KJM 9250

AVIIIHD-800 MHz HSQC, HMBC, SHMBC and H2BC Experiments

Version 5.0

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Windows 7

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1.0 Introduction

^{1}H detected aw coded **HSQC, HMB**C \and **H2BC** parameter sets are set up with 1K or 2K acquired ^{1}H points and 128 to 256 increments.

^{1}H and ^{13}C spectral windows and their midpoints should be determined before setting up **HSQC, HMBC** or **H2BC** experiments. The **SHMBC** experiment has a narrow ^{13}C window (10-20 ppm).

1.1 Processing

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

HMBC experiments are absolute value experiments. Phasing is not required.

The **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 ^{1}H detected **HSQC, HMBC, SHMBC and H2BC** experiments and linked prosol compatible parameter sets have been set up on the **AVIIIHD-800** spectrometer.

2.1	**hsqcetgp**	not multiplicity edited, DEPT45 like
2.2	**hsqcedetgp**	multiplicity edited, DEPT135 like
2.3	**hsqcetedgpsisp2.3-135**	multiplicity edited, DEPT135 like
2.4	**hsqcetedgpsisp2.3-135pr**	with CW presaturation
2.5	**hsqcetgpsisp2.2-45**	not multiplicity edited, DEPT45 like
2.6	**hsqc-tocsy**	not multiplicity edited, DEPT45 like
2.7	**hsqc-dipsi2**	DEPT45 and DEPT135-like variants
2.8	**hsqc-noesy**	
2.9	**hsqc-roesy**	CW spin locked variant
2.10	**hsqc-roesy2**	pulsed spin locked variant
2.11	**hmbc**	with ^{n}Jselection
2.12	**hmbcpr**	with CW presaturation and ^{n}J selection
2.13	**hmbclp2**	with $^{1}J_{min/max}$ filter and ^{n}J selection
2.14	**hmbc-cigar**	with ^{13}C decoupling
2.15	**shmbc**	semi-selective hmbc
2.16	**h2bc**	for ^{2}J correlations

2.1 HSQCETGP

Parameter set: **awhsqcetgp (+ getprosol)**
Pulse programme: **hsqcetgp**

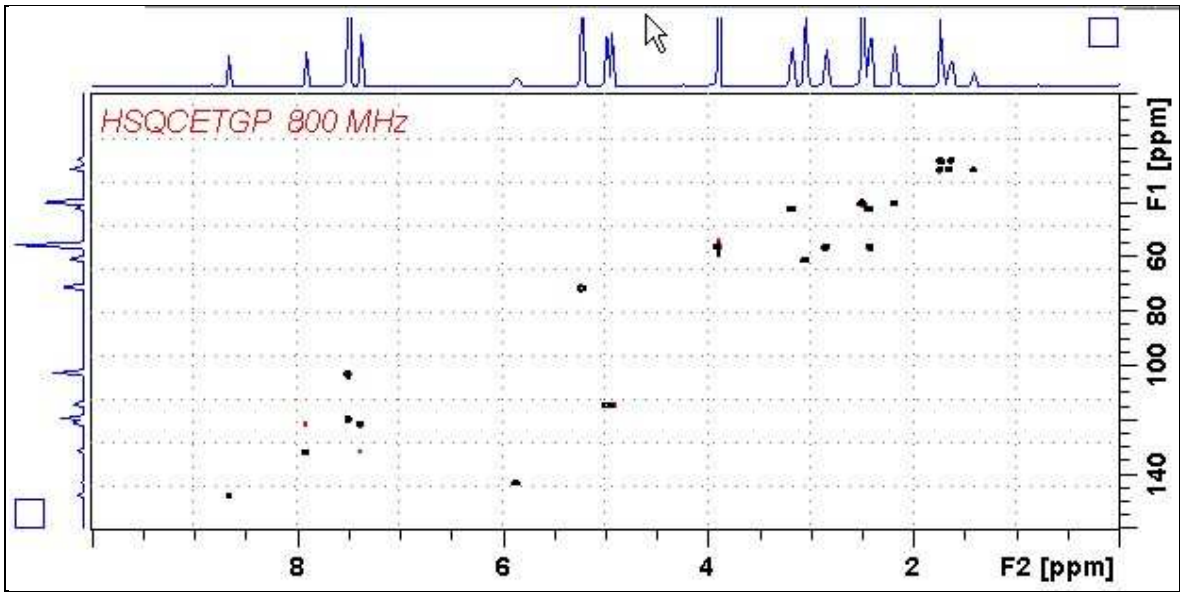
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 = ^{1}J 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



800 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**

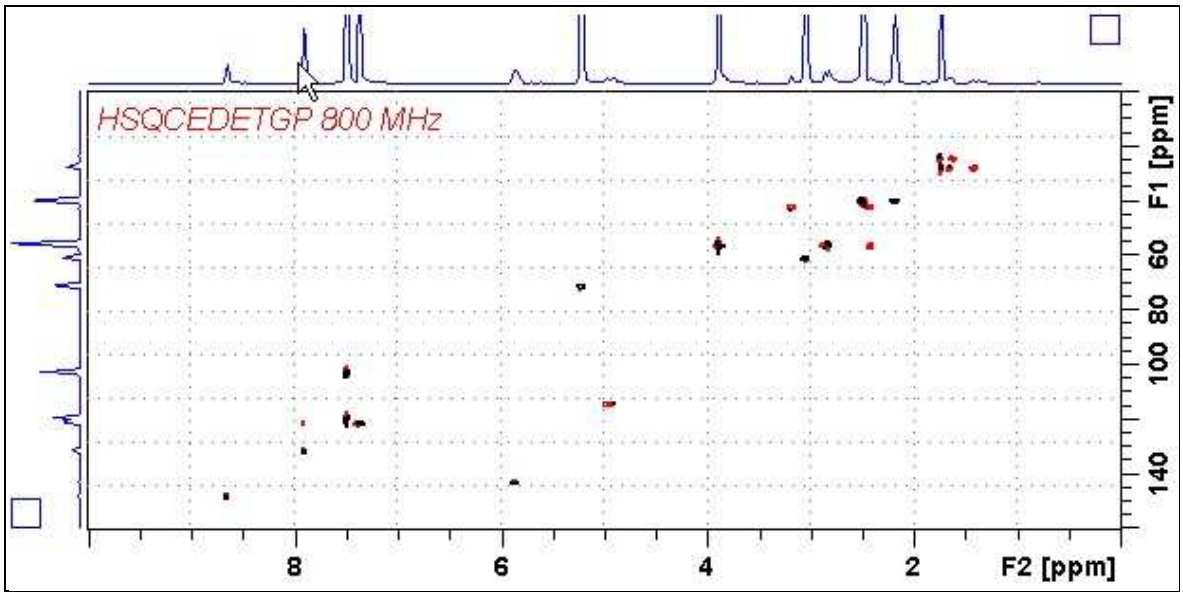
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)**in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 = ^{1}J 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



800 MHz **HSQCEDETGP** spectrum (DEPT135-like) of quinine in D_6-DMSO plotted with CH and CH_3 positive (black) and CH_2 negative (red).

