



KJM 9250

bfprf1bfprf2 Experiments on the AVI 600 and AVII 600

Version 1.0

Topspin 1.3 Windows XP AVI 600

Topspin 3.5 Windows 7 AVII 600



© Professor Emeritus Alistair Lawrence Wilkins,  
University of Waikato, New Zealand.  
February 2018

# bfprf1bfprf2 Experiments on the AVI-600 and AVII-600

## 1.0 Introduction

Bruker pp's with CW presaturation on F1 require that it is applied at O1 = the spectral window midpoint. In cases where target compound signals are in the range 0-6 ppm and the HOD or the other line to be presaturated occurs in the vicinity of 5 ppm, this requires that the presaturation experiment is set up with O1 = 5 ppm and SW = 10 ppm.

*aw coded bfprf1bfprf2 experiments can be used to apply dual CW presaturation at CNST9 Hz on F1 and at CNST21 Hz on F2, independent of one's choice of SW and O1.*

*All power levels, pulse types and pulse times used in aw coded bfprf1bfprf2 2D experiments are by default prosol Table linked and no FQLISTS are required.*

Optimum outcomes are achieved in aw coded bfprf1bfprf2 experiments when the default prosol Table linked F1 and F2 presaturation powers (**PL9** and **PL21** respectively) are adjusted to be sufficient to suppress target signals while not suppressing correlations arising from other nearby signals.

Depending on the proximity of genuine signals this may require the **PL9** and **PL21** power levels to be reduced by 3-12 db from their default prosol Table values. This can be achieved by reducing (*ie* attenuating) the **PL9** and **PL21** power levels by adding 3-12 db to their default prosol Table power levels.

## 2.0 aw Coded bfprf1bfprf2 Parameter Sets

The following **aw coded bfprf1bfprf2** Parameter sets are available on the **AVI-600** and the **AVII-600**:

- |     |                                 |                         |
|-----|---------------------------------|-------------------------|
| 2.1 | <b>awcosyqbfprf1bfprf2</b>      | (no gradients)          |
| 2.2 | <b>awcosybfprf1bfprf2</b>       | (with gradients)        |
| 2.3 | <b>awtoscybfprf1bfprf2</b>      |                         |
| 2.4 | <b>awcleantocsybfprf1bfprf2</b> |                         |
| 2.5 | <b>awdipsi2bfprf1bfprf2</b>     |                         |
| 2.6 | <b>awnoesybfprf1bfprf2</b>      |                         |
| 2.7 | <b>awroesybfprf1bfprf2</b>      | (with CW spin lock)     |
| 2.8 | <b>awroesy2bfprf1bfprf2</b>     | (with pulsed spin lock) |

Prior to setting up **abfprf1bfprf2** experiment determine the frequencies in **Hz** of the two signals to be presaturated in a standard <sup>1</sup>H spectrum and ascertain the desired 2D-spectral window (**SW**) in **ppm** and its intended **O1 value** in **Hz** (= spectral window midpoint).

## 2.1 Cosyqfbfprf1bfprf2 with a P0 excitation pulse, no gradients and CW presaturation on F1 at cnst9 Hz and F2 at cnst21 Hz

Parameter set: **awcosyqfbfprf1bfprf2 (+ getprosol)**

Pulse programme: **awcosyqfbfprf1bfprf2**

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 = O2 = CNST1 in Hz** (*in this order!*) where **O1** = the spectral window midpoint. Enter **CNST9** and **CNST21 in Hz** of the signals to be presaturated on F1 and F2.

