



KJM 9250

AVI 600 and AVII 600 MHz HSQC, HMBC and H2BC
Experiments

Version 5.0

Topspin 2.1 Windows XP AVI 600
Topspin 3.2 Windows 7 AVII 600



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AVI and AVII 600 MHz HSQC, HMBC and H2BC Experiments

1.0 Introduction

^1H detected aw coded **HSQC**, **HMBC** and **H2BC** parameter sets are set up with 1K or 2K acquired ^1H points and 128 to 256 ^{13}C increments. The **SHMBC** experiment (AVII-600 only) has a smaller number of ^{13}C increments.

^1H and ^{13}C spectral windows and their mid points should be determined before setting up **HSQC**, **HMBC**, **SHMBC** or **H2BC** experiments.

1.1 Processing

HSQC experiments are phase sensitive experiments. These spectra should be phased **before** using the **abs1** and **abs2** commands. Low level 2J correlations may occasionally be observed in **HSQC** spectra.

HMBC experiments are absolute value experiments. Phasing is not required

SHMBC and **H2BC** experiments are acquired in phase sensitive mode and transformed to afford an absolute value spectrum using the **xfb** and **xf2m** commands.

2.0 Experiments and Parameter Sets

The following ^1H detected HSQC, HMBC and H2BC experiments and parameter sets have been set up on the AVI and AVII 600 MHz spectrometers.

2.1	hsqcetgp	not multiplicity edited, DEPT45 like
2.2	hsqcedetgp	multiplicity edited, DEPT135 like
2.3	hsqcetedgpsisp2.3-135	
2.4	hsqcetedgpsisp2.3-135pr	with CW presaturation
2.5	hsqcetedgpsisp2.3-135adia	with adiabatic ^{13}C decoupling
2.6	hsqc-tocsy	not multiplicity edited, DEPT45 like
2.7	hsqc-dipsi2.45 and .135	DEPT45 and DEPT135 like variants
2.8	hsqc-noesy	
2.9	hsqc-roesy	CW spin locked
2.10	hsqc-roesy2	pulsed spin locked
2.11	hmbc	with nJ selection
2.12	hmbcpr	with nJ selection and CW presaturation
2.13	hmbclp2	with $^1J_{\text{min/max}}$ filter and nJ selection
2.14	hmbc-cigar	with ^{13}C decoupling
2.15	shmhc	selective hmbc, AVII-600 only
2.16	h2bc	for 2J correlations

2.1 HSQCETGP

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

pulse programme: **hsqcetgp**

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1P** = ^1H spectral window midpoint in ppm.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST2 = 1J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

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

Check gradients are OK.

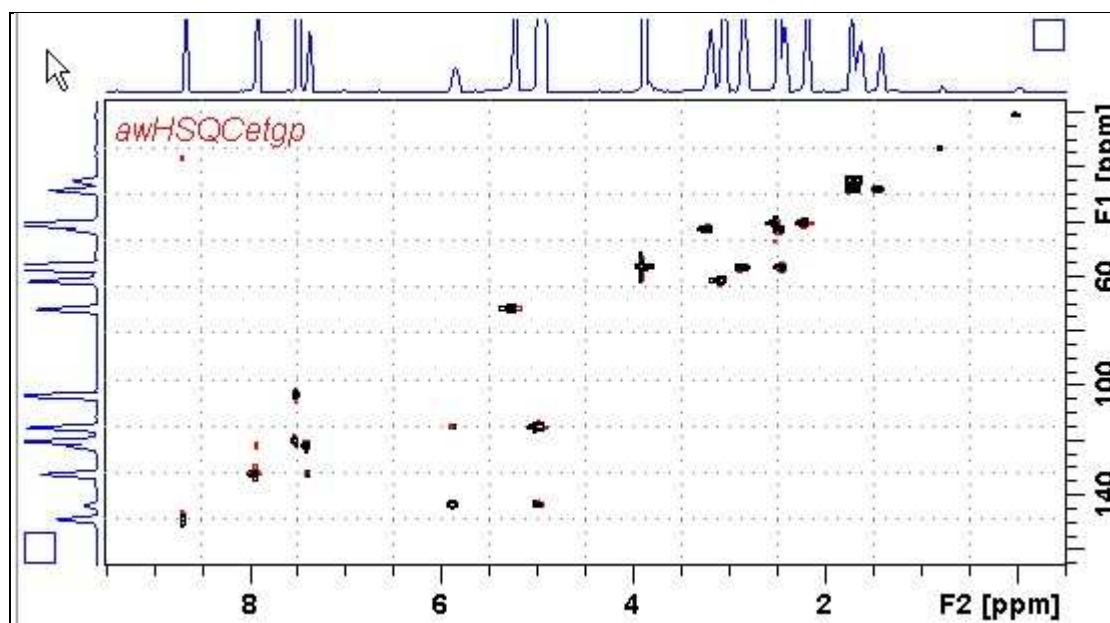
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

xfb, **abs1** and **abs2**



600 MHz **HSQCETGP** spectrum (not edited) of quinine in D_6 -DMSO.

2.2 HSQCEDETGP

Parameter set: **awhsqcedetgp-135** (+ getprosol)

Pulse programme: **awhsqcedetgp-135**

d21 is automatically calculated from **cnst2**

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1P** = ^1H spectral window midpoint in ppm.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST2 = 1J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

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

Check gradients are OK.

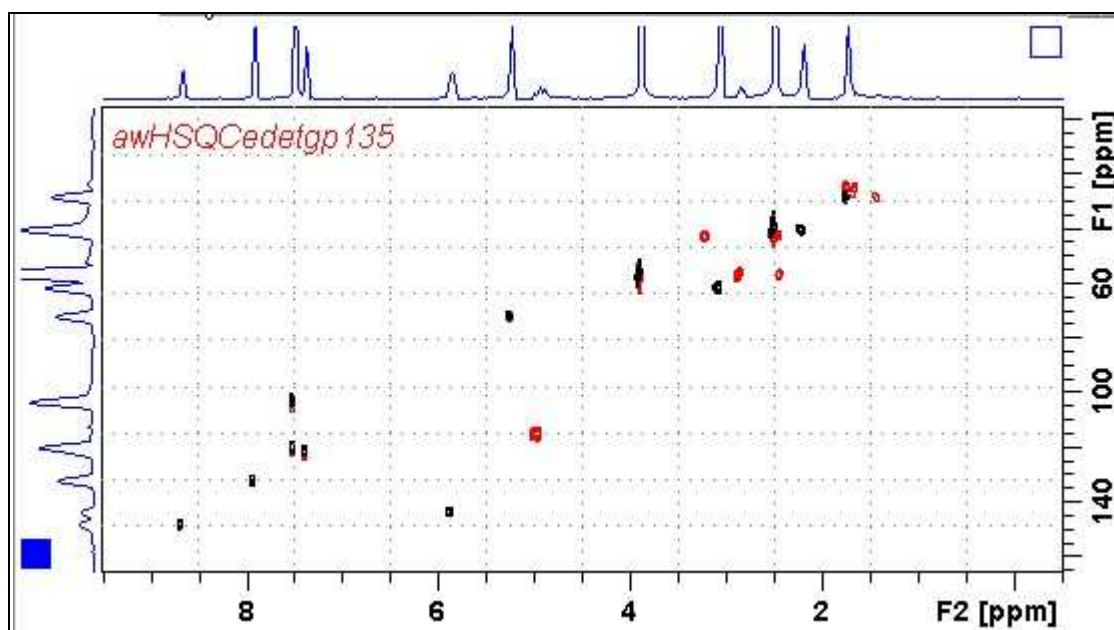
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

xfb, **abs1** and **abs2**



600 MHz **HSQCEDETGP** spectrum (DEPT135-like) of quinine in D₆-DMSO plotted with CH and CH₃ positive (black) and CH₂ negative (red).