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2.3 HSQCEDETGPSISP2.3-135

Parameter set: **awhsqcedetgpsisp2.3-135 (+ getprosol)**
Pulse programme:**awhsqcedetgpsisp2.3-135**
d21 and **d24** are automatically calculated from **cnst2**

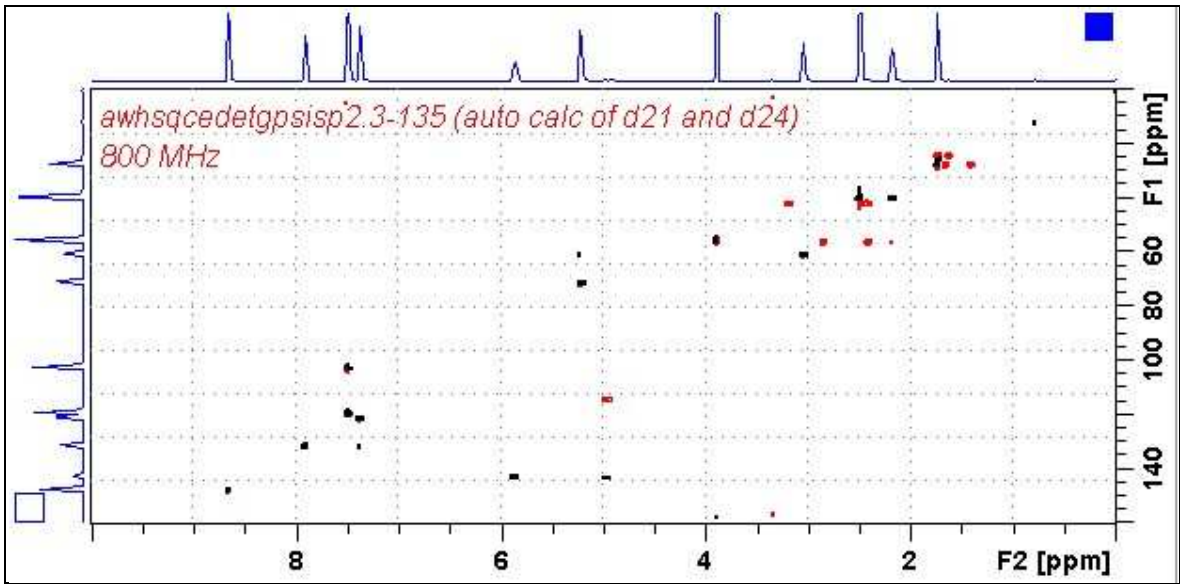
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 = ^{1}J 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



800 MHz **HSQCEDETGPSISP2.3-135** spectrum of quinine in D_6-DMSO plotted with positive CH andCH_3 correlations (black) and negative CH_2 correlations (red).

2.4 HSQCEDETGPSISP2.3-135PR

Parameter set: **awhsqcedetgpsisp2.3-135pr (+ getprosol)**
Pulse programme: **awhsqcedetgpsisp2.3-135pr**
d21 and **d24** are automatically calculated from **cnst2**

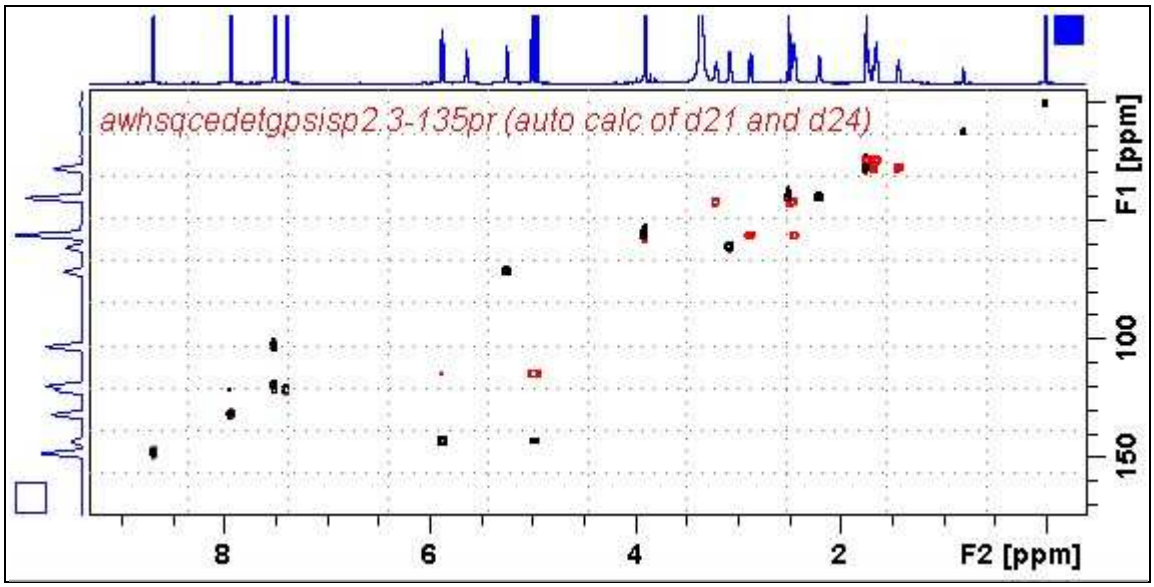
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 = ^{1}J 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



800 MHz **HSQCEDETGPSISP2.3-135PR** spectrum of quinine in D_6-DMSO with CW presaturation of the HOD line at 3.37 ppm. The spectrum is plotted with positive CH and CH_3 correlations (black) and negative CH_2 correlations (red).

