set up

The spectral window (**SW**) width and midpoint should be determined in a standard ^{1}H NMR spectrum before setting up a 2D-COSY, TOCSY, etc, experiment. There should be no signals within 0.5 ppm of the upper or lower ^{1}H ppm limits.

Presaturation (PR) can be used to suppress an HOD or solvent signal. The midpoint of spectral window should be set to the frequency in Hz of the HOD or solvent line to be suppressed. Experiments with **Excitation Sculptured (ES)** peak suppression are described in a separate document.

Presaturation is applied at power level **PLW9(db)** on F1. The presaturation power level can be _decreased by adding 3-12 db_ or _increased by subtracting 3-12 db_ respectively from the prosol Table linked power level value. _6 db = a factor 2._

1.2 Processing

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

The **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 Experiments and Parameter Sets

The following **aw** coded **COSY, TOCSY,** etc, parameter sets have been set up on the **Neo400** spectrometer:

> **2.1 COSY spectrum**
> **2.2 TOCSY spectrum**
> **2.3 DIPSI2 spectrum**
> **2.4 NOESY spectrum**
> **2.5 ROESY spectrum with CW spin lock**
> **2.6 ROESY2 spectrum with pulsed spin lock**
>
> **3.1 COSYPR spectrum with CW presaturation**
> **3.2 TOCSYPR spectrum with CW presaturation**
> **3.3 DIPSI2PR spectrum with CW presaturation**
> **3.4 NOESYPR spectrum with CW presaturation**
> **3.5 ROESYPR spectrum with CW presaturation**
> **3.6 ROESY2PR spectrum with CW presaturation**

2.1 COSY spectrum with a P0 excitation pulse

  parameter set: **awcosy (+ getprosol)**
  pulse programme: **cosygpqf**

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 =** spectral window midpoint in Hz or ppm.
Type **O1** (enter), note the **O1** value in Hz that appears and enter it as **O2** (Hz).

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

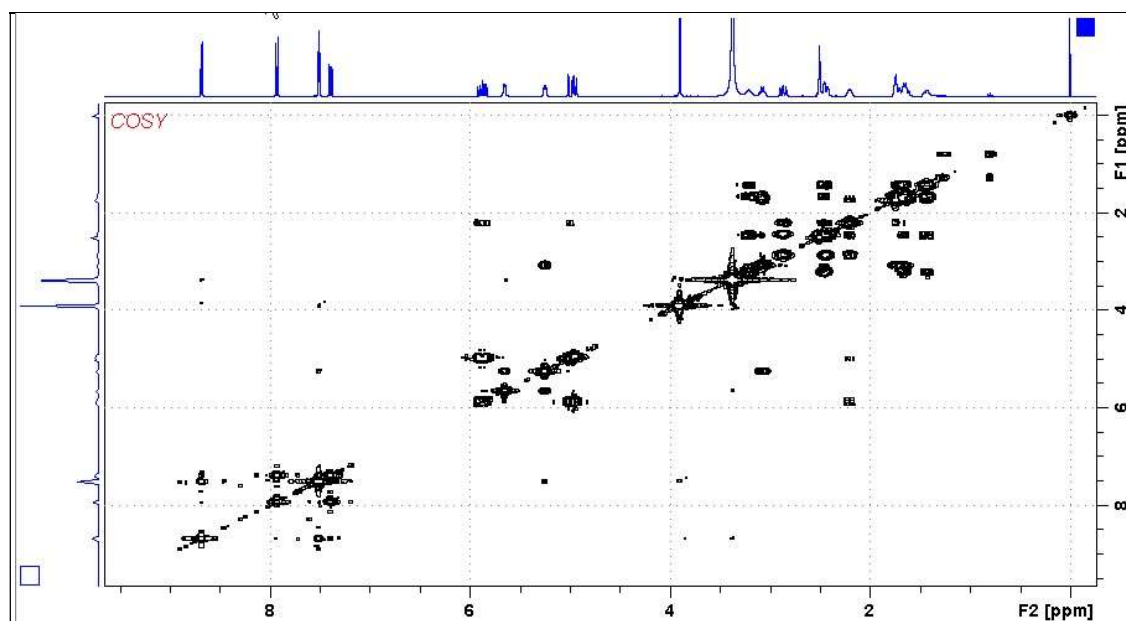Type **ased** (enter) and review parameters used in the job. Check **gradients** are OK.
Set **receiver gain** using **RGA** *(Important!)*.

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**

Neo400 COSY spectrum of quinine in D_6-DMSO. The spectrum is centered at 4.5 ppm.