**TD(F2) = 2K**, **TD(F1) = 128-256** (your choice).

**P0** =  $\theta$  degree excitation pulse time, typically use a  $45^\circ$  or  $90^\circ$  pulse.

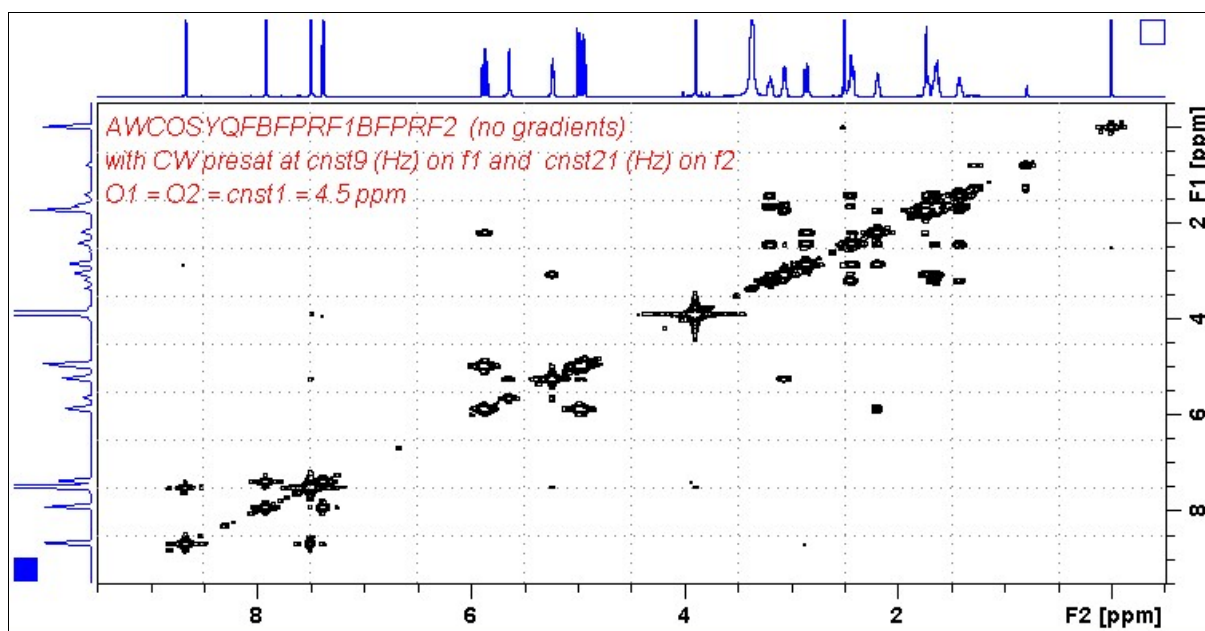
**NS** = 2, 4, 8 (any number is OK), **DS** = 2, 4 or 8.

**D1** = presaturation time = 1.5, 2.0 sec or other time of your choice.

Type **ased** (enter) and review parameters used in the job including **CNST1**, **CNST9** and **CNST21**. Check the **PL9** and **PL21** presaturation power levels are OK and if required adjust them appropriately.

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

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



AVI-600 **Cosyqfbfprf1bfprf2** 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 4.5 ppm ( $O1 = O2 = CNST1 = 2700.59$  Hz).

## 2.2 Cosybfprf1bfprf2with gradients and a P0 excitation pulse and CW presaturation on F1 at cnst9 Hz and F2 at cnst21 Hz

Parameter set: **awcosybfprf1bfprf2 (+ getprosol)**

Pulse programme: **awcosygpqfbfprf1bfprf2**

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 = O2 = CNST1 in Hz (in this order!)** where **O1** = the spectral window midpoint. Enter **CNST9** and **CNST21 in Hz** of the signals to be presaturated on F1 and F2\.