2.3 HSQCEDETGPSISP2.3-135

parameter set: **awhsqcedetgpsisp2.3-135** (+ **getprosol**)

fast load: **awhsqc135** (+ **getprosol**)

pulse programme: **awhsqcedetgpsisp2.3-135**

d21 and **d24** are automatically calculated from **cnst2**

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1P** = ^1H spectral window midpoint in ppm.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST2 = 1J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

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

Check gradients and shaped pulses are OK.

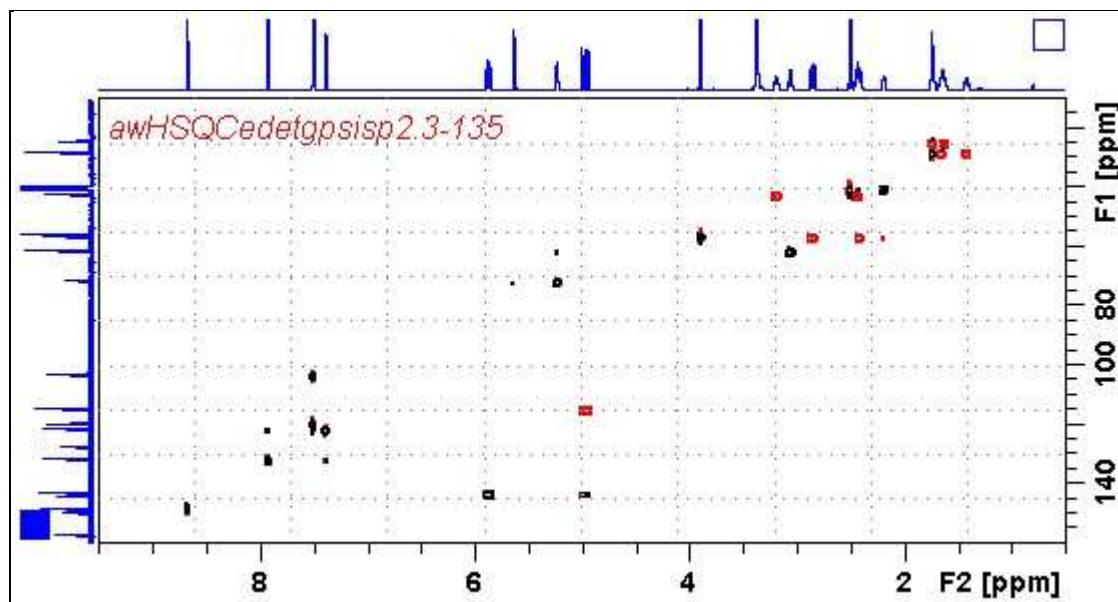
Set receiver gain using **RGA** (*Important!*).

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

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

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

xfb, **abs1** and **abs2**



600 MHz **HSQCEDETGPSISP2.3-135** spectrum of quinine in D6-DMSO plotted with CH and CH_3 correlations positive (black) and CH_2 correlations negative (red).

2.4 HSQCEDETGPSISP2.3-135PR

Parameter set: **awhsqcedetgpsisp2.3-135pr** (+ **getprosol**)

Fast load: **awhsqc135pr** (+ **getprosol**)

Pulse programme: **awhsqcedetgpsisp2.3-135pr**

d21 and **d24** are automatically calculated from **cnst2**

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1** = ^1H frequency to be presaturated during **D1**.

Check **SW** = spectral window is wide enough.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

PL9 = CW presaturation power level.

CNST2 = 1J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

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

Check gradients and shaped pulses are OK.

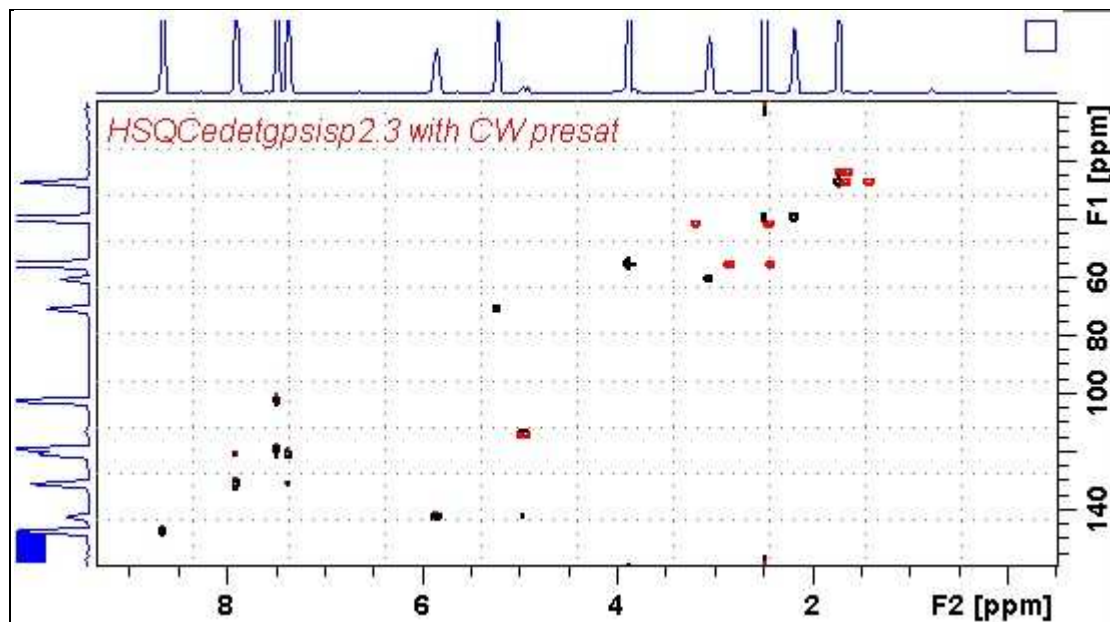
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

xfb, **abs1** and **abs2**



600 MHz **HSQCEDETGPSISP2.3-135PR** spectrum of quinine in D_6 -DMSO with CW presaturation of the HOD line. The spectrum is plotted with positive CH and CH_3 correlations (black) and negative CH_2 correlations (red).