2.2 TOCSY Spectrum

parameter set: **awtocsy (+ getprosol)**
pulse programme: **mlevph**

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(F2)** box. Check **SWH(F1) = SWH(F2)** in Hz including all dp's.

Enter **O1 =** spectral window midpoint in Hz or ppm.
Type **O1** (enter), note the **O1** value in Hz that appears and enter it as **O2** (Hz).

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

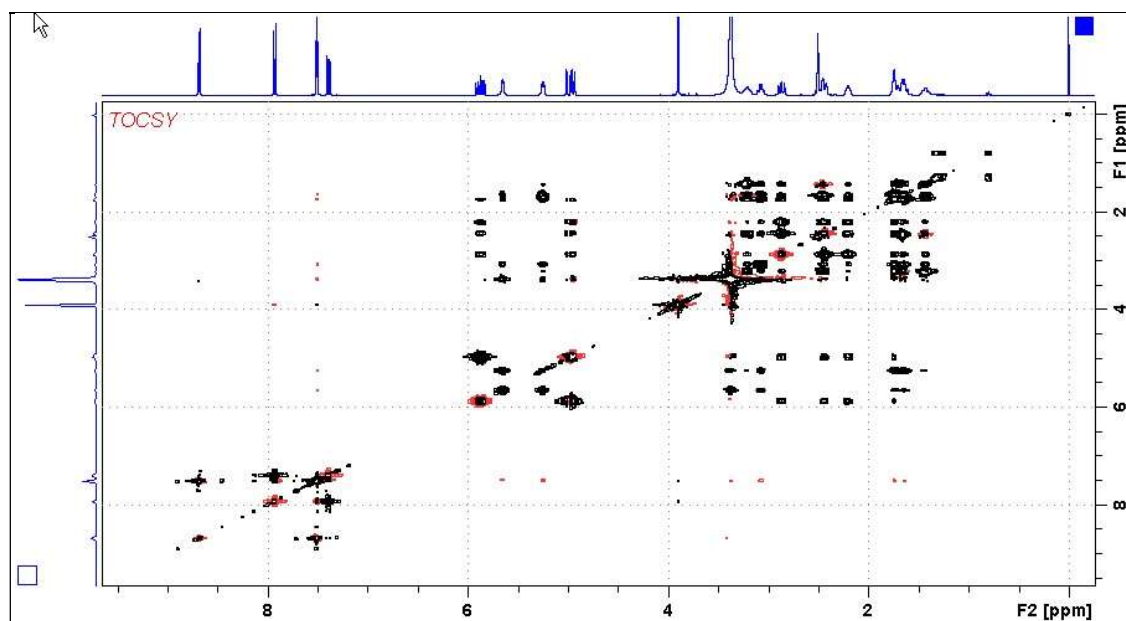Type **ased** (enter) and review parameters used in the job.
Set **receiver gain** using **RGA** *(Important!)*.

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**

Neo400 TOCSY spectrum of quinine in D_6-DMSO. The spectrum is centered at 4.7 ppm.

2.3 DIPSI2 Spectrum

parameter set: **awdipsi2 (+ getprosol)**
pulse programme: **dipsi2ph**

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(F1) = SWH(F2)** in Hz including all dp's.

Enter **O1 =** spectral window midpoint in Hz or ppm.
Type **O1** (enter), note the **O1** value in Hz that appears and enter it as **O2** (Hz).

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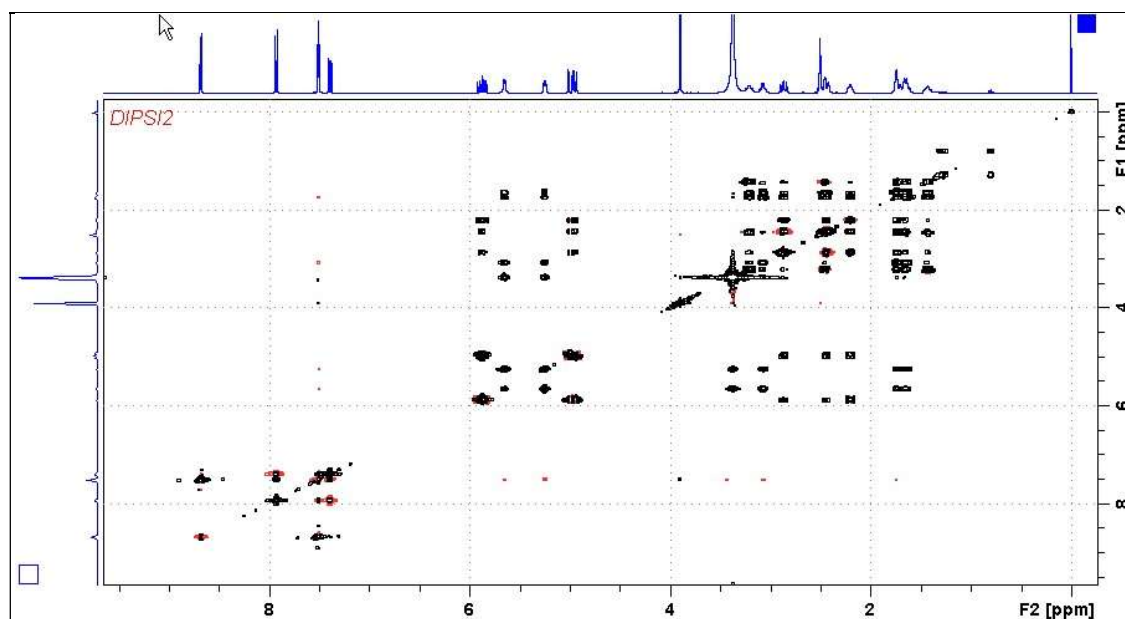**NS** = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
D1 = repletion time = **1.5 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