2.5 HSQCEDETGPSISP2.2-45

Parameter set: **awhsqcetgpsisp2.2-45 (+ getprosol)**
Pulse programme: **awhsqcetgpsisp2.2-45**
d24 is automatically calculated from **cnst2**

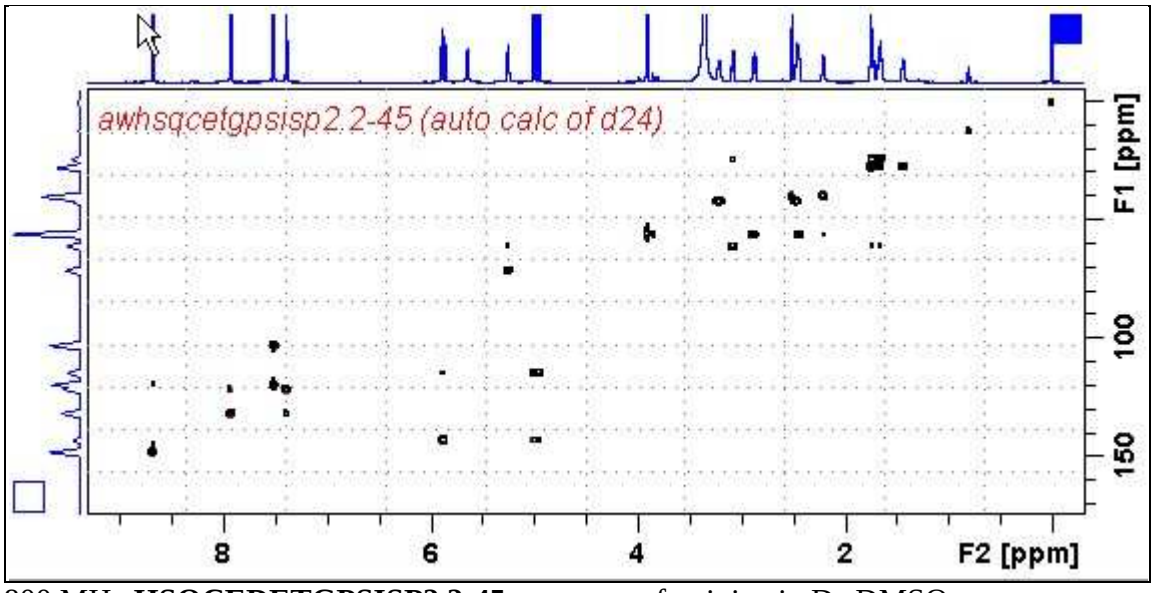
Type **eda** (enter) and enter **SW (^{1}H)** and **SW(^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 = ^{1}J 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



800 MHz **HSQCEDETGPSISP2.2-45** spectrum of quinine in D_6-DMSO.

2.6 HSQC-TOCSY

Parameter set: **awhsqc-tocsy (+ getprosol)**
Pulse programme: **hsqcetgpml**

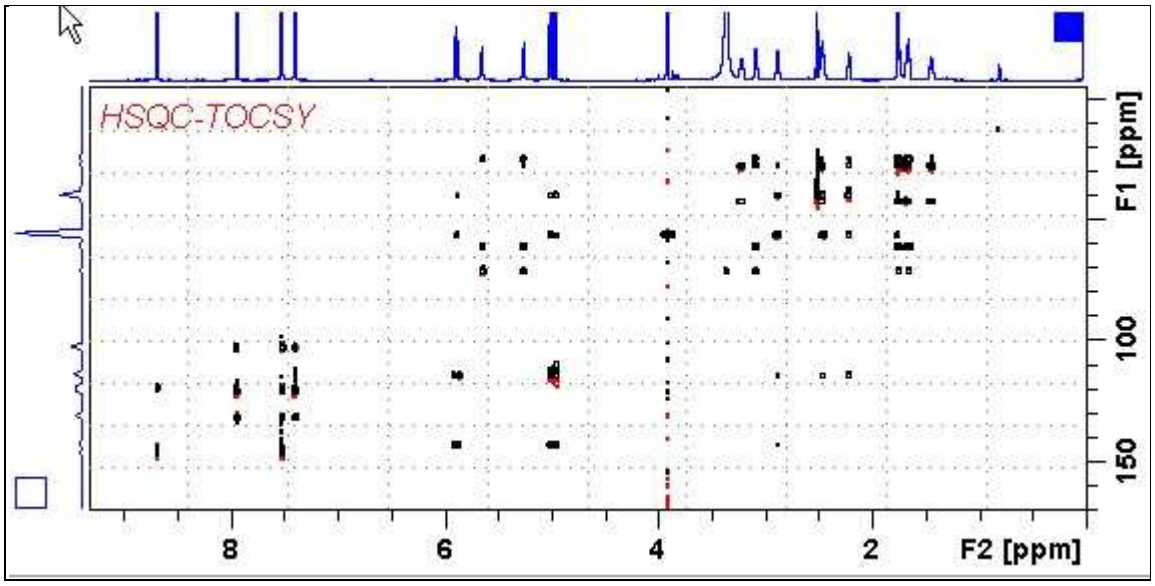
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 = ^{1}J 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



800 MHz **HSQC-TOCSY** spectrum of quinine in D_6-DMSO. HSQC and correlated TOCSY peaks are positively phased.

2.7.1 HSQC-DIPSI2.45

Parameter set: **awhsqc-dipsi2.45 (+ getprosol)**
Pulse programme: **awhsqcdietgpsisp.2-45**
With auto calculation of **d24** from **cnst2**