**TD(F2) = 2K**, **TD(F1) = 128-256** (your choice).

**P0** =  $\theta$  degree excitation pulse time, typically use a  $45^\circ$  or  $90^\circ$  pulse.

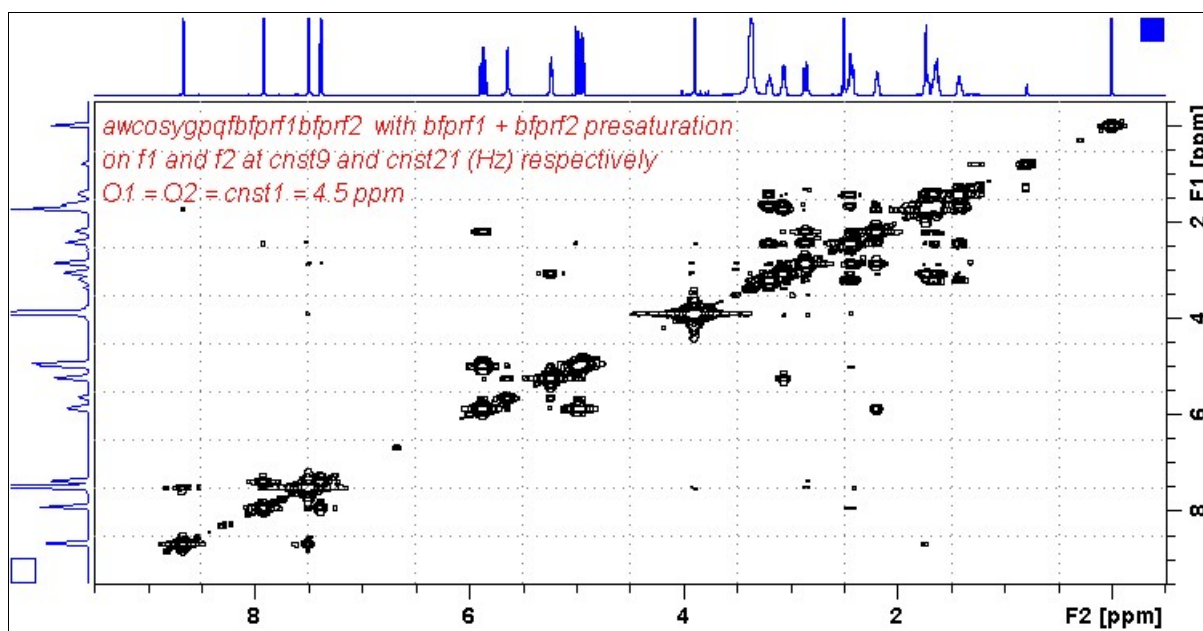
**NS** = 2, 4, 8 (any number is OK), **DS** = 2, 4 or 8.

**D1** = presaturation time = 1.5, 2.0 sec or other time of your choice.

Type **ased** (enter) and review parameters used in the job including **CNST1**, **CNST9** and **CNST21**. Check gradient and **PL9** and **PL21** presaturation power levels are OK and if required adjust them appropriately.

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

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



AVI-600 **Cosybfprf1bfprf2** 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 4.5 ppm ( $O1 = O2 = CNST1 = 2700.59$  Hz).

### 2.3 Tocsybfprf1bfprf2 with CW presaturation on F1 at cnst9 Hz and F2 at cnst21 Hz

Parameter set: **awtocsybfprf1bfprf2 (+ getprosol)**

Pulse programme: **awtocsybfprf1bfprf2**

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 = O2 = CNST1 in Hz** (*in this order!*) where **O1** = the spectral window midpoint. Enter **CNST9** and **CNST21 in Hz** of the signals to be presaturated on F1 and F2.

**TD(F2) = 2K**, **TD(F1) = 128-256** (your choice).

**NS = 4, 8, 16** (multiple of 4 or 8 recommended), **DS = 4 or 8**.

**D1** = presaturation time = 1.5, 2.0 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 including **CNST1**, **CNST9** and **CNST21**. Check the **PL9** and **PL21** presaturation power levels are OK and if required adjust them appropriately.