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

Neo400 DIPSI2 spectrum of quinine in D_6-DMSO. The spectrum is centered at 4.7 ppm.

2.4 NOESY Spectrum

  parameter set: **awnoesy (+ getprosol)**
  pulse programme: **noesygpph**

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(F1) = SWH(F2)** in Hz including all dp's.

Enter **O1 =** spectral window midpoint in Hz or ppm.
Type **O1** (enter), note the **O1** value in Hz that appears and enter it as **O2** (Hz).

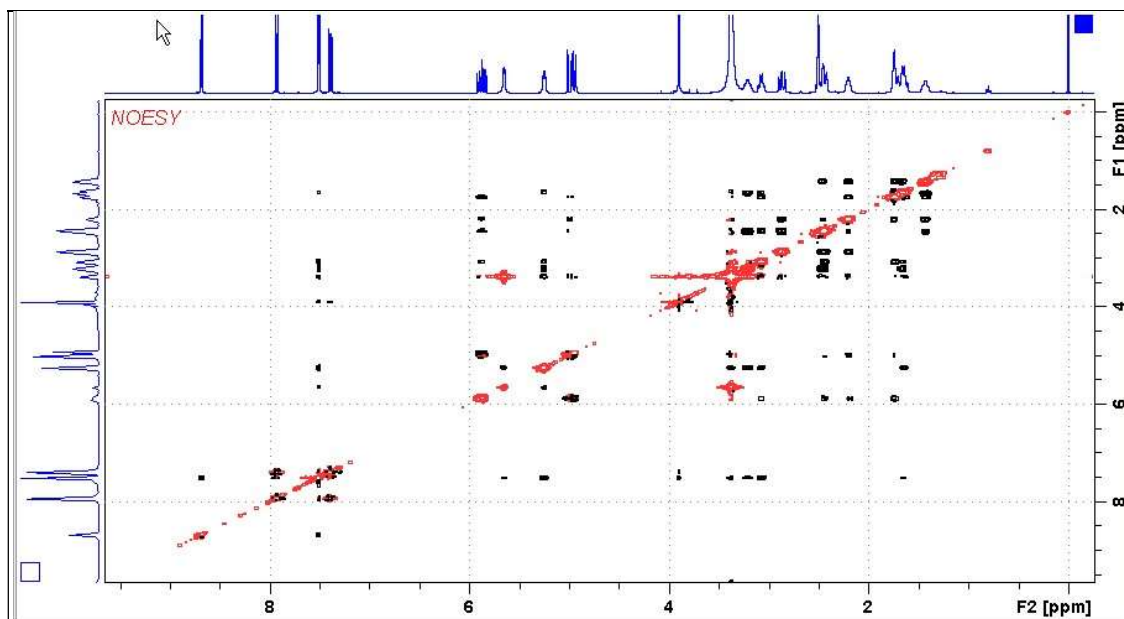**TD(F2)** = 1K or 2K, **TD(F1)** = 128 - 256 (your choice).
NS =multiple of 4 or 8, **DS** = 4 or 8.
D1 = repletion time = **1.5 sec** or other time of your choice.
D8 = NOE mixing time = **0.5 sec** or other time of your choice.

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

Neo400 NOESY spectrum of quinine in D_6-DMSO. The spectrum is centered at 4.7 ppm.

2.5 ROESY Spectrum

  parameter set: **awroesy (+ getprosol)**
  pulse programme: **roesyph** (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(F1) = SWH(F2)** in Hz including all dp's.

