



KJM 9250

**XHDEPT, HETCOR and COLOC experiments on the AVI-600  
Spectrometer**

Version 7.3

Topspin 1.3 Windows XP AVI600



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## **XHDEPT, HETCOR and COLOC Experiments on the AVI-600**

### **1.0 Introduction**

<sup>13</sup>C detected aw coded **XHDEPT, HETCOR and COLOC** parameter sets are set up with 2K acquired <sup>13</sup>C points and 128 to 256 <sup>1</sup>H increments. <sup>1</sup>H and <sup>13</sup>C 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 <sup>1</sup>H detected **HXDEPT, HETCOR and COLOC** experiments and parameter sets have been set up on the AVI- 600 spectrometer.

- 2.1 HXDEPT45, HXDEPT90 and HXDEPT135** spectra
- 2.2 HXDEPTQF** spectrum
- 2.3 HETCOR (= HXCOQF)** spectrum
- 2.4 COLOC** spectrum

## 2.1 HXDEPT45, HXDEPT90 and HXDEPT135 spectra

Parameter sets: **awhxdept45**, **awhxdept90** or **awhxdept135** (+ **getprosol**)  
pulse programmes: **awhxdept45**, **awhxdept90** or **awhxdept135**

Type **eda** (enter) and enter **SW (<sup>1</sup>H)** and **SW (<sup>13</sup>C)** in ppm.

Enter **O1P** = <sup>13</sup>C spectral window midpoint in ppm.

Enter **O2P** = <sup>1</sup>H 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.

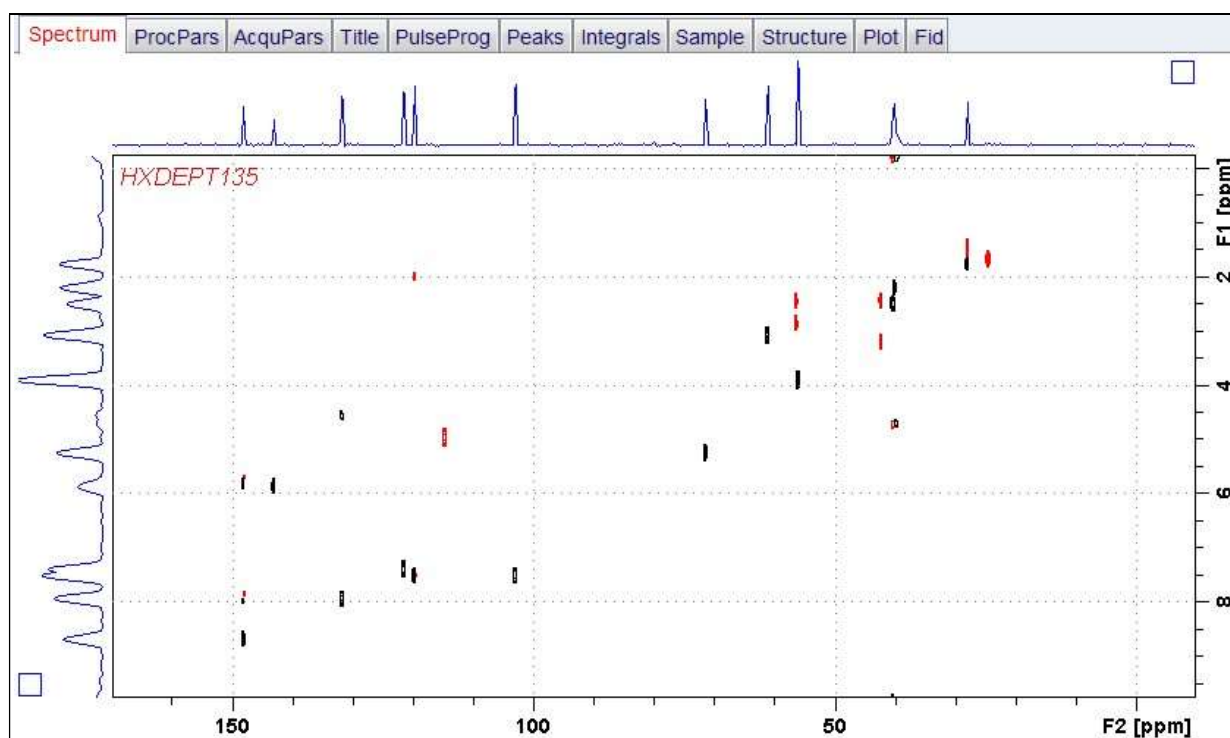
**D1** = repetition delay = **1.5 sec** or other time of your choice.

**CNST2** = <sup>1</sup>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.

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**



AVI-600 HXDEPT135 spectrum of quinine in D<sub>6</sub>-DMSO.

## 2.2 HXDEPTQF

Parameter set: **awhxdeptqf (+ getprosol)**  
pulse programme: **hxdeptqf**

Type **eda** (enter) and enter **SW (<sup>1</sup>H)** and **SW (<sup>13</sup>C)** in ppm.