2.5 HSQCEDETGPSISP2.3-135ADIA

Parameter set: **awhsqcedetgpsisp2.3-135adia**

Pulse programme: **awhsqcedetgpsisp2.3-135**

d21 and **d24** are automatically calculated from **cnst2**

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm

Enter **O1P** = ^1H spectral window midpoint in ppm.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128 - 256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST2 = 1J coupling constant = **145 Hz** or other value of your choice.

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

Check **CPDPRG2** = **bi_p5m4sp_4sp.2** for adiabatic ^{13}C decoupling.

Check gradients and shaped pulses are OK.

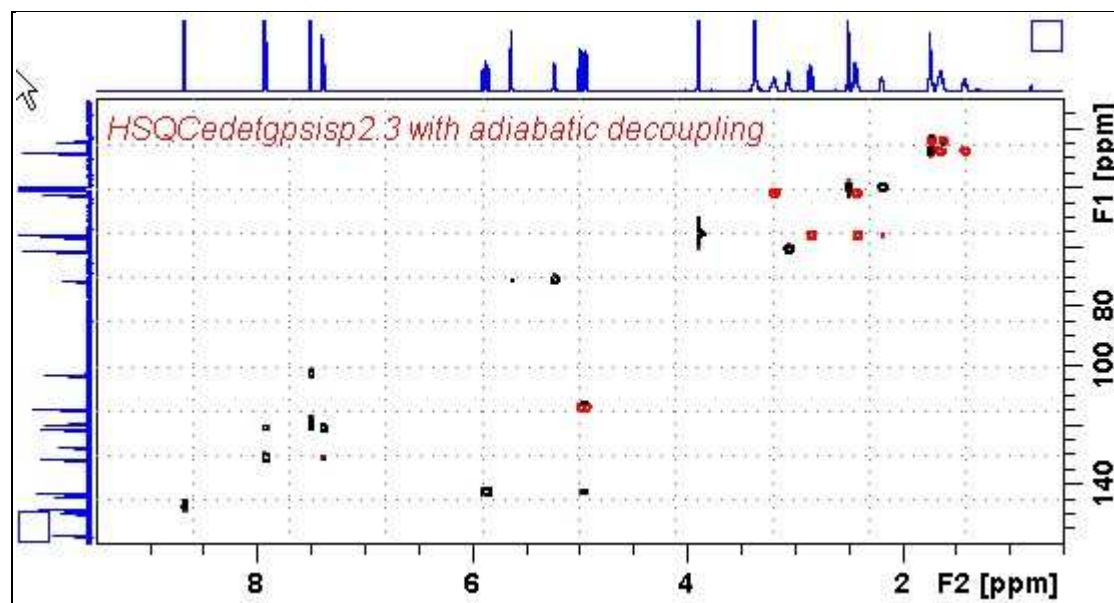
Set receiver gain using **RGA** (*Important!*).

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

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

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

xfb, **abs1** and **abs2**



600 MHz **HSQCEDETGPSISP2.3-135ADIA** spectrum of quinine in D_6 -DMSO with adiabatic ^{13}C decoupling. The spectrum is plotted with positive CH and CH_3 correlations (black) and negative CH_2 correlations (red).

2.6 HSQC-TOCSY

Parameter set: **awhscq-tocsy (+ getprosol)**

Pulse programme: **hscqetgpml**

Type **eda** (enter) and enter **SW (¹H)** and **SW (¹³C)** in ppm.

Enter **O1P** = ¹H spectral window midpoint in ppm.

Enter **O2P** = ¹³C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

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

CNST2 = ¹J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

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

Check gradients are OK.

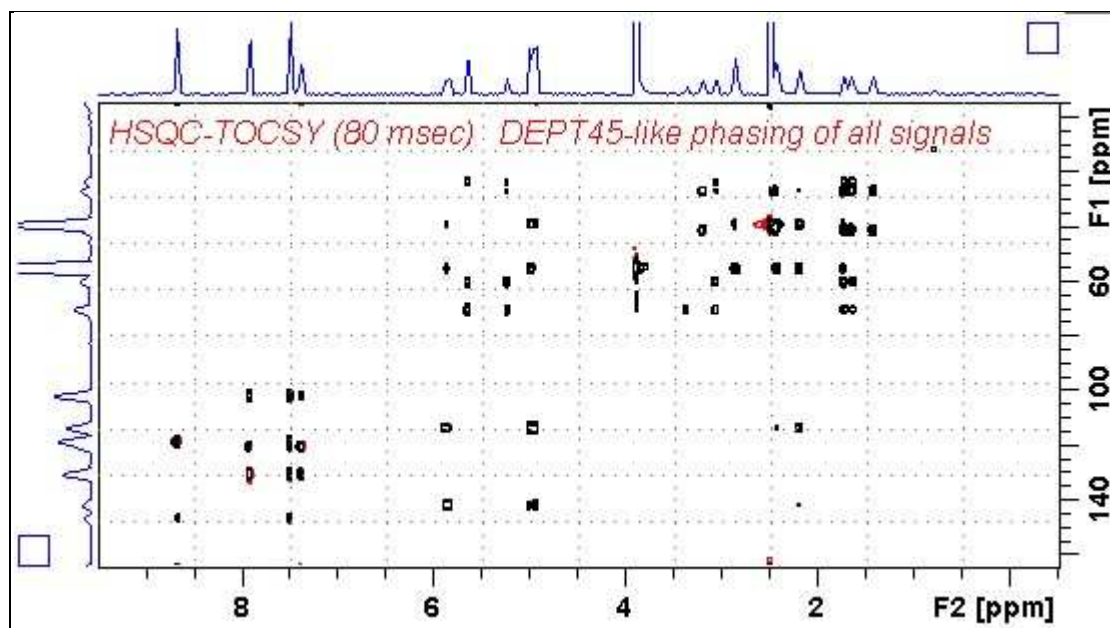
Set receiver gain using **RGA** (*Important!*).

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

WDW(F1) = WDW(F2) = QSINE

SSB(F2) = SSB(F1) = 2

xfb, abs1 and abs2



600 MHz **HSQC-TOCSY** spectrum of quinine in D6-DMSO. HSQC and correlated TOCSY peaks are positively phased.

2.7.1 HSQC-DIPSI2.45

Parameter set: **awhsqc-dipsi2.45** (+ **getprosol**)

Pulse programme: **awhsqcdipsi2.45**

With auto calculation of **d24** from **cnst2**

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1P** = ^1H spectral window midpoint in ppm.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

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

CNST2 = 1J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

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

Check gradients and shaped pulses are OK.

