



KJM 9250

XHDEPT, HETCOR and COLOC Experiments on the
AVI 600 and AVII 600 Spectrometers

Version 5.0

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



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XHDEPT, HETCOR and COLOC Experiments on the AVI-600 and AVII-600 Spectrometers

1.0 Introduction

¹³C detected aw coded **XHDEPT, HETCOR and COLOC** parameter sets are set up with 2K acquired ¹³C points and 128 to 256 ¹H increments. ¹H and ¹³C spectral windows and their midpoints should be determined before setting up these experiments.

1.1 Processing

HXDEPT45, HXDEPT90 and HXDEPT135 experiments are phase sensitive experiments. These spectra should be phased **before** using the **abs1** and **abs2** commands.

The **HXDEPTQF, HETCOR and COLOC** experiments are absolute value experiments. Phasing is not required.

2.0 Experiments and Parameter Sets

The following ¹H detected **HXDEPT, HETCOR and COLOC** experiments and parameter sets have been set up on the AVI and AVII 600 MHz spectrometers.

- 2.1 HXDEPT45, HXDEPT90 and HXDEPT135** spectra
- 2.2 HXDEPTQF** spectrum
- 2.3 HETCOR (= HXCOQF)** spectrum
- 2.4 HETCORLR** spectrum
- 2.5 COLOCQF** spectrum
- 2.6 COLOCLR** spectrum with auto calculation of d6 and d18 from J_{LR}

2.1 HXDEPT45, HXDEPT90 and HXDEPT135 spectra

Parameter sets (both 600's): **awhxdept45**, **awhxdept90** or **awhxdept135** (+ **getprosol**)

AVI-600 pulse programmes: **awhxdept45**, **awhxdept90** or **awhxdept135**

AVII-600 pulse programme: **hxdeptph**

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

Enter **O1P** = ^{13}C spectral window midpoint in ppm.

Enter **O2P** = ^1H spectral window midpoint in ppm.

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

NS = 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).

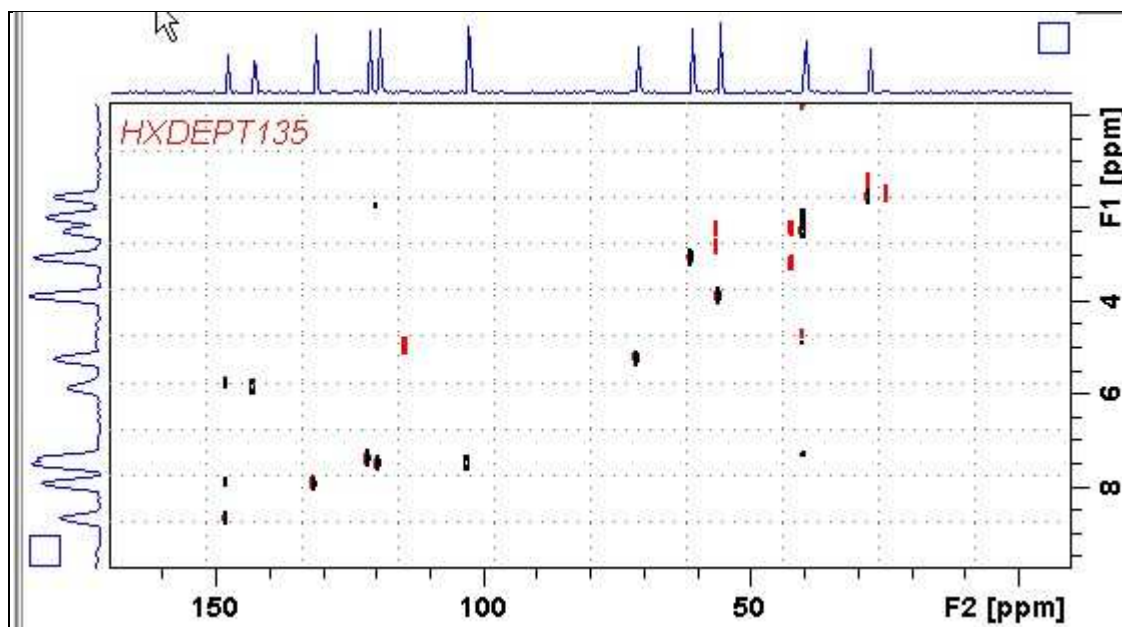
AVI-600/TS2.1: **p0** = **p3*** **0.5**, **1.0** or **1.5** for **45°**, **90°** or **135°** pulses.