Enter **O1P** = <sup>13</sup>C spectral window midpoint in ppm.

Enter **O2P** = <sup>1</sup>H 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.

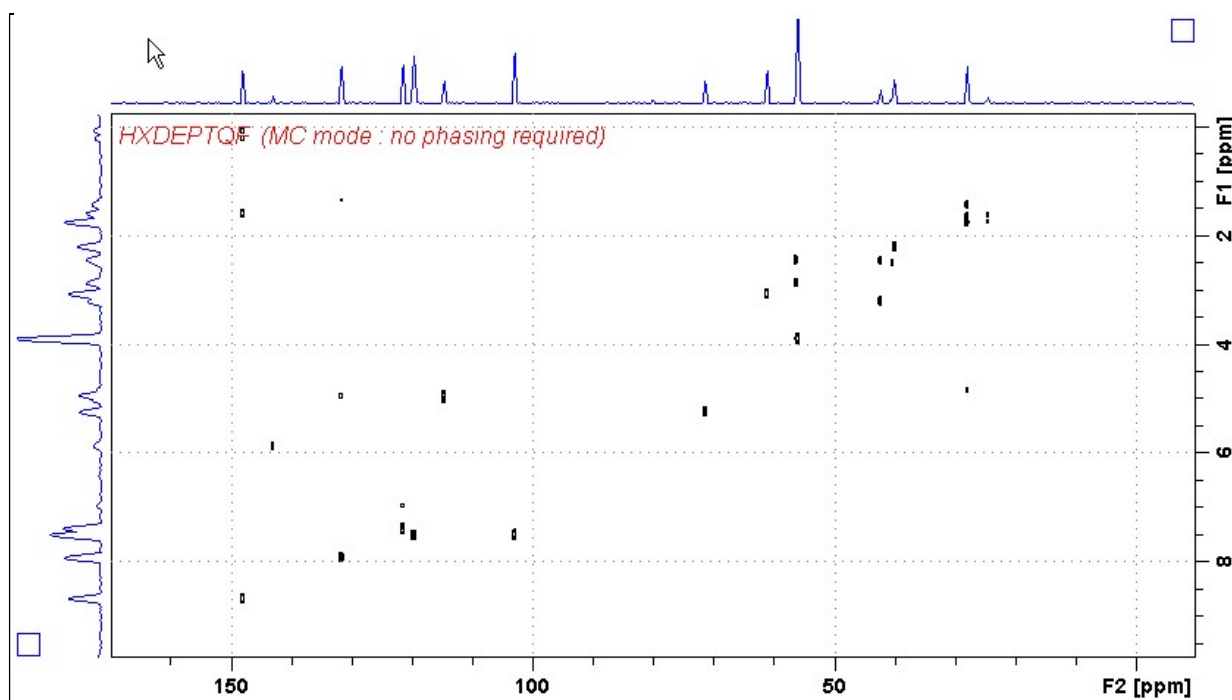
**CNST2** = <sup>1</sup>J coupling constant = **145 Hz** or other value of your choice (eg 125-160 Hz).

With a **p3\*0.5** pulse for a DEPT45 like outcome.

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**



AVI-600 HXDEPTQF spectrum of quinine in D<sub>6</sub>-DMSO.

## 2.3 HETCOR spectrum

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

Pulse programme: **hxcoqf**

Type **eda** (enter) and enter **SW (<sup>1</sup>H)** and **SW (<sup>13</sup>C)** in ppm.

Enter **O1P** = <sup>13</sup>C spectral window midpoint in ppm.

Enter **O2P** = <sup>1</sup>H 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** = <sup>1</sup>J 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.

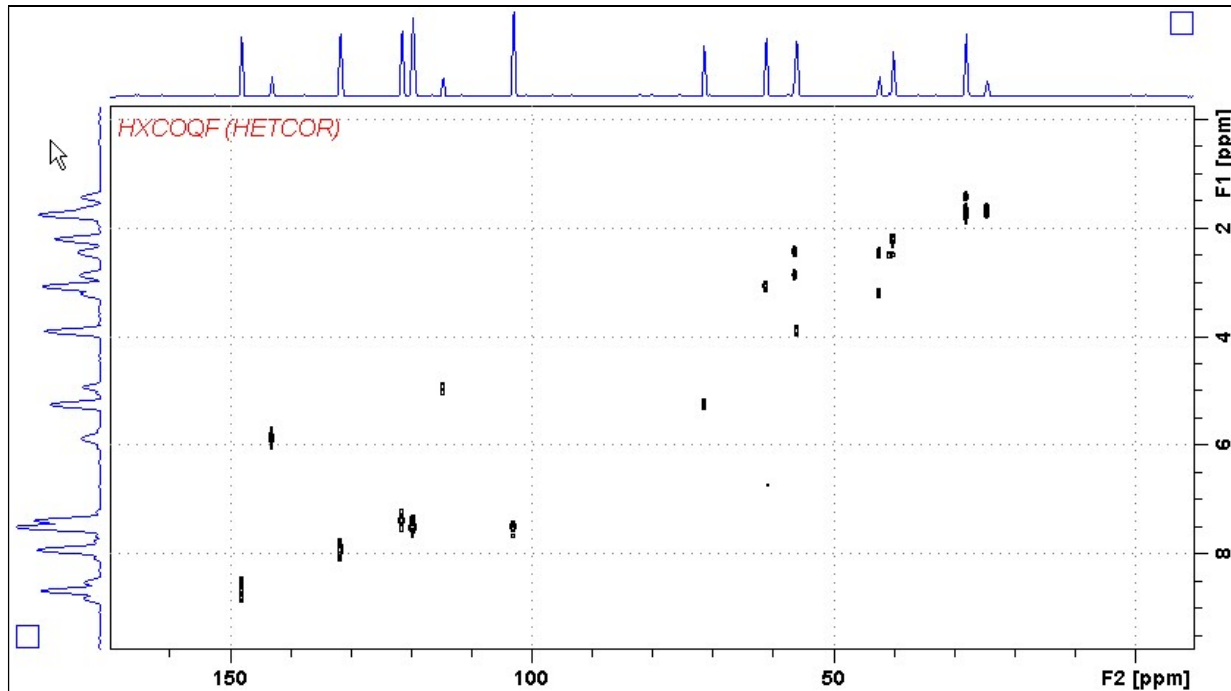
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