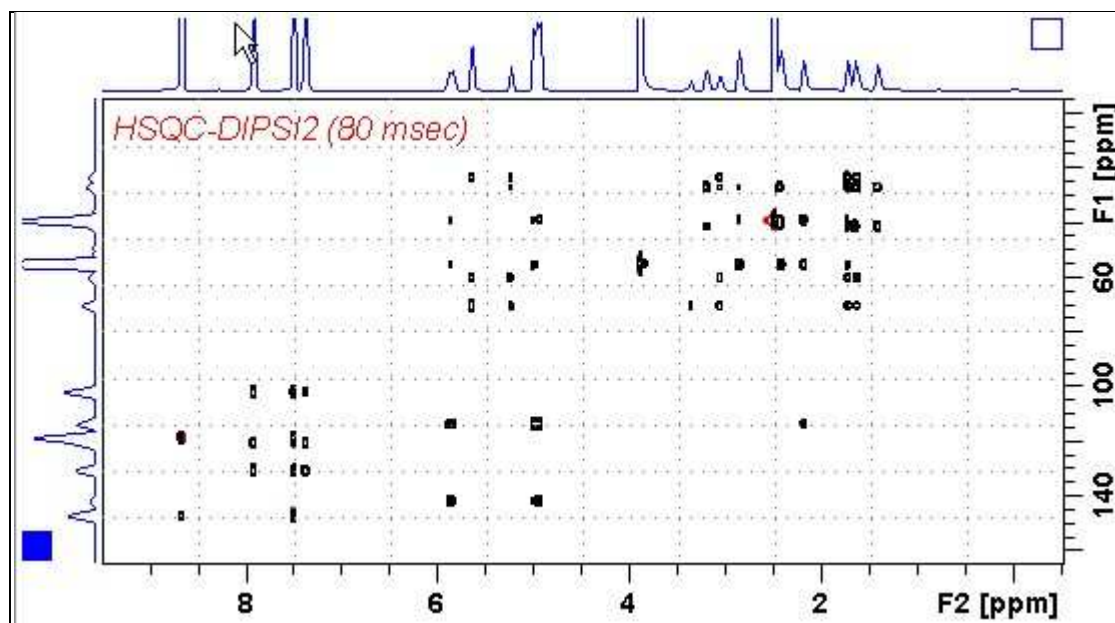
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

xfb, **abs1** and **abs2**



600 MHz **HSQC-DIPSI2.45** spectrum of quinine in D_6 -DMSO.

2.7.2 HSQC-DIPSI2.135

Parameter set: **awhsqc-dipsi2.135** (+ getprosol)

Pulse programme: **awhsqcdipsi2.135**

With auto calculation of **d24** from **cnst2**

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1P** = ^1H spectral window midpoint in ppm.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

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

CNST2 = 1J coupling constant = **145 Hz** or other value of your choice (eg: 122-160 Hz).

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

Check gradients and shaped pulses are OK.

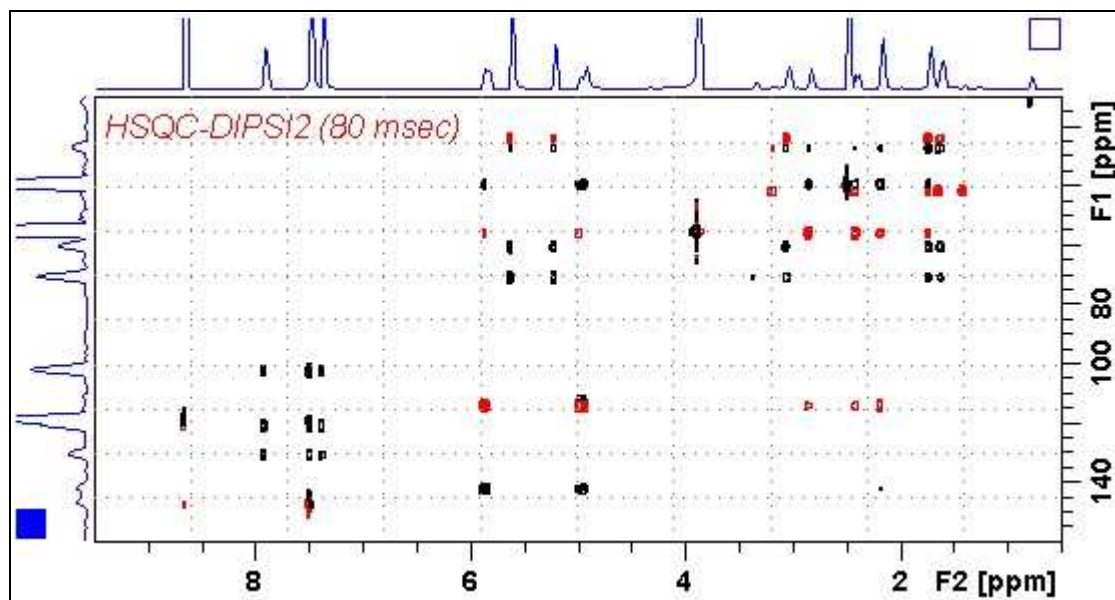
Set **receiver gain** using **RGA** (*Important!*).

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

WDW(F1) = WDW(F2) = QSINE

SSB(F2) = SSB(F1) = 2

xfb, abs1 and abs2



600 MHz **HSQC-DIPSI2.135** spectrum of quinine in D_6 -DMSO. CH and CH_3 signals and correlated DIPSI2 signals are positive (black). CH_2 signals and correlated DIPSI2 signals are negative (red).

2.8 HSQC-NOESY

Parameter set: **awhsqc-noesy (+ getprosol)**

Pulse programme: **hsqcetgnosp**

Type **eda** (enter) and enter **SW (¹H)** and **SW (¹³C)** in ppm.

Enter **O1P** = ¹H spectral window midpoint in ppm.

Enter **O2P** = ¹³C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

D8 = NOESY correlation time = **0.5 sec** or other value of your choice (0.3-0.8 sec),

CNST2 = ¹J coupling constant = **145 Hz** or other value of your choice (eg: 125-160 Hz).

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

Check gradients and the shaped pulse are OK.

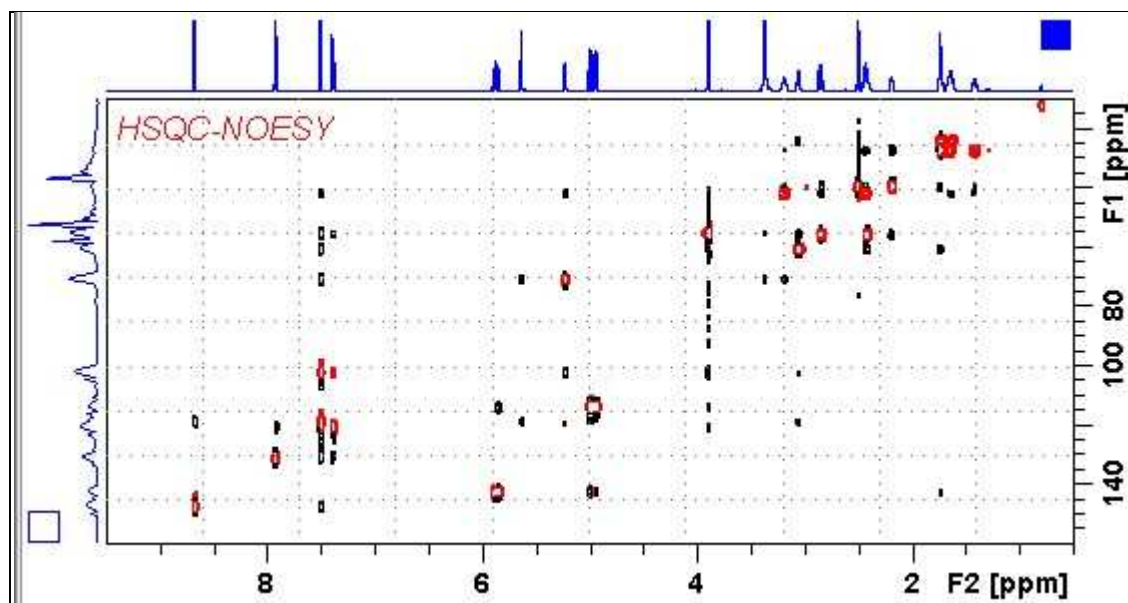
Set **receiver gain** using **RGA** (*Important!*).