AVII-600/TS3.2 **P0** = **45°**, **90°** or **135°** pulses.

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** and **abs2**



600 MHz **HXDEPT135** spectrum of quinine in D_6 -DMSO.

Some low level artifact peaks (of unknown origin) may be observed in HXDEPT experiments.

2.2 HXDEPTQF

Parameter set (both 600's): **awhxdeptqf(+ getprosol)**
pulse programmes (both 600's): **hxdeptqf**

Type **eda** (enter) and enter **SW (¹H)** and **SW (¹³C)** in ppm.
Enter **O1P** = ¹³C spectral window midpoint in ppm.
Enter **O2P** = ¹H spectral window midpoint in ppm.

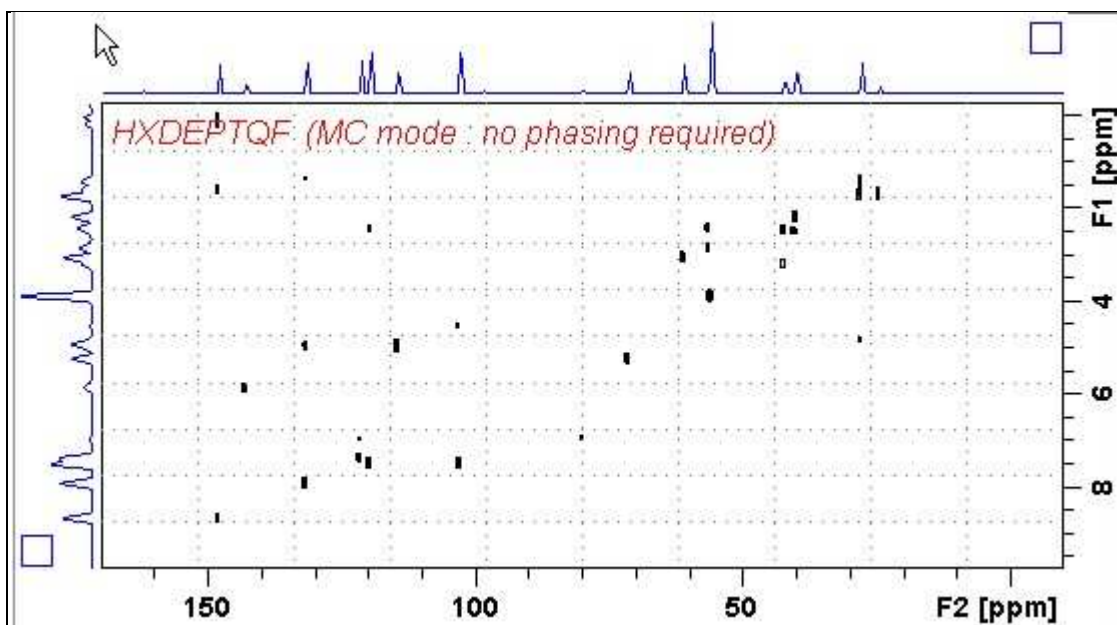
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 8, 16 (multiple of 4 or 8 recommended), **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.
CNST2 = ¹J coupling constant = **145 Hz** or other value of your choice (eg 125-160 Hz).

AVI-600/TS2.1: **p0** defined as **p3*0.5** for a DEPT45 like outcome.
AVII-600/TS3.2: **p0** = 45 degree pulse for a DEPT45-like outcome.
As defined in the AVI and AVII version of the parameter set

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



HXDEPTQF spectrum of quinine in D₆-DMSO.