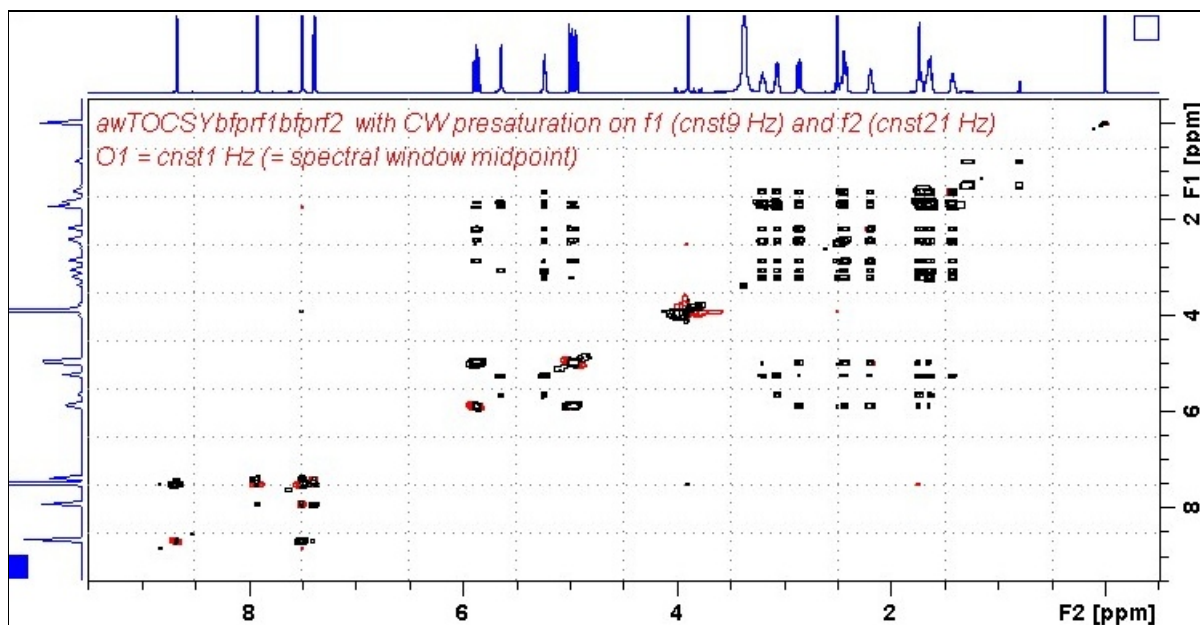
Set **receiver gain** using **RGA** (*important!*).

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

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

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

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



AVI-600 **Tocsybfprf1bfprf2** 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 4.5 ppm (O1 = O2 = CNST1 = 2700.59 Hz).

## 2.4 Clean-tocsybfprf1bfprf2 with CW presaturation on F1 at cnst9 Hz and F2 at cnst21 Hz

Parameter set: **awcleantocsybfprf1bfprf2 (+ getprosol)**

Pulse programme: **awclmlevbfprf1bfprf2**

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 = O2 = CNST1 in Hz** (*in this order!*) where **O1** = the spectral window midpoint. Enter **CNST9** and **CNST21 in Hz** of the signals to be presaturated on F1 and F2.

**TD(F2) = 2K**, **TD(F1) = 128-256** (your choice).

**NS = 4, 8, 16** (multiples of 4 or 8 recommended), **DS = 4 or 8**.

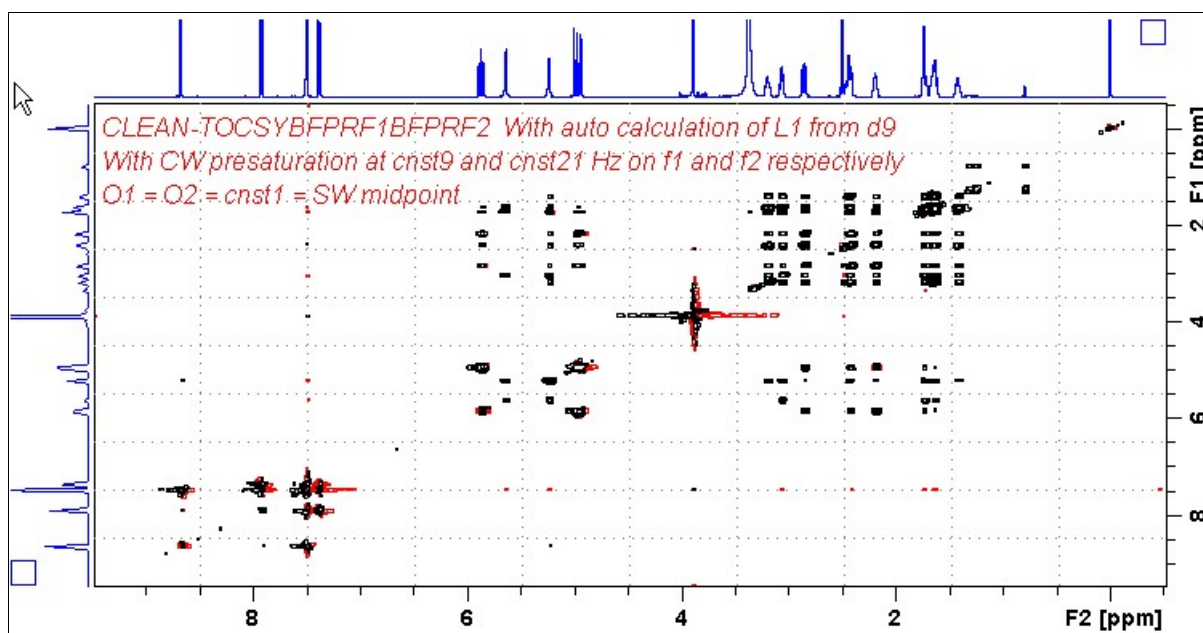
**D1** = presaturation time = 1.5, 2.0 sec or other time of your choice.