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

WDW(F1) = WDW(F2) = QSINE

SSB(F2) = SSB(F1) = 2

xfb, abs1 and abs2



600 MHz **HSQC-NOESY** spectrum of quinine in D6-DMSO. HSQC signals (red) are negatively phased. Correlated NOESY signals (black) are positively phased. HSQC signal levels were reduced by a factor of 10-20 relative to NOESY signals levels using the **edlev** command.

2.9 HSQC-ROESY

Parameter set: **awhsqc-roesy (+ getprosol)**

Pulse programme: **hsqcetgprosp** (with CW spin lock)

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1P** = ^1H spectral window midpoint in ppm.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST2 = 1J coupling constant = **145 Hz** or other value of your choice.

P15 = ROESY correlation time **200000** or **250000** usec (= 200 or 250 msec).

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

Check gradients and shaped pulses are OK.

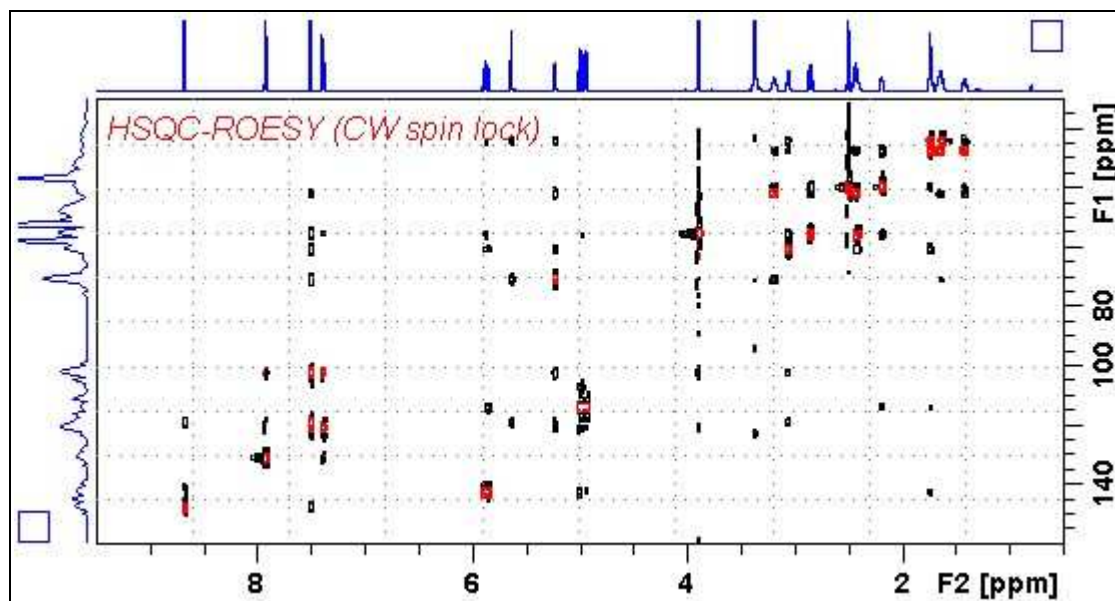
Set **receiver gain** using **RGA** (*Important!*).

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

WDW(F1) = WDW(F2) = QSINE

SSB(F2) = SSB(F1) = 2

xfb, abs1 and abs2



600 MHz **HSQC-ROESY** spectrum of quinine in D6-DMSO. HSQC signals (red) are negatively phased. Correlated ROESY signals (black) are positively phased. HSQC signal levels were reduced by a factor of 10 relative to ROESY signal levels using the **edlev** command.

2.10 HSQC-ROESY2

Parameter set: **awhsqc-roesy2** (+ **getprosol**)

Pulse programme: **hsqcetgprosp.2** (with pulsed spin lock)

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1P** = ^1H spectral window midpoint in ppm.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST2 = 1J coupling constant = **145 Hz** or other value of your choice

P15 = ROESY correlation time = **200000** or **250000** usec (= 200 or 250 msec).

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

Check gradients and shaped pulses are OK.

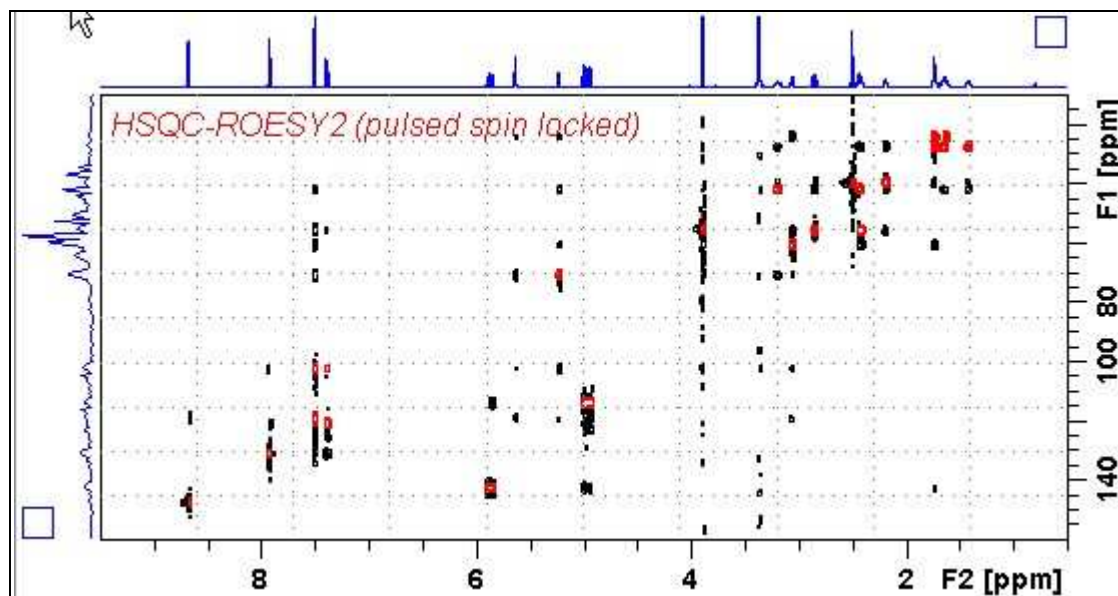
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

xfb, **abs1** and **abs2**



600 MHz **HSQC-ROESY2** spectrum of quinine in $\text{D}_6\text{-DMSO}$. HSQC signals (red) are negatively phased. Correlated ROESY2 signals (black) are positively phased. HSQC signal levels were reduced by a factor of 10 relative to ROESY2 signal levels using the **edlev** command.