Some low level artifact peaks (of unknown origin) may be observed in HXDEPT experiments.

2.3 HETCOR spectrum

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

Pulse programme: **hxcoqf**

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

Enter **O1P** = ¹³C spectral window midpoint in ppm.

Enter **O2P** = ¹H spectral window midpoint in ppm.

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

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

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

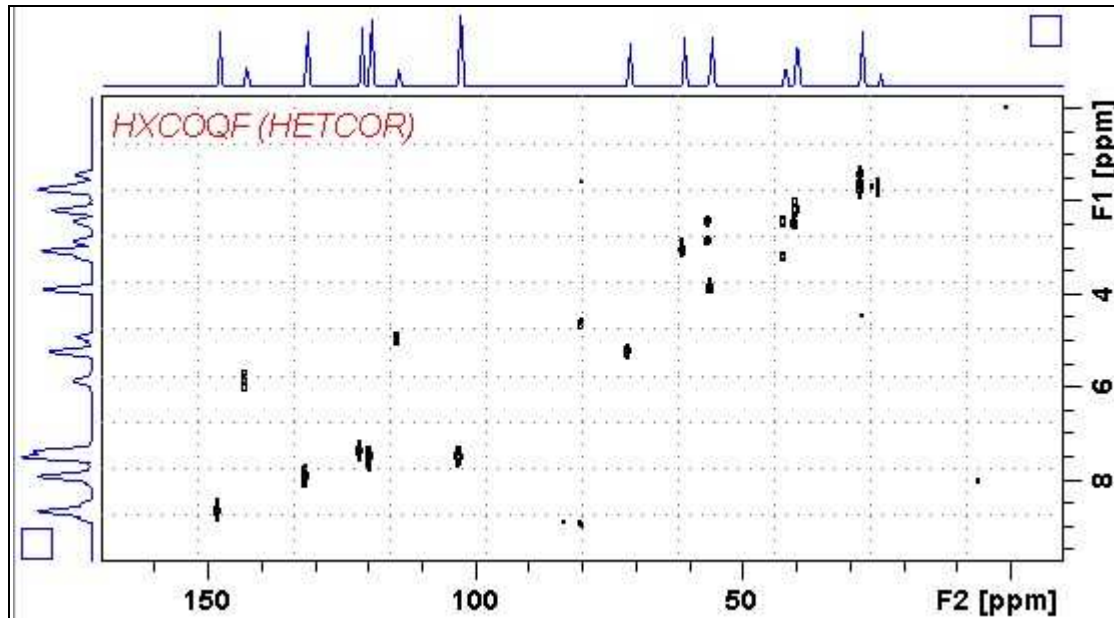
CNST2 = ¹J coupling constant = **145 Hz** or other value of your choice (eg: 125-160Hz).

CNST11 = **3** (used to auto calculate **D3**).

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



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

2.4 HETCORLR spectrum

Parameter sets: **awhetcorlr** (+ **getprosol**)

Pulse programme: **hxcoqf**

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

Enter **O1P** = ¹³C spectral window midpoint in ppm.

Enter **O2P** = ¹H spectral window midpoint in ppm.

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

NS = 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 = ⁿJ coupling constant = **10 Hz** or other value of your choice (eg: 6-14 Hz).

CNST11 = **3** (used to auto calculate **D3**).