**xfb, abs1 and abs2**



AVI-600 HETCOR spectrum of quinine in D<sub>6</sub>-DMSO.

## 2.4 COLOC spectrum

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

Pulse programme: **colocqf**

Type **eda** (enter) and enter **SW (<sup>1</sup>H)** and **SW (<sup>13</sup>C)** in ppm.

Enter **O1P** = <sup>13</sup>C spectral window midpoint in ppm.

Enter **O2P** = <sup>1</sup>H 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** = 50-80 msec or other delay for <sup>n</sup>J evolution.

**D18** = 30 msec or other delay for <sup>n</sup>J evolution.

Parameter set **D6** and **D18** delay values are those for <sup>n</sup>J = ~ 8-10 Hz.

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

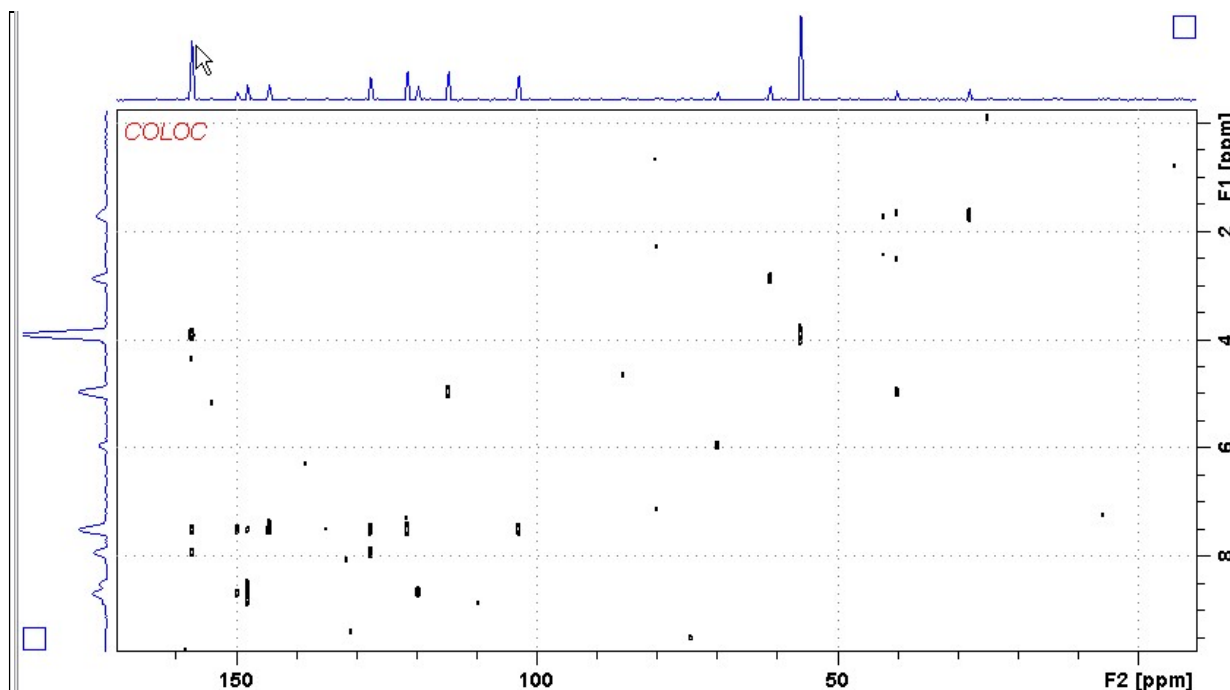
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

**xfb, abs1 and abs2**



AVI-600 COLOC spectrum of quinine in D<sub>6</sub>-DMSO optimized for <sup>n</sup>J = ~10 Hz.