2.11 HMBC

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

Pulse programme: **hmbcglpndqf**

Type **eda** (enter) and enter **SW (¹H)** and **SW (¹³C)** in ppm.

Enter **O1P** = ¹H spectral window midpoint in ppm.

Enter **O2P** = ¹³C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST2 = ¹J coupling constant = **145 Hz** or other value of your choice.

CNST13 = ⁿJ selection filter = **8 Hz** or other value of your choice.

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

Check gradients are OK.

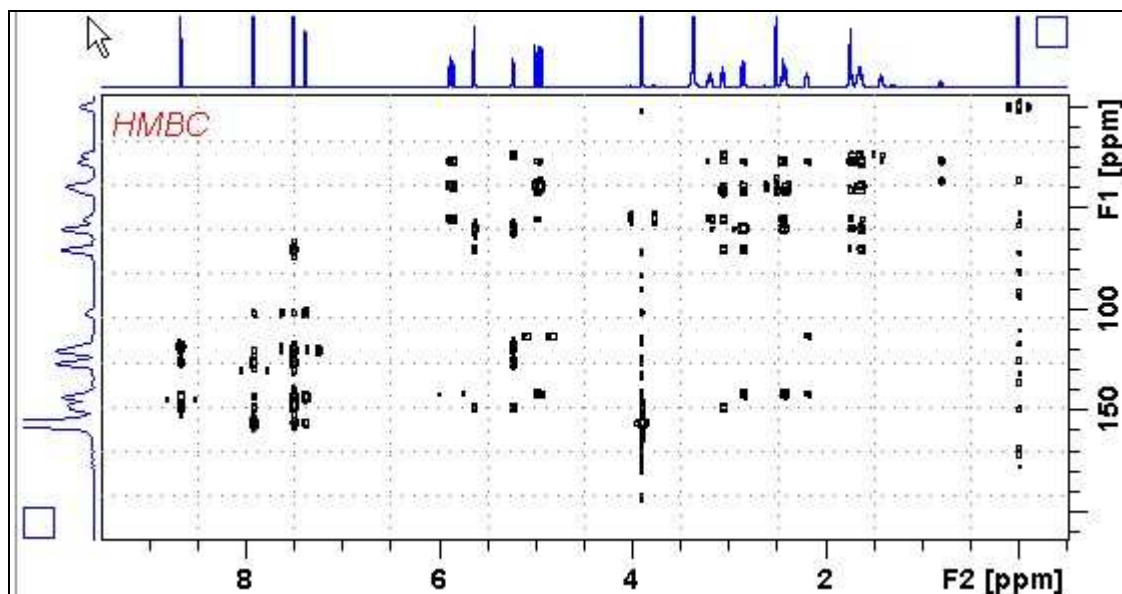
Set **receiver gain** using **RGA** (*Important!*).

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

WDW(F1) = WDW(F2) = SINE

SSB(F2) = SSB(F1) = 0

xfb, abs1 and abs2



600 MHz **HMBC** spectrum of quinine in D₆-DMSO.

2.12 HMBCPR

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

Pulse programme: **awhmbcgplpndprqf**

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1** = ^1H frequency to be presaturated during **D1**.

Check **SW** = spectral window is wide enough.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

PL9 = CW presaturation power applied during **D1**.

CNST2 = 1J coupling constant = **145 Hz** or other value of your choice.

CNST13 = nJ selection filter = **8 Hz** or other value of your choice.

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

Check gradients are OK.

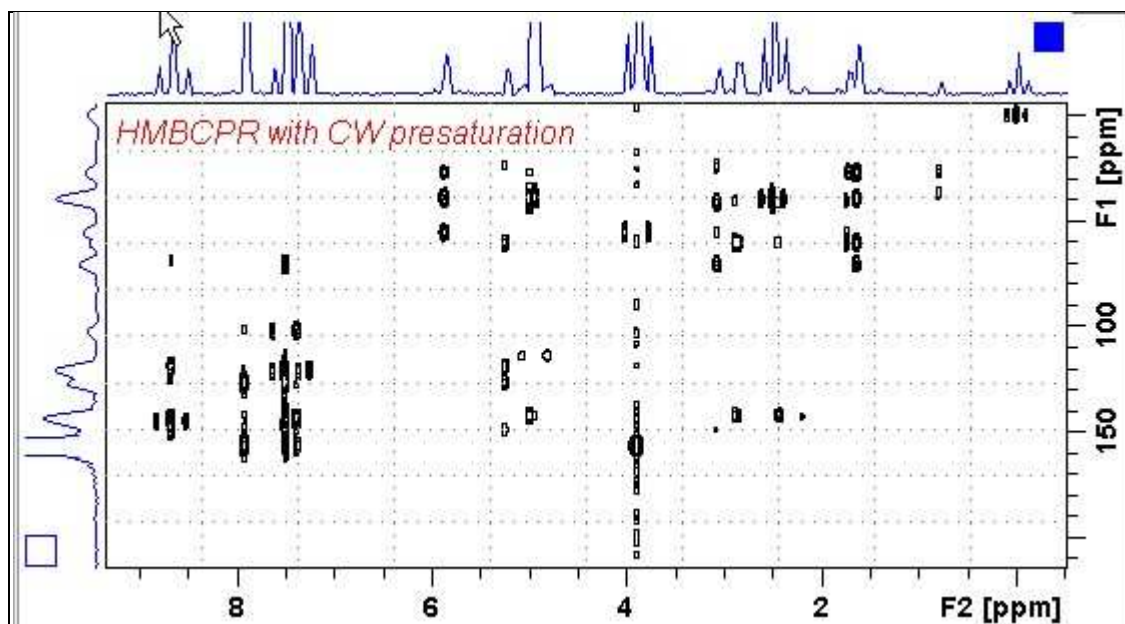
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

xfb, **abs1** and **abs2**



600 MHz **HMBCPR** spectrum of quinine in $\text{D}_6\text{-DMSO}$ with CW presaturation of the HOD signal at 3.37 ppm.

2.13 HMBCL2

Parameter set: **awhmbcl2** (+ **getprosol**)

Pulse programme: **hmbcgp12ndqf**

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1P** = ^1H spectral window midpoint in ppm.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST6 = min. 1J coupling constant = **125 Hz** or other value of your choice.

CNST7 = max. 1J coupling constant = **165 Hz** or other value of your choice.

CNST13 = nJ selection filter = **8Hz** or other value of your choice

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

Check gradients are OK.