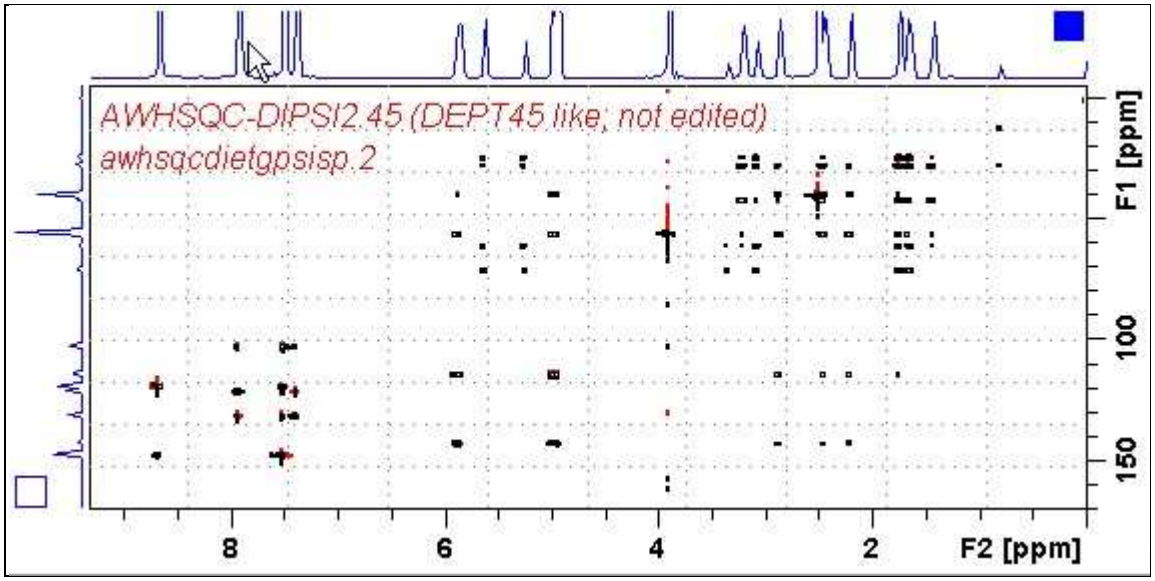
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)**in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 = ^{1}J 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



800 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**: awhsqcdiedetgpsisp.2-135**
With auto calculation of **d24** from **cnst2**

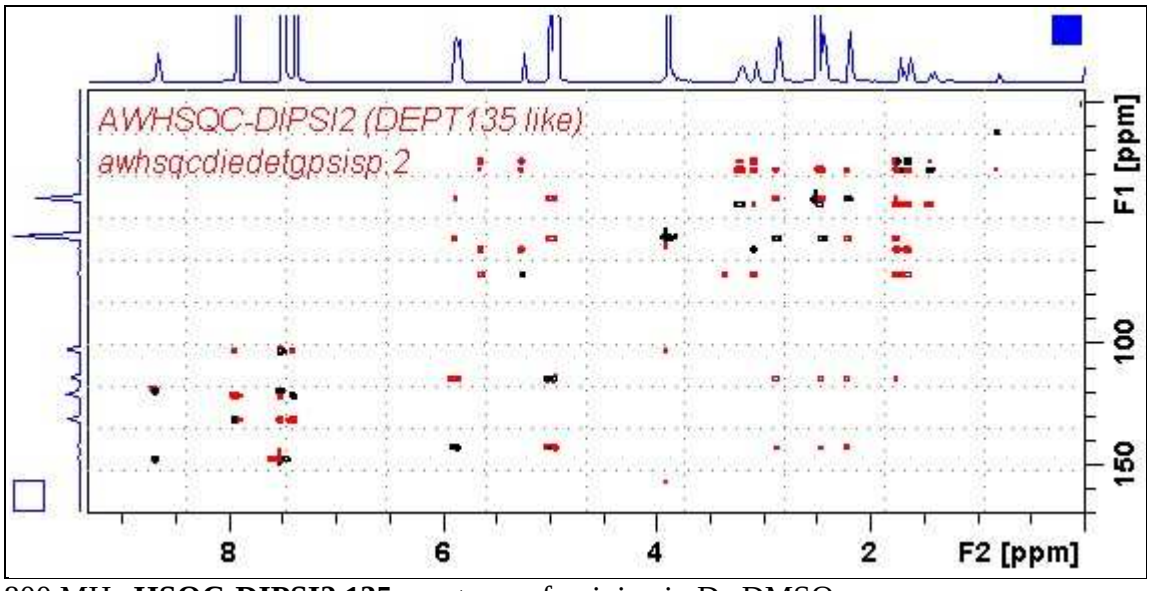
Type **eda** (enter) and enter **SW (**^{1}**H)** and **SW (**^{13}**C i**n ppm.
Enter **O1P =** ^{1}**H** spectral window midpoint in ppm.
Enter **O2P =** ^{13}**C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 = ^{1}J 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



800 MHz **HSQC-DIPSI2.135** spectrum of quinine in D_6-DMSO.

2.8HSQC-NOESY

Parameter set: **awhsqc-noesy (+ getprosol)**
Pulse programme: **hsqcetgpnosp**

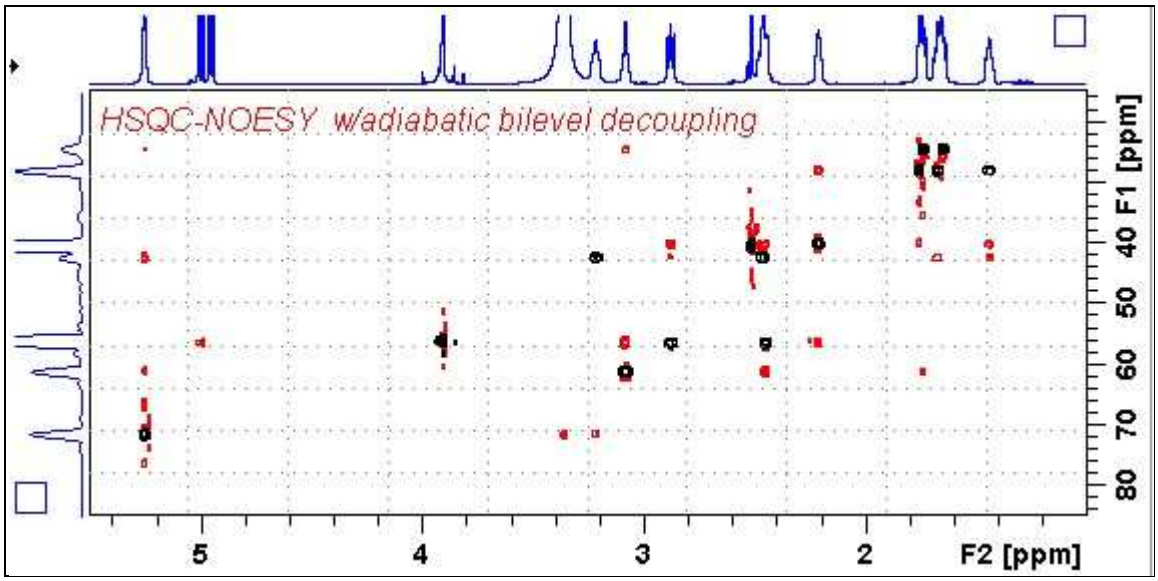
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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.
D8 = NOESY correlation time = **0.5 sec** or other value of your choice (0.3-0.8 sec),
CNST2 = ^{1}J 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



800 MHz **HSQC-NOESY** spectrum (expansion of the 1.0-5.5 ppm/10-85 ppm region) of quinine in D_6-DMSO. Positively phased HSQC signals (black) are scaled down by a factor of 10 using the **edlev** command relative to less intense negatively phased NOESY correlations (red).