Enter **O1 =** spectral window midpoint in Hz or ppm.
Type **O1** (enter), note the **O1** value in Hz that appears and enter it as **O2** (Hz).

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

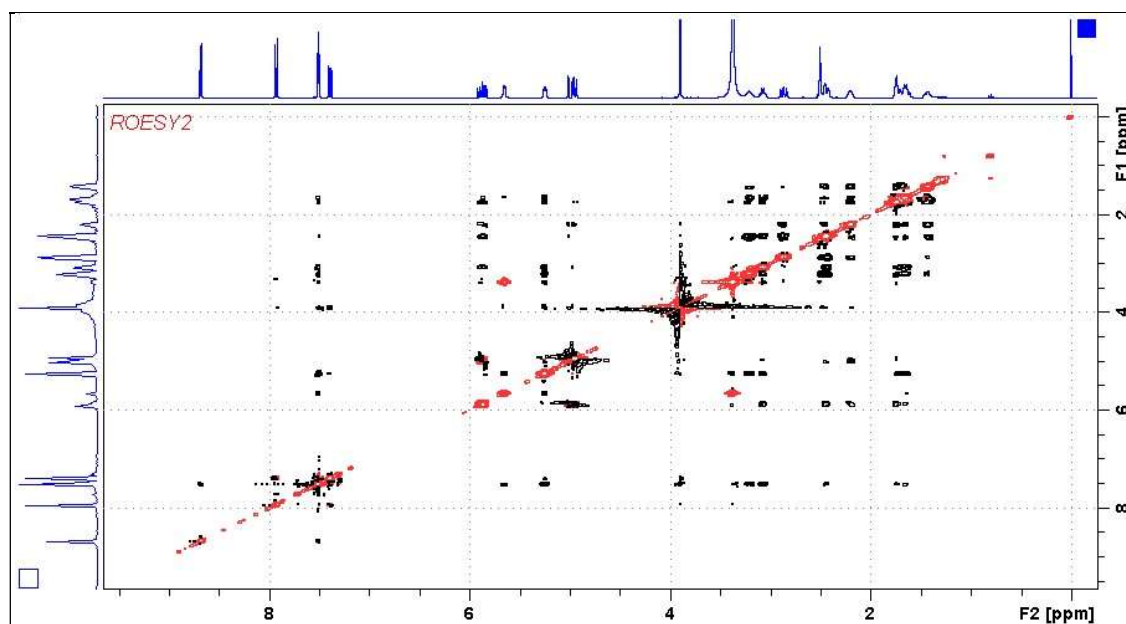Type **ased** (enter) and review parameters used in the job.
Set **receiver gain** using **RGA** *(Important!)*.

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**

400 MHz ROESY spectrum of quinine in D_6-DMSO. The spectrum is centered at 4.5 ppm.

2.6 ROESY2 Spectrum

parameter set: **awroesy2 (+ getprosol)**
pulse programme: **roesyph.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(F1) = SWH(F2)** in Hz including all dp's.

Enter **O1 =** spectral window mid point in Hz or ppm.
Type **O1** (enter), note the **O1** value in Hz that appears and enter it as **O2** (Hz).

TD(F2) = 1K or 2K, **TD(F1)** = 128 - 256 (your choice).
NS = multiple of 4 or 8, **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).

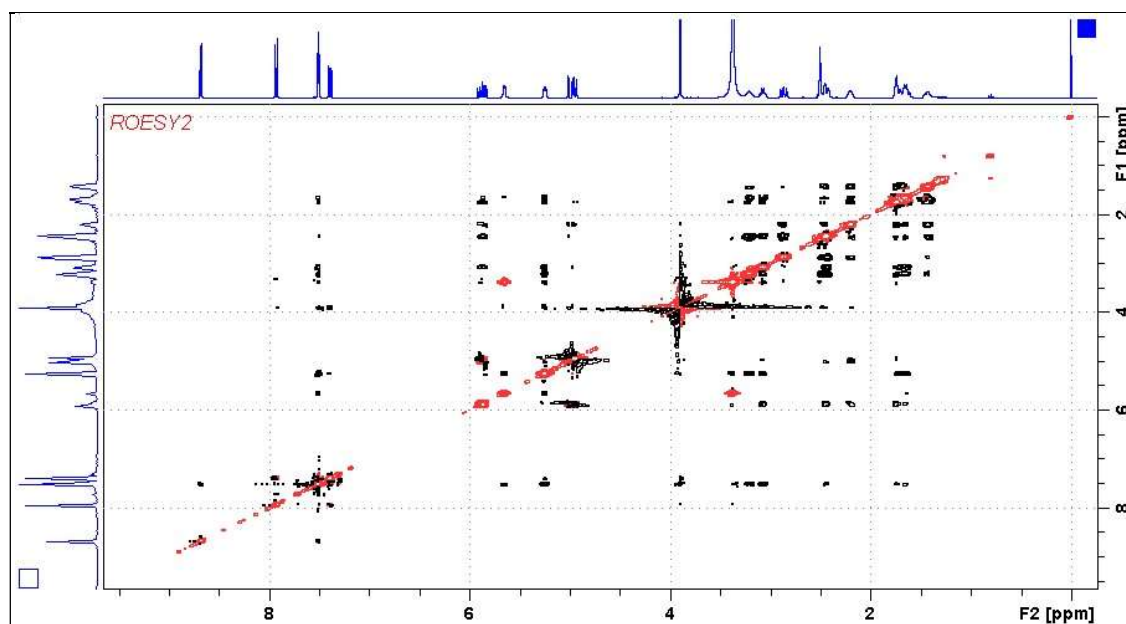Type **ased** (enter) and review parameters used in the job.
Set **receiver gain** using **RGA** *(Important!)*.