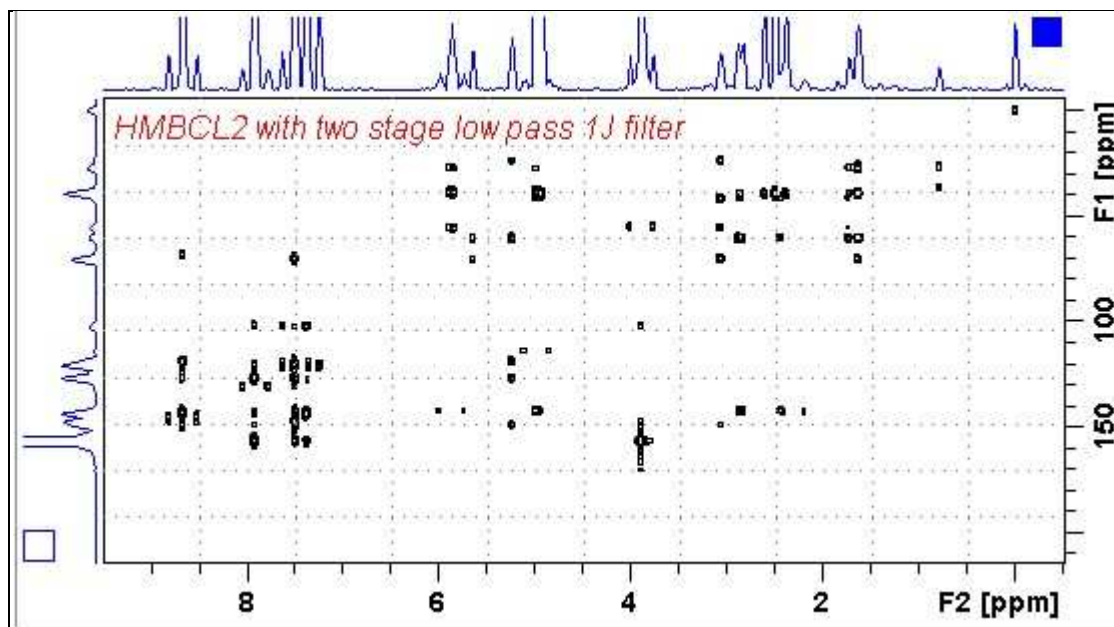
Set receiver gain using **RGA** (*Important!*).

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

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

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

xfb, **abs1** and **abs2**



600 MHz HMBCL2 spectrum of quinine in D₆-DMSO with a two stage 1J filter.

2.14 HMBC-CIGAR

Parameter set: **awhmbc-cigar** (+ **getprosol**)

Pulse programme: **hmbcacgplpqf**

Spectrum is acquired with ^{13}C decoupling

Type **eda** (enter) and enter **SW** (^1H) and **SW** (^{13}C) in ppm.

Enter **O1P** = ^1H spectral window midpoint in ppm.

Enter **O2P** = ^{13}C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST6 = 125 Hz, **CNST7** = 160 Hz = min/max 1J selection filter range.

CNST14 = 4 Hz, **CNST15** = 12 Hz min/max nJ selection filter range.

CNST16 = 1.0 = J scale factor.

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

Check gradients are OK.

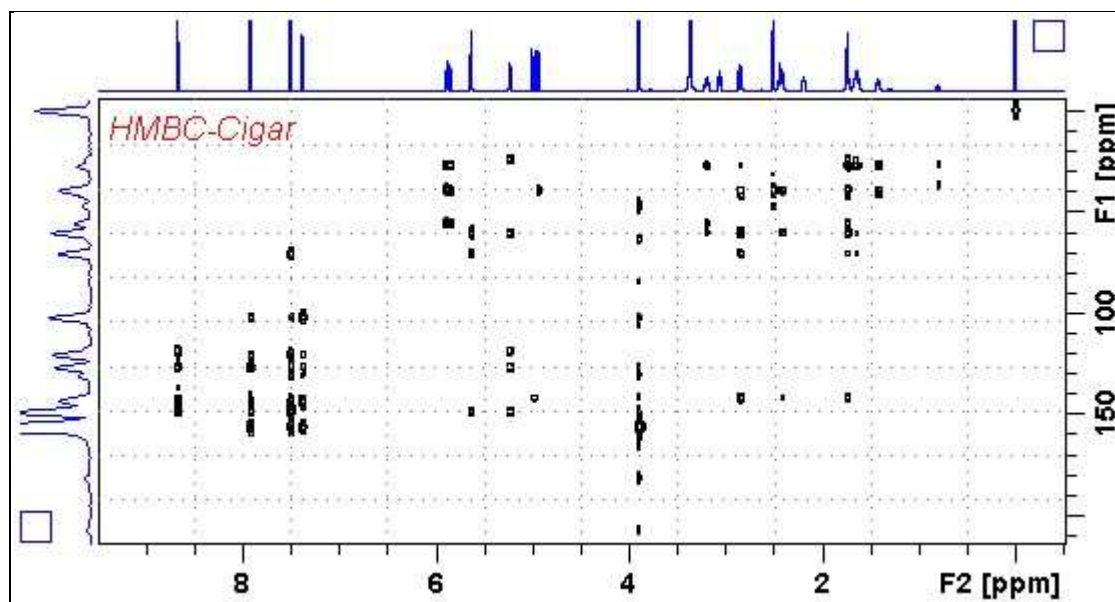
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

xfb, **abs1** and **abs2**



2.15 SHMBC (AVII-600 only)

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

Pulse programme: **shmbcctetgpl2nd**

SW (¹H) = ¹H spectral window = 10 ppm or other value of your choice).

O1P = ¹H spectral window midpoint in ppm.

SW(¹³C) = ¹³C spectral window = 20-30 ppm.

O2P = ¹³C spectral window point.

TD(F2) (¹H) = 1K or 2K, **TD(F1) (¹³C)** = 64-80 or other value of your choice.

SI(F1) (¹H) = 1K or 2K, **SI(F2) (¹³C)** = 128-160.

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST6 = **120 Hz**, **CNST7** = **170 Hz** = min/max ¹J coupling constants.

CNST13 = ⁿJ selection filter = **8 Hz** or other value of your choice (eg: 6-14 Hz).

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

Check gradients are OK.

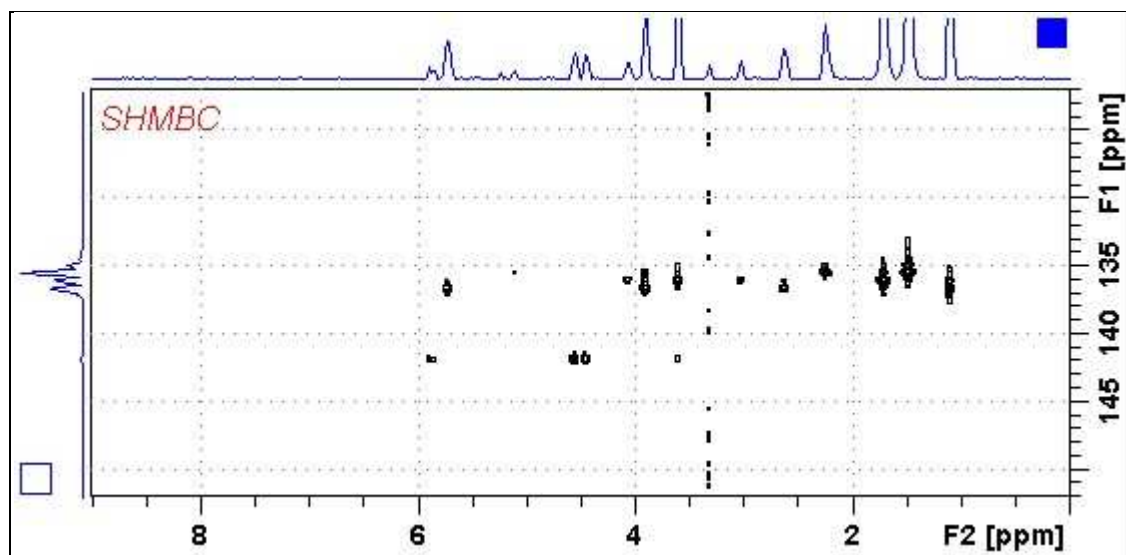
Set **receiver gain** using **RGA** (*Important!*).