2.9 HSQC-ROESY

Parameter set: **awhsqc-roesy (+ getprosol)**
Pulse programme: **hsqcetgprosp**

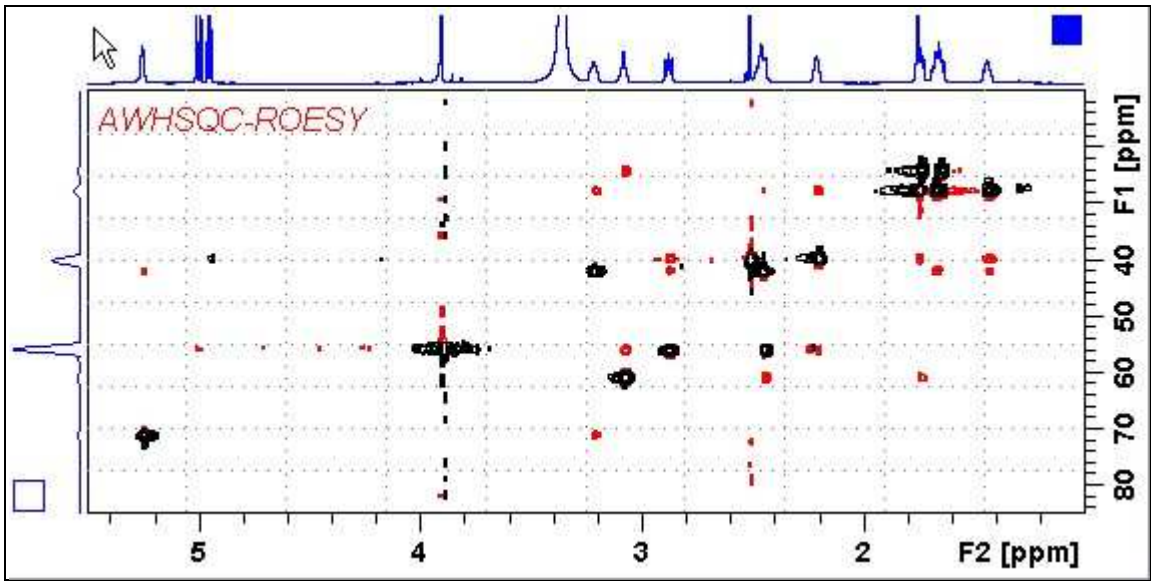
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 = ^{1}J 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



800 MHz **HSQC-ROESY** spectrum (expansion of the 1.0-5.5 ppm/10-85 ppm region) of quinine in D6-DMSO. HSQC signals (black are positively phased. Correlated ROESY signals (red) are negatively 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**

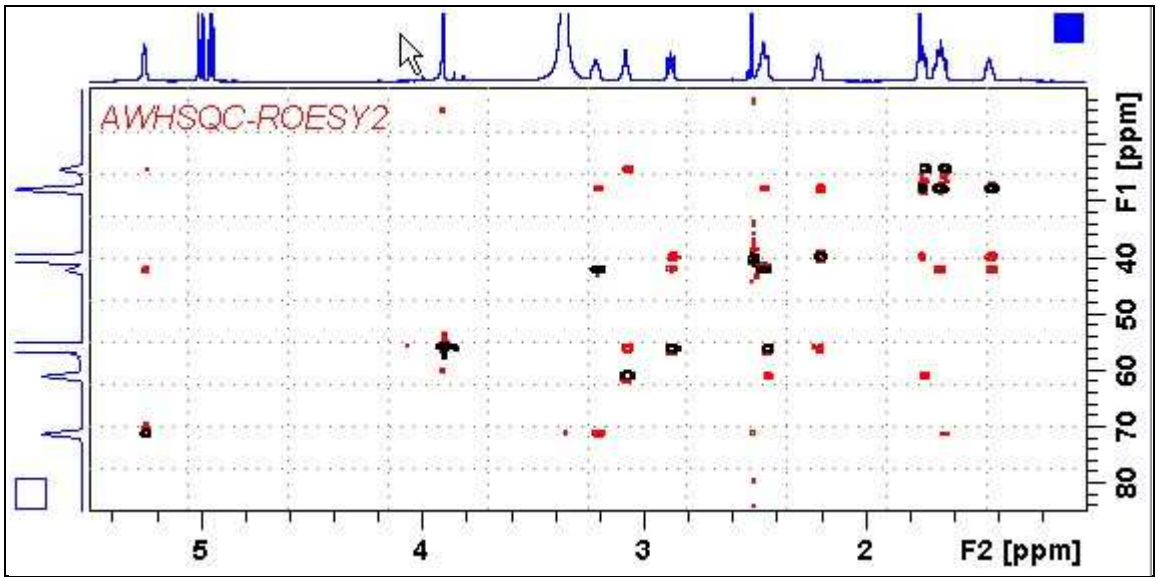
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 = ^{1}J 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



800 MHz **HSQC-ROESY2** spectrum (expansion of the 1.0-5.5 ppm/10-85 ppm region) of quinine in D_6-DMSO. HSQC signals (black) are positively phased. Correlated ROESY signals (red) are negatively phased. HSQC signal levels were reduced by a factor of 10 relative to ROESY signal levels using the **edlev** command.