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**

Neo400 ROESY2 spectrum of quinine in D_6-DMSO. The spectrum is centered at 4.5 ppm.

3.1 COSYPR Spectrum with CW Presaturation

  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(F1) = SWH(F2)** 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 = multiple of 2, 4 or 8, **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 **PLW9(db)** 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
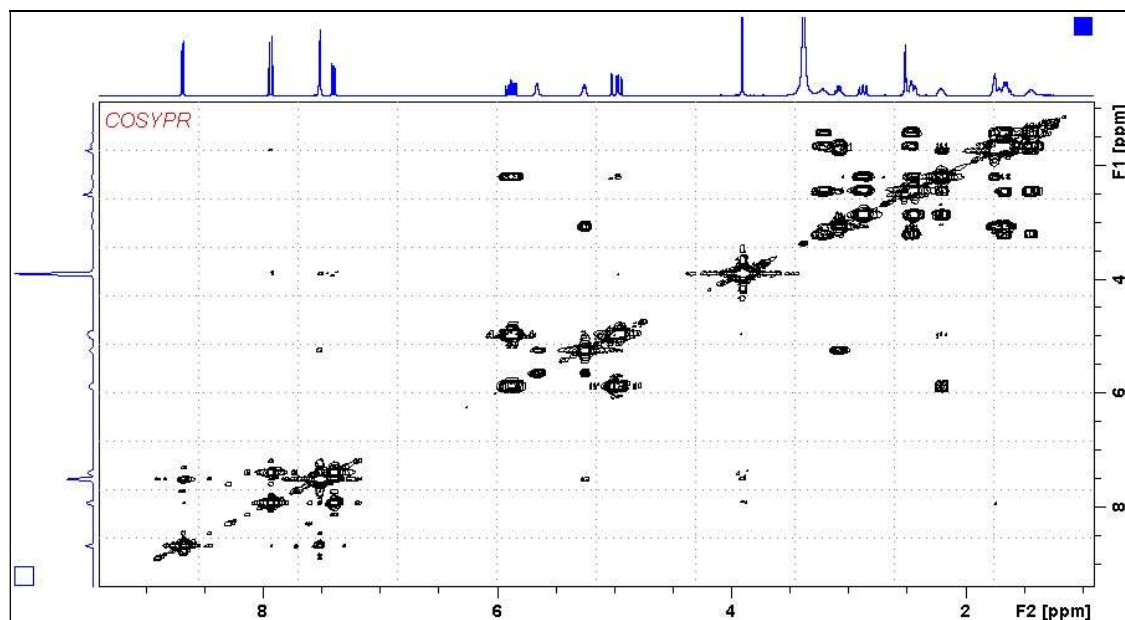
0.9-9.4 ppm region of the **Neo400 COSYPR** spectrum of quinine in D_6-DMSO with the HOD line at 3.37 ppm suppressed.