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

Type **ased** (enter) and review parameters used in the job including **CNST1**, **CNST9** and **CNST21**. Check the **PL9** and **PL21** presaturation power levels are OK and if required adjust them appropriately.

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

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



AVI-600 **Clean-tocsybfprf1bfprf2** 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 4.5 ppm ( $O1 = O2 = CNST1 = 2700.59$  Hz).



## 2.5 Dipsi2bfprf1bfprf2 with CW presaturation on F1 at cnst9 Hz and F2 at cnst21 Hz

Parameter set: **awdipsi2bfprf1bfprf2 (+ getprosol)**

Pulse programme: **awdipsi2phbfprf1bfprf2**

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 = O2 = CNST1 in Hz** (*in this order!*) where **O1** = the spectral window midpoint. Enter **CNST9** and **CNST21 in Hz** of the signals to be presaturated on F1 and F2.

**TD(F2) = 2K**, **TD(F1) = 128-256** (your choice).

**NS = 4, 8, 16** (multiples of 4 or 8 recommended), **DS = 4 or 8**.

**D1 = presaturation time = 1.5, 2.0 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 including **CNST1**, **CNST9** and **CNST21**. Check the **PL9** and **PL21** presaturation power levels are OK and if required adjust them appropriately.

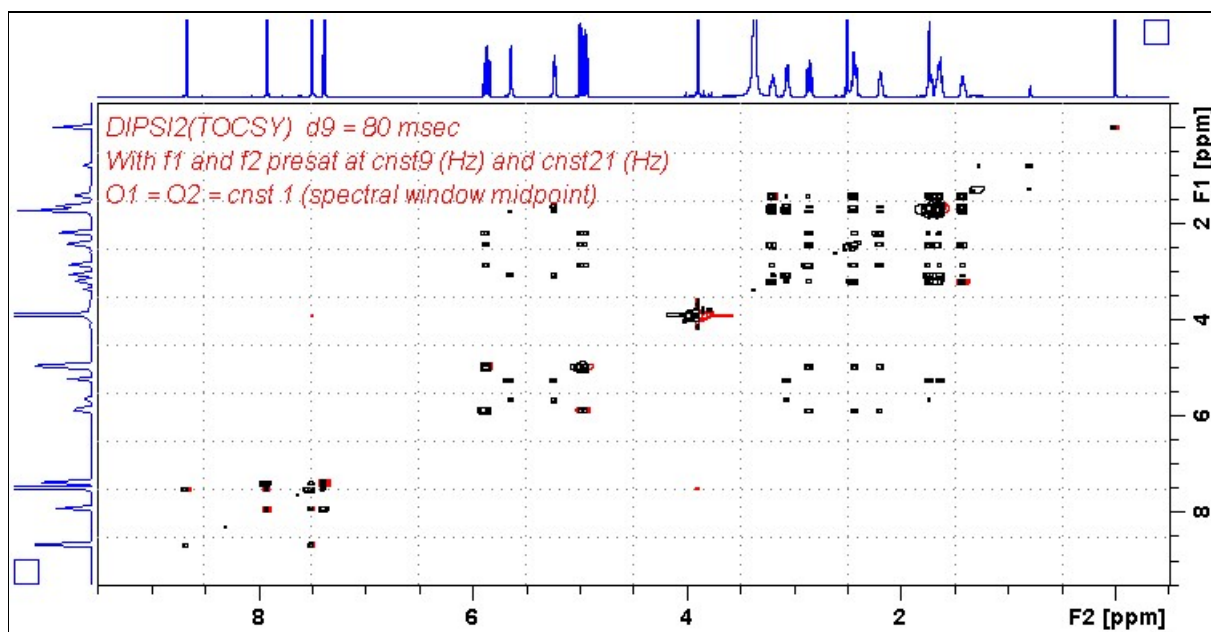
Set **receiver gain** using **RGA** (*important!*).