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

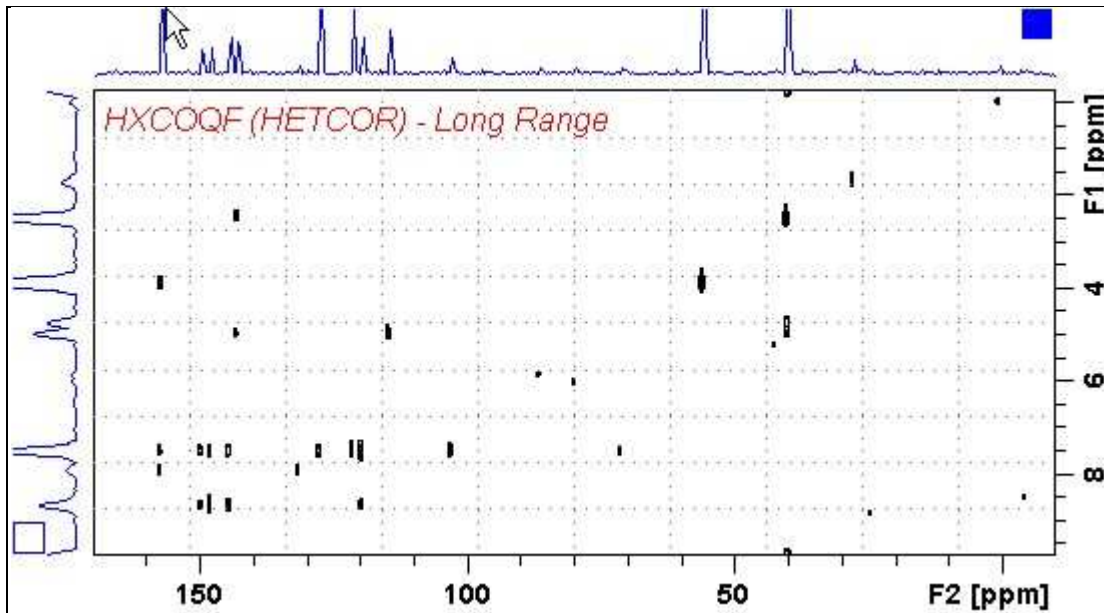
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

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



600 MHz **HETCORLR** spectrum of quinine in D₆-DMSO optimized for ⁿJ = 10 Hz (**D2** = 50 msec, **D3** = 33 msec).

2.5 COLOC spectrum

Parameter sets: **awcoloc** (+ **getprosol**)

Pulse programme: **colocqf**

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

Enter **O1P** = ¹³C spectral window midpoint in ppm.

Enter **O2P** = ¹H spectral window midpoint in ppm.

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

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

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

D6 = 50 msec or other delay for ⁿJ evolution [D6= 1000/(2* ⁿJ) msec].

D18 = 30 msec or other delay for ⁿJ evolution [D18= 1000/(3* ⁿJ) msec].

Parameter set **D6** and **D18** delay values are those for ⁿJ = ~10 Hz.

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

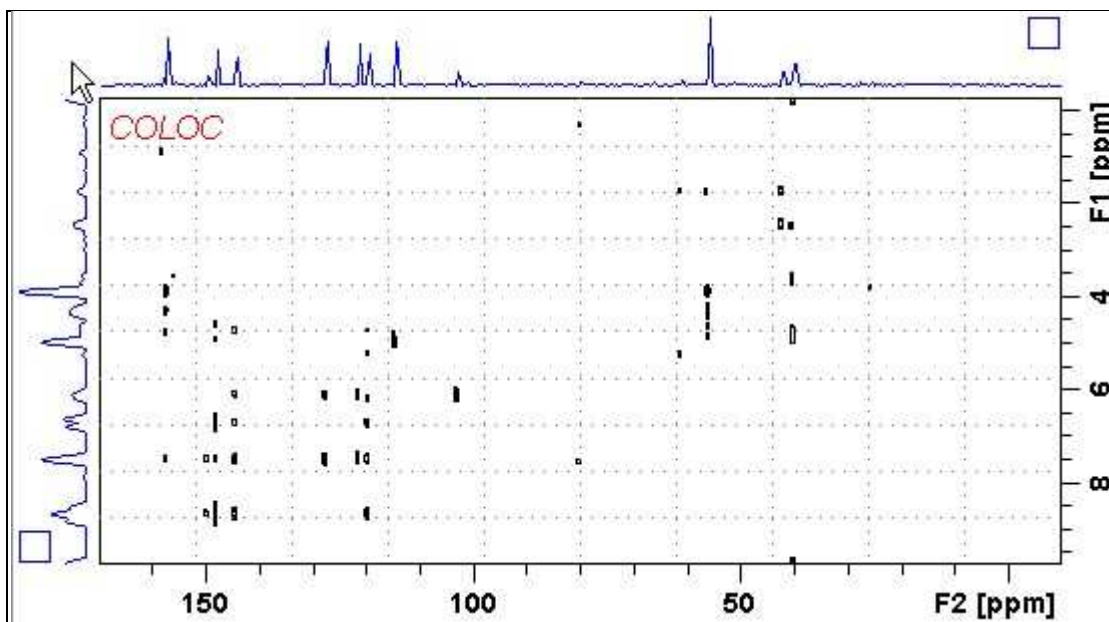
Set **receiver gain** using **RGA** (*Important!*).