3.2 TOCSYPR Spectrum with CW Presaturation

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(F1) = SWH(F2)** 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 = multiple of 2, 4 or 8, **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 **PLW9(db)** 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**
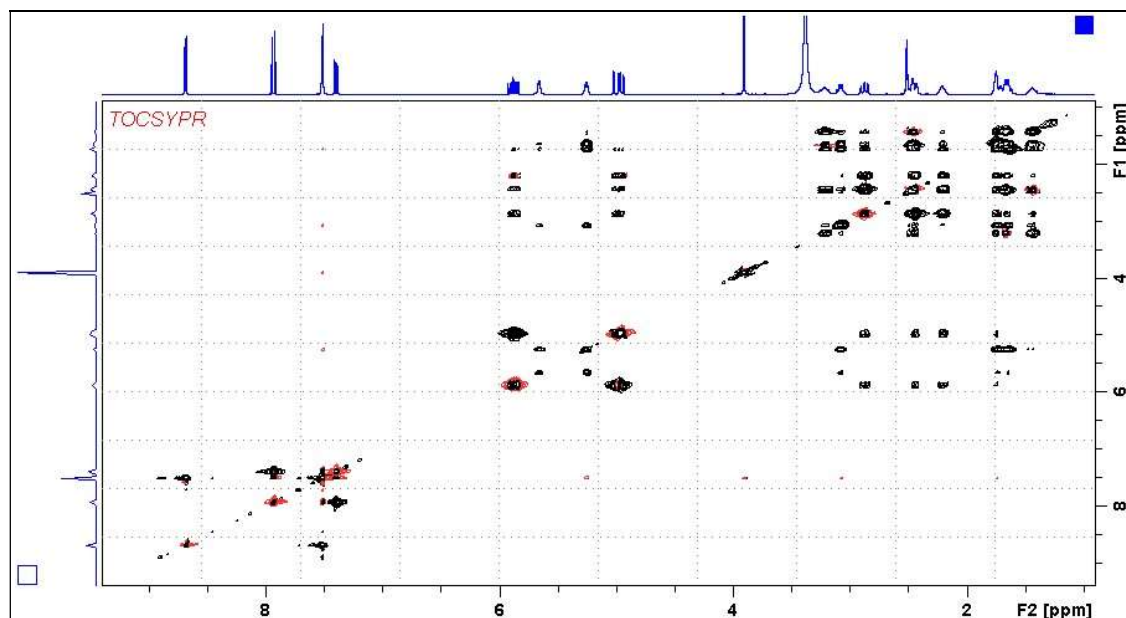
0.9-9.4 ppm region of the **Neo400 TOCSYPR** spectrum of quinine in D_6-DMSO with the HOD line at 3.37 ppm suppressed.

3.2 DIPSI2PR Spectrum with CW Presaturation

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(F1) = SWH(F2)** 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 = multiple of 4 or 8, **DS** = 4 or 8.
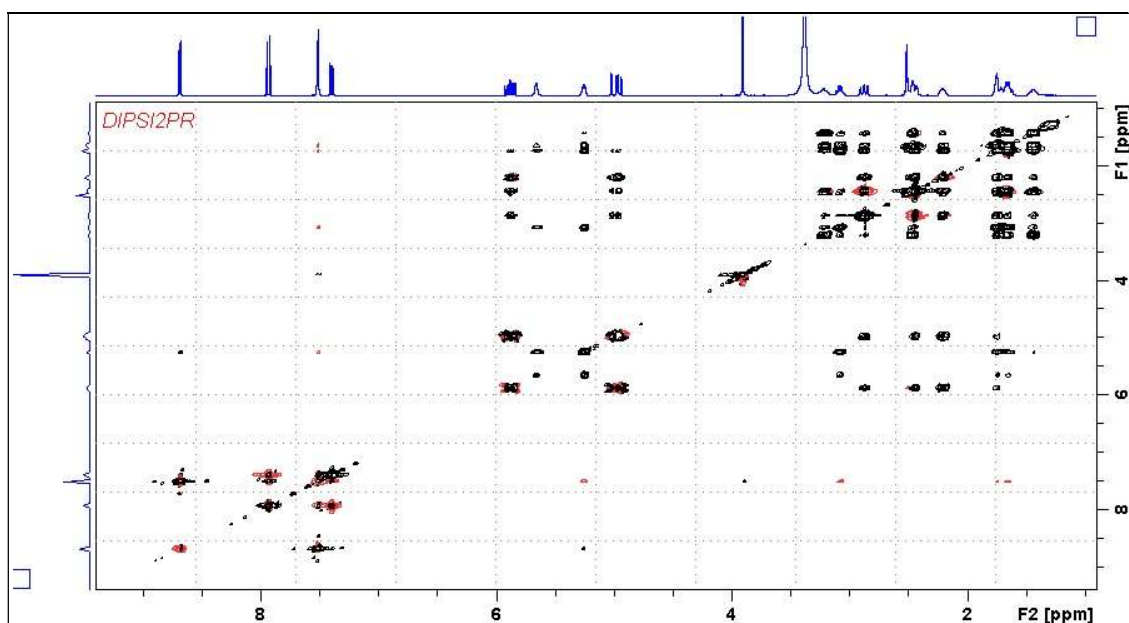**D1** = presaturation time = **2 sec** or other time of your choice.
D9 = correlation time = **80 msec** or other time of your choice (6-240 msec).