2.11HMBC

Parameter set: **awhmbcgplpndqf (+ getprosol)**
Pulse programme: **hmbcgplpndqf**

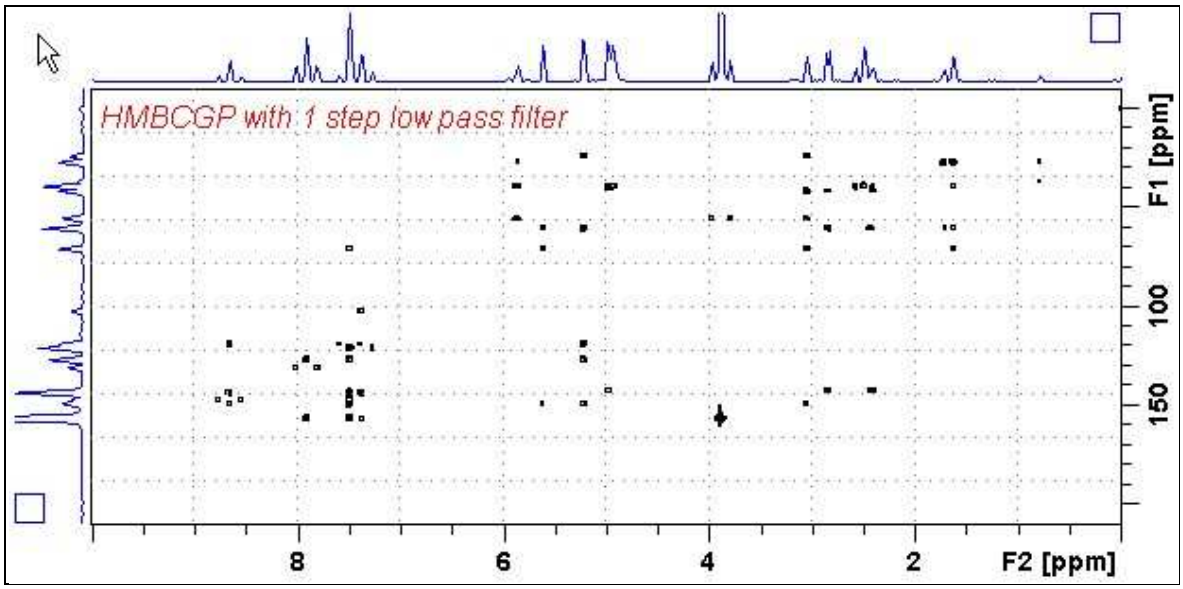
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K,**TD(F1)** = 128-256 (your choice).

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 = ^{1}J coupling constant = **145 Hz** or other value of your choice.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice.

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) = SINE
SSB(F2) = SSB(F1) = 0
xfb, abs1 and abs2



800 MHz **HMBC** spectrum of quinine in D_6-DMSO.

2.12 HMBCPR

Parameter set: **awhmbcpr (+ getprosol)**
Pulse programme: **awhmbcgplpndqfpr**

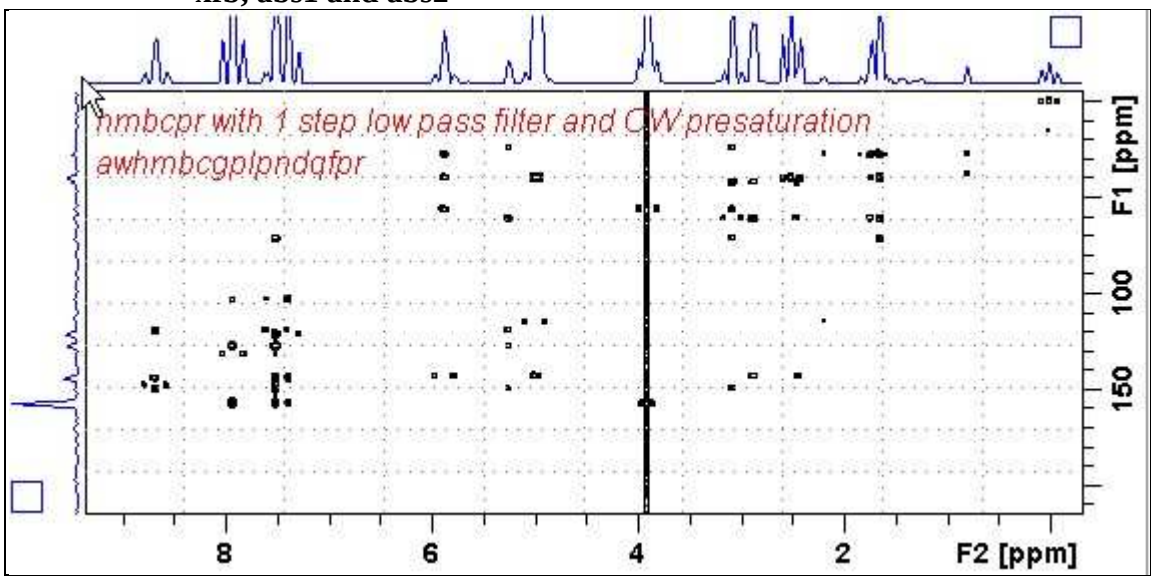
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K,**TD(F1)** = 128-256 (your choice).

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 = ^{1}J coupling constant = **145 Hz** or other value of your choice.
CNST13= ^{n}J selection filter = **8 Hz** or other value of your choice.

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) = SINE
SSB(F2) = SSB(F1) = 0
xfb, abs1 and abs2



800 MHz **HMBC** spectrum of quinine in D_6-DMSO with CW presaturation of the HOD signal at 3.37 ppm,

2.13 HMBCL2

Parameter set: **awhmbcgpl2ndqf (+ getprosol)**
Pulse programme: **hmbcgpl2ndqf**

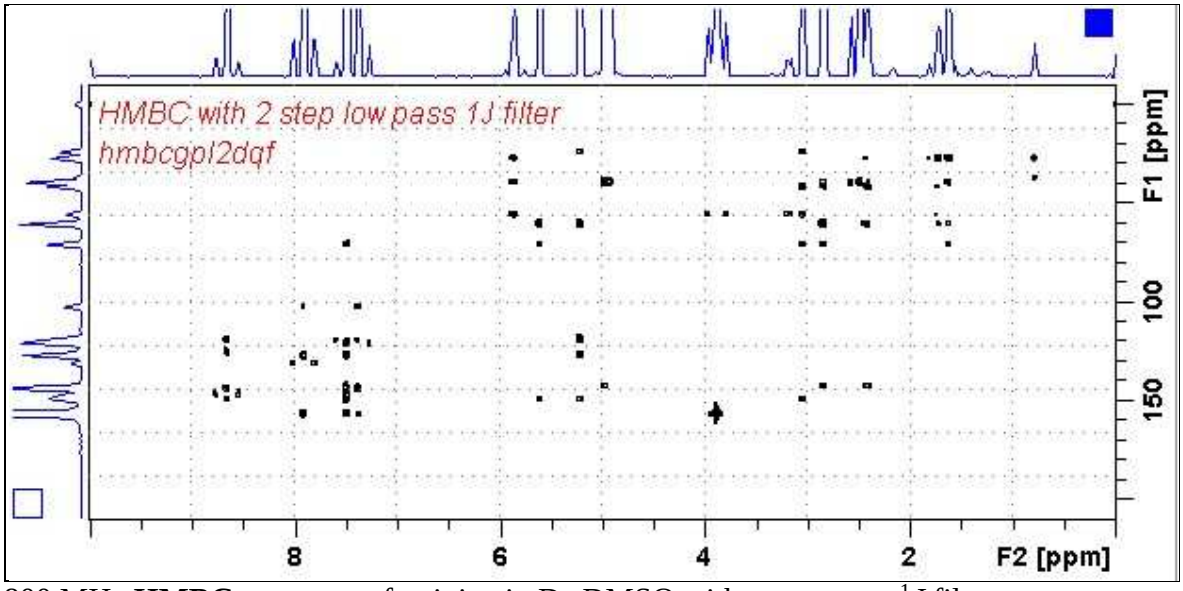
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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.^{1}J coupling constant = **125** Hz or other value of your choice.
CNST7 = max.^{1}J coupling constant = **165** Hz or other value of your choice.
CNST13 = ^{n}J selection filter = **8 Hz** or other value of your choice