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

WDW(F1) = WDW(F2) = SINE

SSB(F2) = SSB(F1) = 0

xfb, abs1 and abs2



600 MHz COLOC spectrum of quinine in D₆-DMSO optimized for ⁿJ = ~10 Hz (**D6** = 50 msec, **D18** = 30 msec).

2.6 COLOCLR spectrum

Note: Currently this experiment may not be set up on the AVI-600

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

Pulse programme: **awcolocqf**

d6 and **d18** are auto calculated from J_{LR} entered as **cnst21**

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

Enter **O1P** = ¹³C spectral window midpoint in ppm.

Enter **O2P** = ¹H spectral window midpoint in ppm.

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

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

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

CNST21 = J_{LR} = **10 Hz** or other value of your choice.

D6 = $1000/(2 * ^nJ)$ msec and **D18** = $1000/(3 * ^nJ)$ msec are auto calculated from **CNST21** (Hz).

D6 = 50 msec, **D18** = 33 msec for **CNST21** = 10 Hz.

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

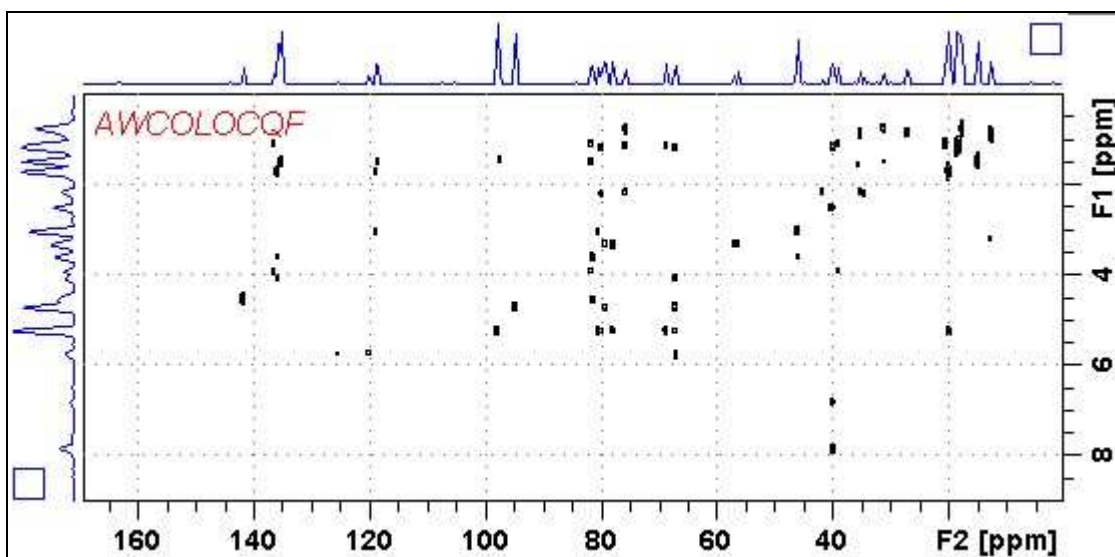
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

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



AVII-600 COLOCLR spectrum of ivermectin-B1A in D₆-DMSO with CNST21 = 10 Hz.