Type **ased** (enter) and review parameters used in the job.
The **PLW9(db)** 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**

0.9-9.4 ppm region of the **Neo400 DIPSI2PR** spectrum of quinine in D_6-DMSO with the HOD line at 3.37 ppm suppressed.

3.4 NOESYPR Spectrum with CW Presaturation

  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(F1) = SWH(F2)** 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 = multiple of 4 or 8, **DS** = 4 or 8.
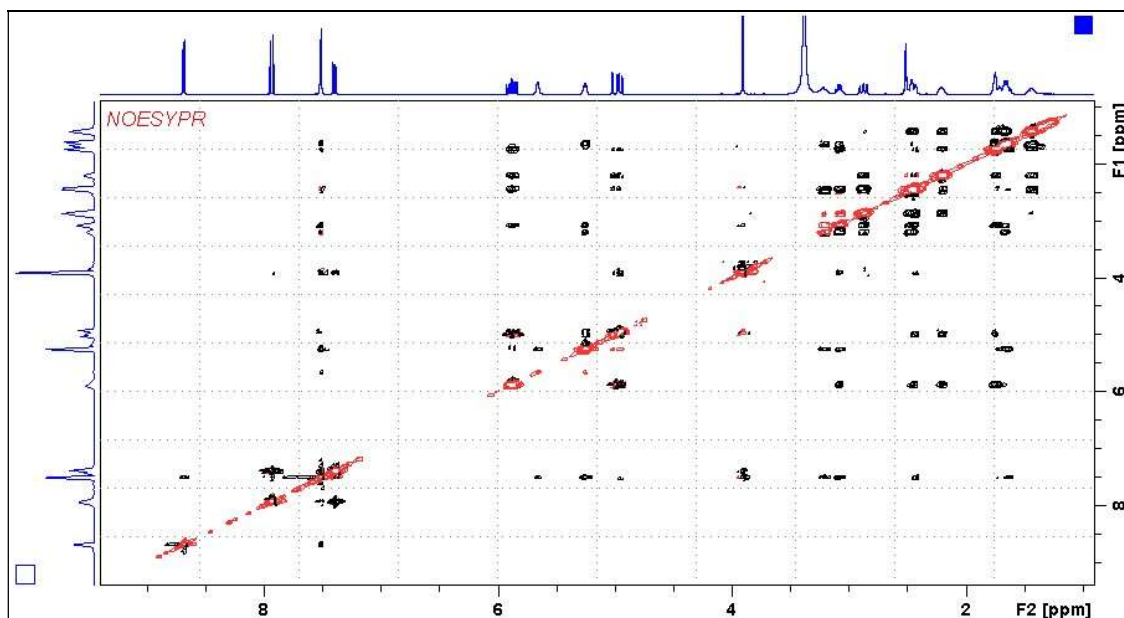**D1** = presaturation time = **2 sec** or other time of your choice.
D8 = NOE mixing time **= 0.5 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job and check gradients are OK.
The **PLW9(db)** 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**

0.9-9.4 ppm region of the **Neo400 NOESYPR** spectrum of quinine in D_6-DMSO with the HOD line at 3.37 ppm suppressed.