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) = SINE
SSB(F2) = SSB(F1) = 0
xfb, abs1 and abs2



800 MHz **HMBC** spectrum of quinine in D_6-DMSO with a two stage ^{1}J filter.

2.14 HMBC-CIGAR

Parameter set: **awhmbc-cigar (+ getprosol)**
Pulse programme: **hmbcacgplpqf**
Spectrum is acquired with ^{13}C decoupling

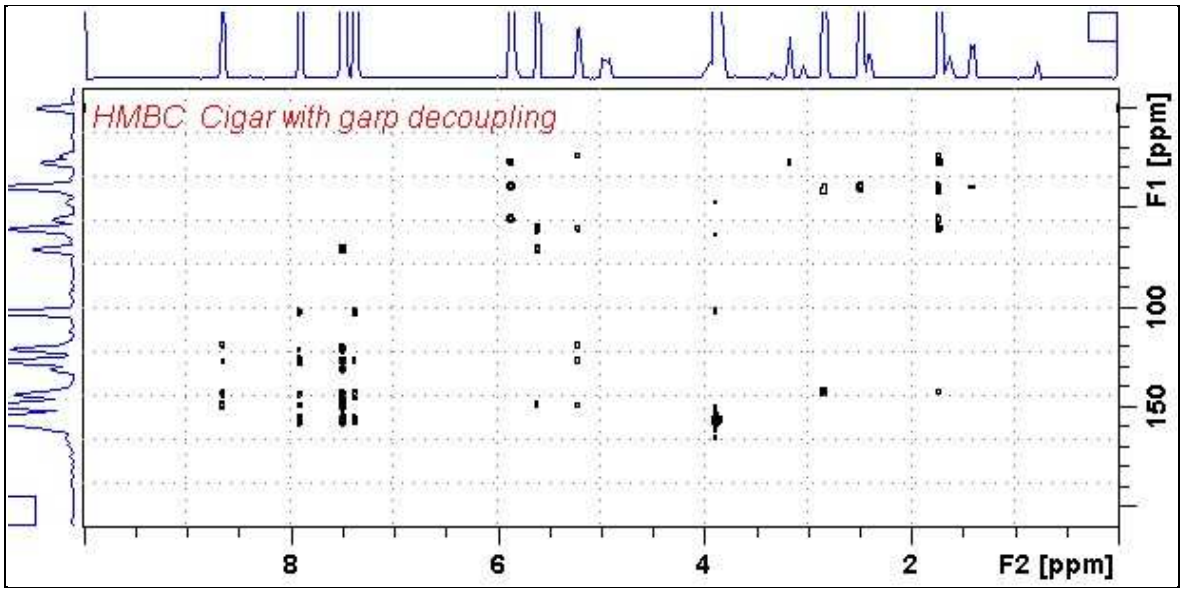
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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 ^{1}J selection filter range.
CNST14 = 4 Hz**, CNST15** =12 Hz = min/max ^{n}J selection filter range.
CNST16 = 1.0 = *J* scale factor.

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) = SINE
SSB(F2) = SSB(F1) = 0
xfb, abs1 and abs2



800 MHz **HMBC-CIGAR** spectrum of quinine in D_6-DMSO.

2.15 SHMBC

Parameter set: **awshmbc (+ getprosol)**
Pulse programme: **shmbcctetgpl2nd**

SW (^{1}H) = ^{1}H spectral window = 10 ppm or other value of your choice).
O1P = ^{1}H spectral window midpoint in ppm.

SW(^{13}C) = ^{13}C spectral window = 20-30 ppm.
O2P = **^{13}C** spectral widow point.

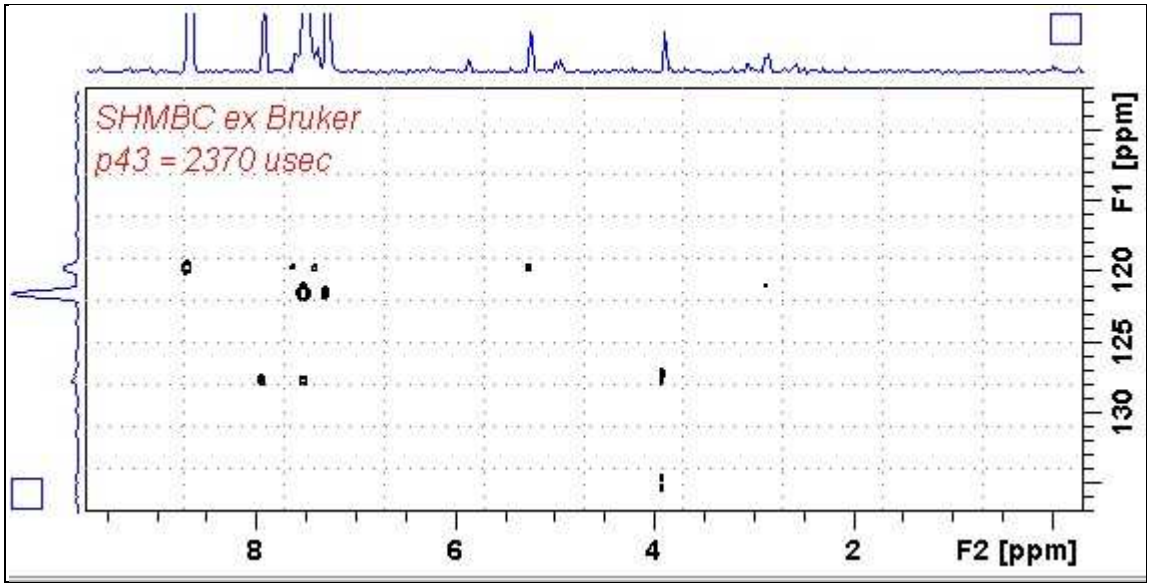
TD(F2) (^{1}H) = 1K or 2K, **TD(F1) (**^{13}C) = 64-80 or other value of your choice.
SI(F1) (^{1}H) = 1K or 2K, **SI(F2)** (^{13}C) = 128-160.