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

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

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

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



AVI-600 **Dipsi2bfprf1bfprf2** 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 4.5 ppm (O1 = O2 = CNST 1 = 2700.59 Hz).

## 2.6 Noesybfprf1bfprf2 with CW presaturation on F1 at cnst9 Hz and F2 at cnst21 Hz

Parameter set: **awnoesybfprf1bfprf2 (+ getprosol)**

Pulse programme: **awnoesygpphbfprf1bfprf2**

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 = O2 = CNST1 in Hz** (*in this order!*) where **O1** = the spectral window midpoint. Enter **CNST9** and **CNST21 in Hz** of the signals to be presaturated on F1 and F2.

**TD(F2) = 2K**, **TD(F1) = 128-256** (your choice).

**NS = 4, 8, 16** (multiples of 4 or 8 recommended), **DS = 4 or 8**.

**D1 = presaturation time = 1.5, 2.0 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 including **CNST1**, **CNST9** and **CNST21**. Check the **PL9** and **PL21** presaturation power levels are OK and if required adjust them appropriately.

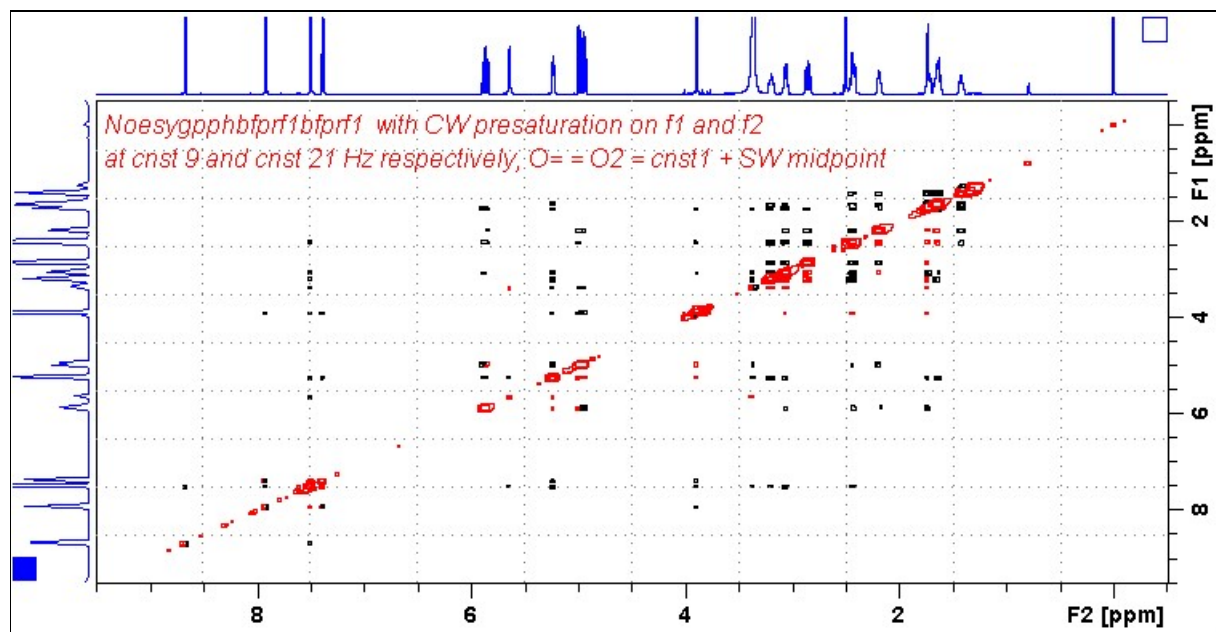
Set **receiver gain** using **RGA** (*important!*).