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

WDW(F1) = WDW(F2) = QSINE

SSB(F2) = SSB(F1) = 2

xfb, xf2m, abs1 and abs2



AVII-600MHz **SHMBC** spectrum of ivermectim-B1A in D₆-DMSO. The ¹³C axis was centered at 137 ppm.

The ¹³C spectral window can be adjusted via the time and power of the **P43 SP32** shaped pulse as described on the next page

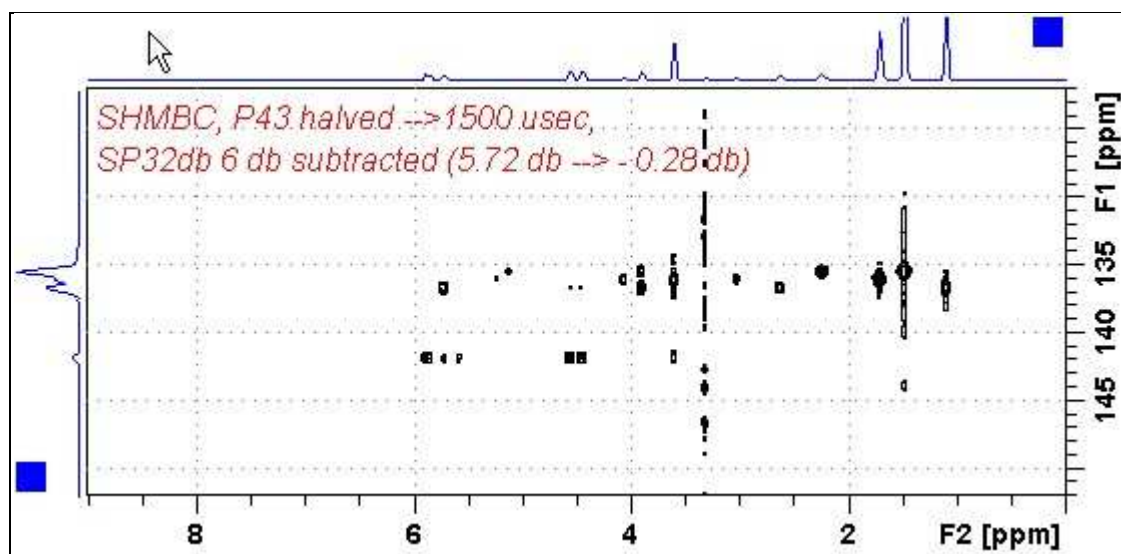
AVII-600 SHMBC Experiment with ^{13}C spectral window adjustment

The ^{13}C spectral window of the **shmbcctetgpl2nd** pulse programme can be increased from ~ 10 ppm (± 5 ppm) to ~ 20 ppm (± 10 ppm) by halving the time and doubling the power (= subtract 6 db from it) of the frequency selective **P43 SP32** shaped pulse.

Eg: **Standard values** for ~ 10 ppm ^{13}C window: **P43 = 3000 usec, SP32 = 5.72 db**

Adjusted values for ~ 20 ppm ^{13}C window: **P43 = 1500 usec, SP32 = -0.28 db**

No change(s) are required to the other shaped pulse times and powers used in the pulse programme.



800 MHz SHMBC spectrum of quinine in D_6 -DMSO with adjustment of the **P43 SP32** shaped pulse time and power. The ^{13}C axis was centered at 137 ppm.

16 H2BC spectrum (+ getprosol)

Parameter set: **awh2bc (+ getprosol)**

Pulse programme: **h2bcetgpl3**

Type **eda** (enter) and enter **SW (¹H)** and **SW (¹³C)** in ppm.

Enter **O1P** = ¹H spectral window midpoint in ppm.

Enter **O2P** = ¹³C spectral window midpoint in ppm.

TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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

D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST6 = 125 Hz, **CNST7** = 165 Hz = min/max ¹J selection filter range.

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

Check gradients are OK.

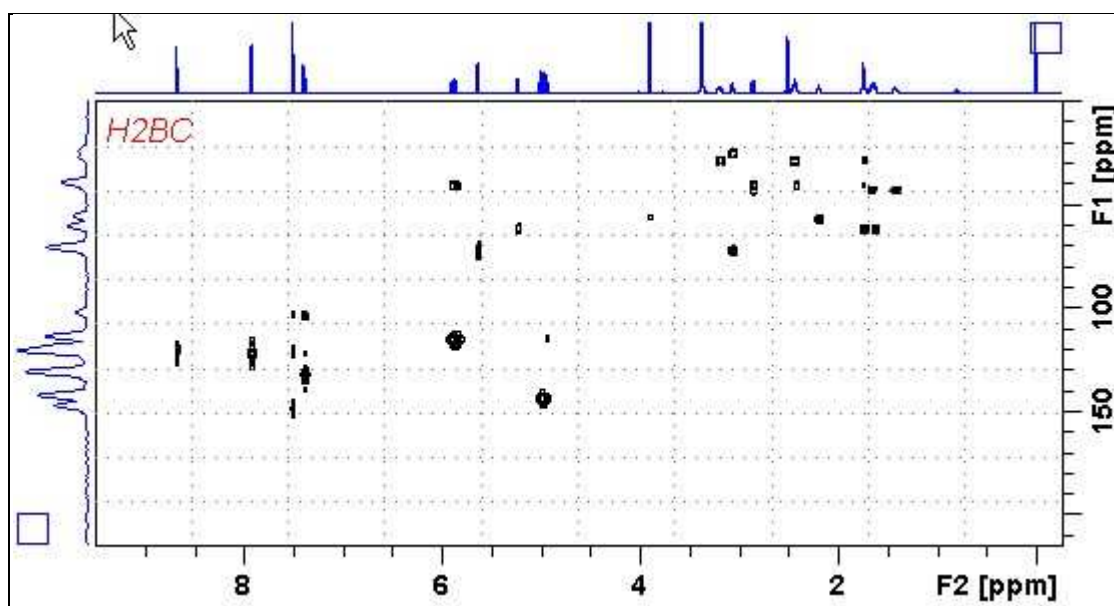
Set **receiver gain** using **RGA** (*Important!*).

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

WDW(F1) = WDW(F2) = SINE

SSB(F2) = SSB(F1) = 0

xfb, xf2m, abs1 and abs2



600 MHz **H2BC** spectrum of quinine in D₆-DMSO.