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 ^{1}J coupling constants.
CNST13 = ^{n}J 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 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, xf2m, abs1 and abs2



800 MHz **SHMBC** spectrum of quinine in D_6-DMSO. The ^{13}C axis was centered at 122 ppm.

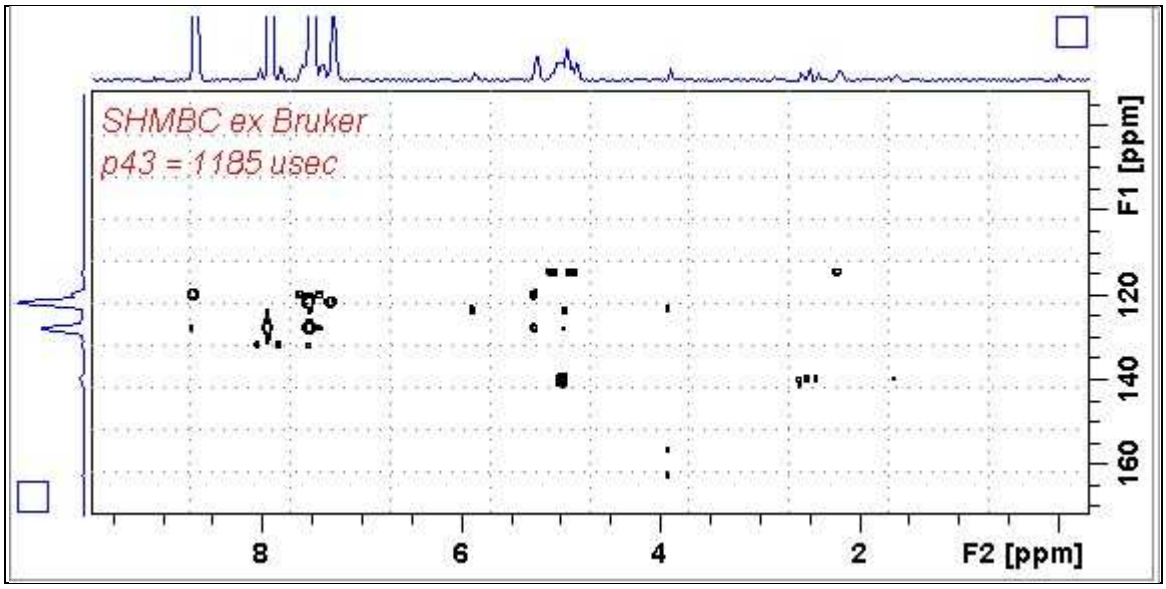
The ^{13}C spectral window can be adjusted via the time and power of the **P43 SP32** shaped pulse as described on the next page.\

SHMBC Experiment ^{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 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 = 2370 usec, SP32 = 0.04 db**
Adjusted values for ~ 20 ppm ^{13}C window: **P43 = 1185 usec, SP32 = -5.96 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 122 ppm.

2.16 H2BC spectrum (+ getprosol)

Parameter set: **awh2bc (+ getprosol)**
Pulse programme: **h2bcetgpl3**

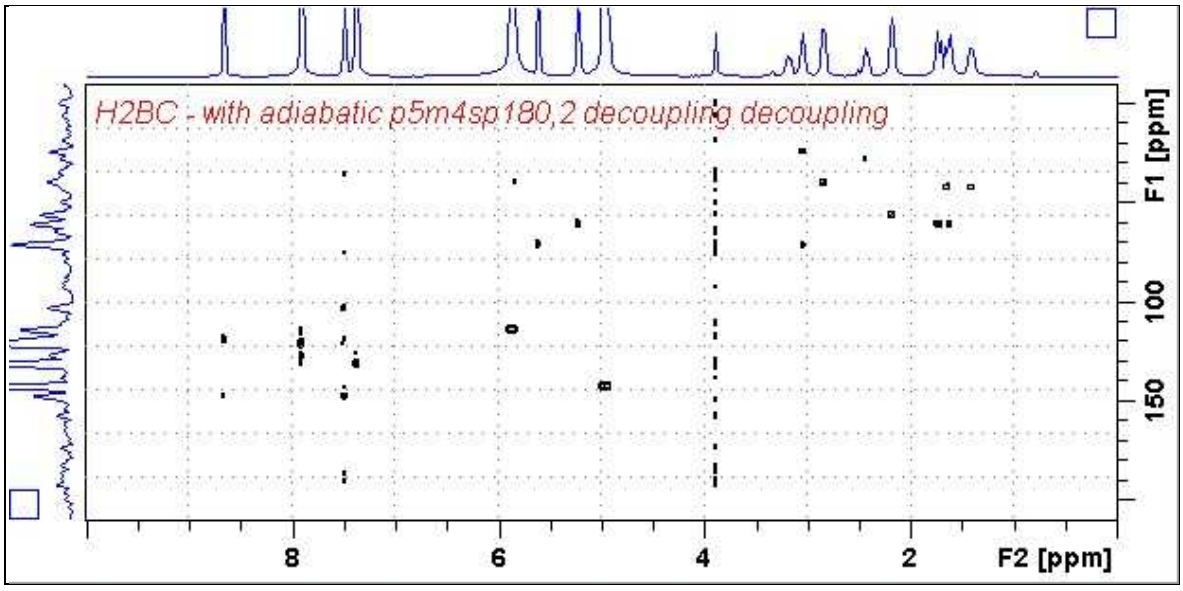
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{1}H** spectral window midpoint in ppm.
Enter **O2P = ^{13}C** spectral window midpoint in ppm.
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).

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** =165 Hz = min/max ^{1}J selection filter range.

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, xf2m, abs1 and abs2



800 MHz **H2BC** spectrum of quinine in D_6-DMSO.