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

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

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

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



AVI-600 **Noesybfprf1bfprf2** 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 4.5 ppm ( $O1 = O2 = CNST 1 = 2700.59$  Hz).



## 2.7 Roesybfprf1bfprf2 with CW presaturation on F1 at cnst9 Hz and F2 at cnst21 Hz

Parameter set: **awroesybfprf1bfprf2 (+ getprosol)**

Pulse programme: **awroesyphbfprf1bfprf2** (with CW spinlock)

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 = O2 = CNST1 in Hz** (*in this order!*) where **O1** = the spectral window midpoint. Enter **CNST9** and **CNST21 in Hz** of the signals to be presaturated on F1 and F2.

**TD(F2) = 2K**, **TD(F1) = 128-256** (your choice).

**NS = 4, 8, 16** (multiples of 4 or 8 recommended), **DS = 4 or 8**.

**D1** = presaturation time = 1.5, 2.0 sec or other time of your choice.

**P15** = spinlock time = **200000 usec** or **250000 usec** = 250 or 200 msec.

Type **ased** (enter) and review parameters used in the job including **CNST1**, **CNST9** and **CNST21**. Check the **PL9** and **PL21** presaturation power levels are OK and if required adjust them appropriately.

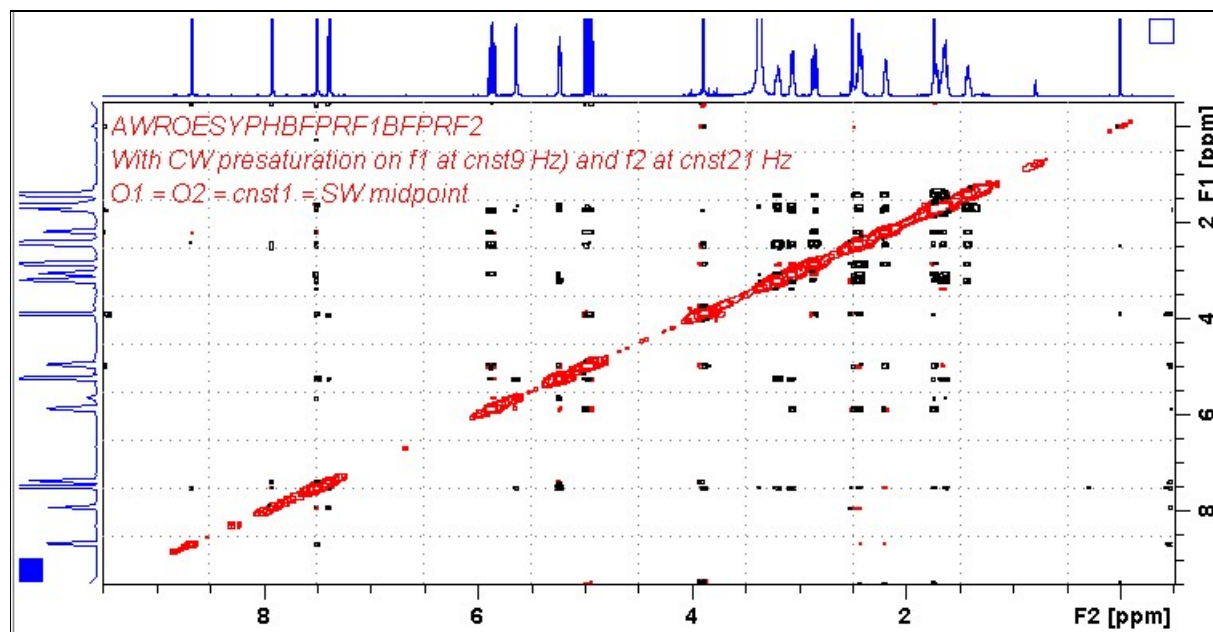
Set **receiver gain** using **RGA** (*important!*).