3.5 ROESYPR Spectrum with CW Presaturation

    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(F1) = SWH(F2)** 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 = multiple of 4 or 8, **DS** = 4 or 8.
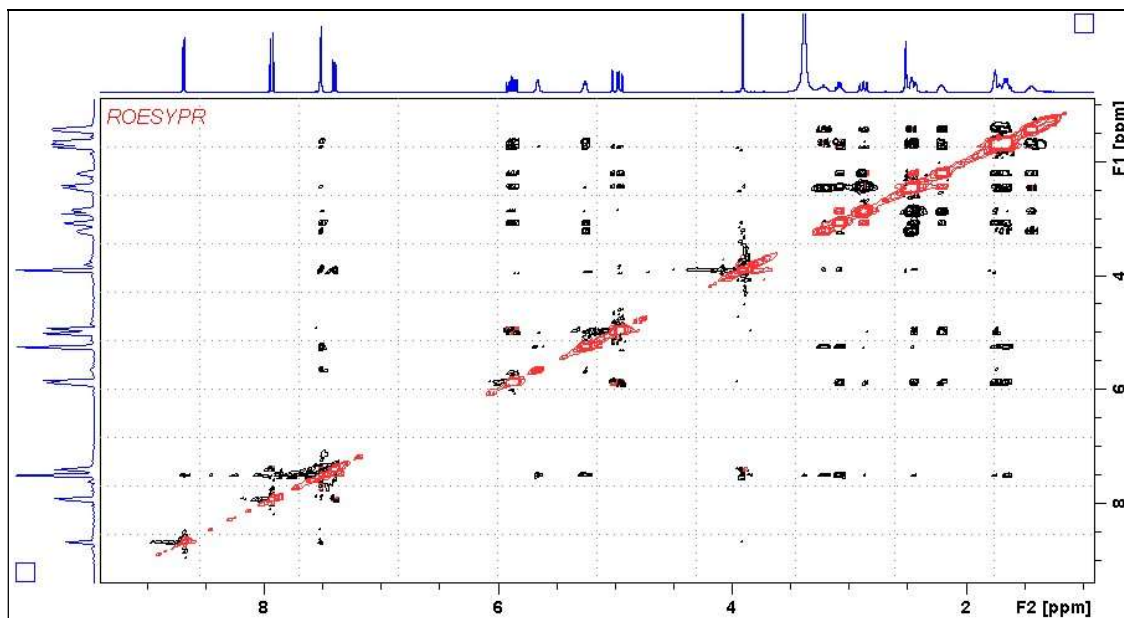**D1** = presaturation time = **2 sec** or other time of your choice.
P15 = spin lock time = **200000** or **250000 usec** (200 or 250 msec).

Type **ased** (enter) and review parameters used in the job.
The **PLW9(db)** 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**

0.9-9.4 ppm region of the **Neo400 ROESYPR** spectrum of quinine in D_6-DMSO with the HOD line at 3.37 ppm suppressed.

3.6 ROESY2PR with CW Presaturation 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(F1)** = **SWH(F2)** 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 = multiple of 4 or 8, **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.
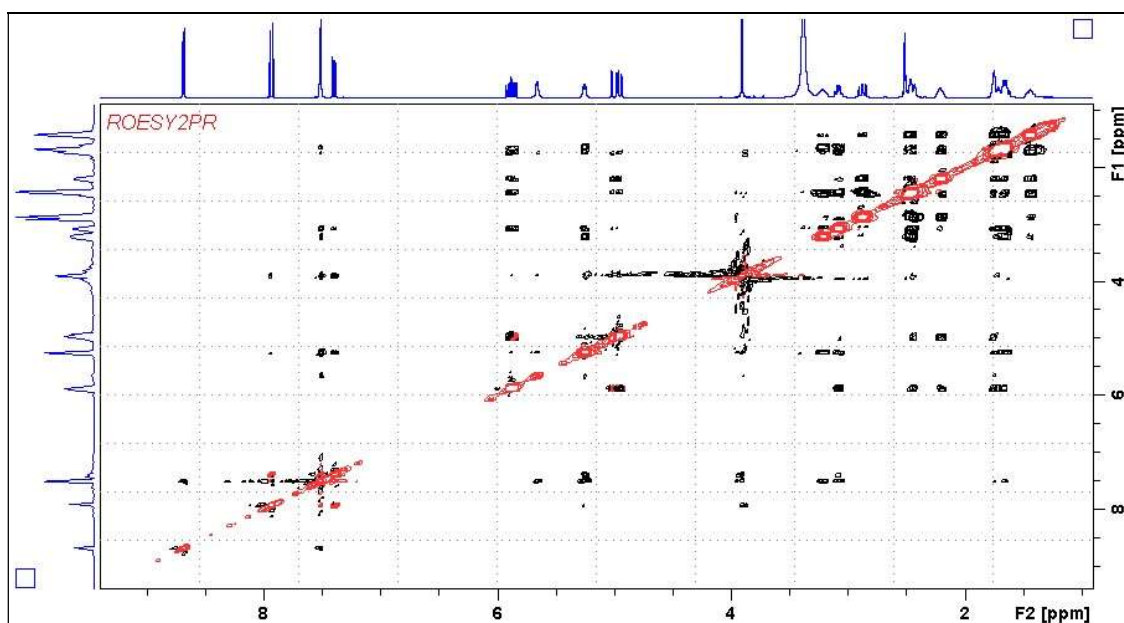The **PLW9(db)** presaturation power level can be adjusted if required
Set **receiver gain** using **RGA** *(important!)*.

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**

0.9-9.4 ppm region of the **Neo400 ROESYPR** spectrum of quinine in D_6-DMSO with the HOD line at 3.37 ppm suppressed.