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

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

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

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



AVI-600 **Roesybfprf1bfprf2** 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 4.5 ppm (**O1 = O2 = CNST1 = 2700.59 Hz**).

## 2.8 Roesy2bfprf1bfprf2 with CW presaturation on F1 at cnst9 Hz and F2 at cnst21 Hz

Parameter set: **awroesy2bfprf1bfprf2 (+ getprosol)**

Pulse programme: **awroesy2bfprf1bfprf2**(with pulsed spinlock)

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 = O2 = CNST1 in Hz** (*in this order!*) where **O1** = the spectral window midpoint. Enter **CNST9** and **CNST21 in Hz** of the signals to be presaturated on F1 and F2.

**TD(F2) = 2K**, **TD(F1) = 128-256** (your choice).

**NS = 4, 8, 16** (multiples of 4 or 8 recommended), **DS = 4 or 8**.

**D1** = presaturation time = 1.5, 2.0 sec or other time of your choice.

**P15** = spinlock time = **200000 usec** or **250000 usec** = 200 or 250 msec.

Type **ascd** (enter) and review parameters used in the job including **CNST1**, **CNST9** and **CNST21**. Check the **PL9** and **PL21** presaturation power levels are OK and if required adjust them appropriately.

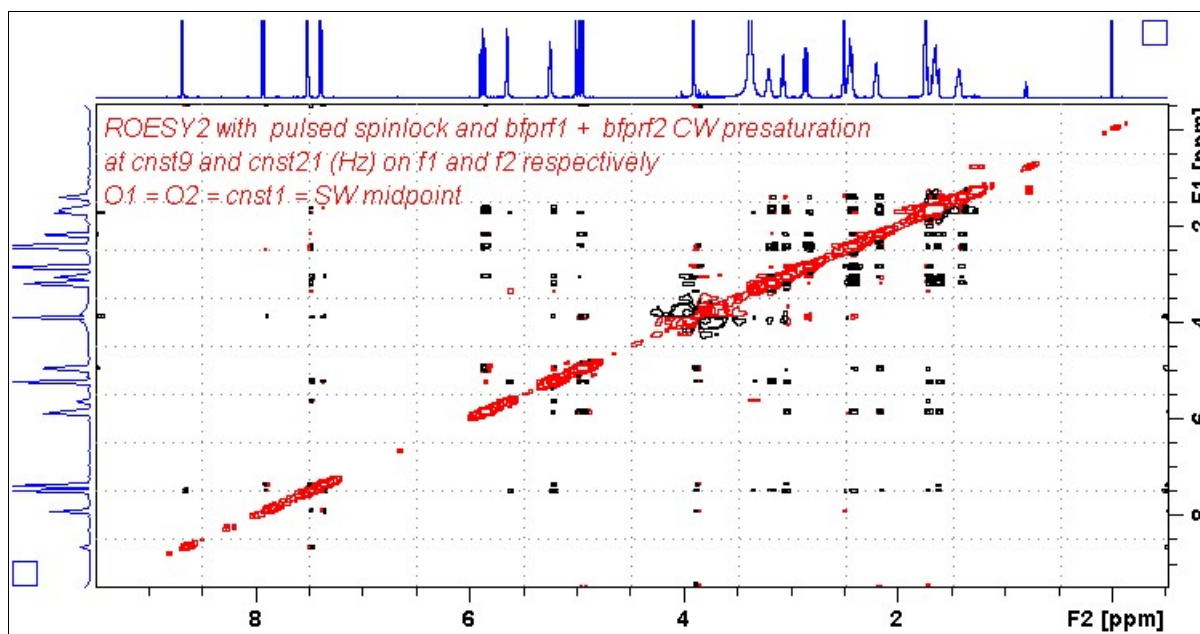
Set **receiver gain** using **RGA** (*important!*).

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

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

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

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



AVI-600 Roesy2bfprf1bfprf2 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 4.5 ppm (O1 = O2 = CNST 1 = 2700.59 Hz).