



KJM 9250

$^{13}\text{C}$  Detected XHDEPT, HETCOR and COLOC  
Experiments on the AVIIIHD-800 Spectrometer

Version 1.0

Topspin 3.5

Windows 7



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# **<sup>13</sup>C Detected XHDEPT, HETCOR and COLOC Experiments on the AVIIIHD-800 Spectrometer**

## **1.0 Introduction**

<sup>13</sup>C detected aw coded **XHDEPT, HETCOR and COLOC** parameter sets are set up with 1K or 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 Which 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 AVIIIHD-800 MHz spectrometer.

- 2.1 HXDEPT45, HXDEPT90 and HXDEPT135** spectra
- 2.2 HXDEPTQF** spectrum
- 2.3 HETCOR (= HXCOQF)** spectrum
- 2.4 HETCORLR** spectrum
- 2.5 COLOCQF** spectrum with manual or auto calculation of **d6** and **d18**.

## 2.1 HXDEPT45, HXDEPT90 and HXDEPT135 spectra

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

Pulse programme: **hxdept**

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.

**CNST12** = **0.5**, **1.0** or **1.5** for **P0** = **45°**, **90°** or **135°** as saved in parameter sets.

**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.

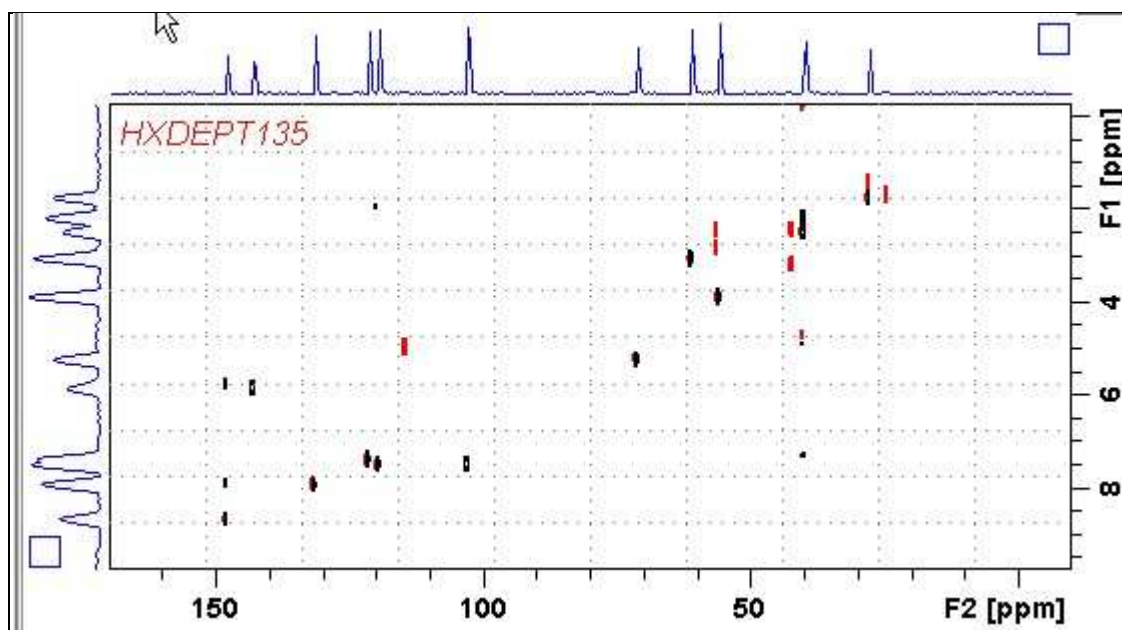
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

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



800 MHz **HXDEPT135** spectrum of quinine in D<sub>6</sub>-DMSO.

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

## 2.2 HXDEPTQF spectrum

Parameter sets: **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).

**CNST12** = **0.5** for DEPT45-like outcome.

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

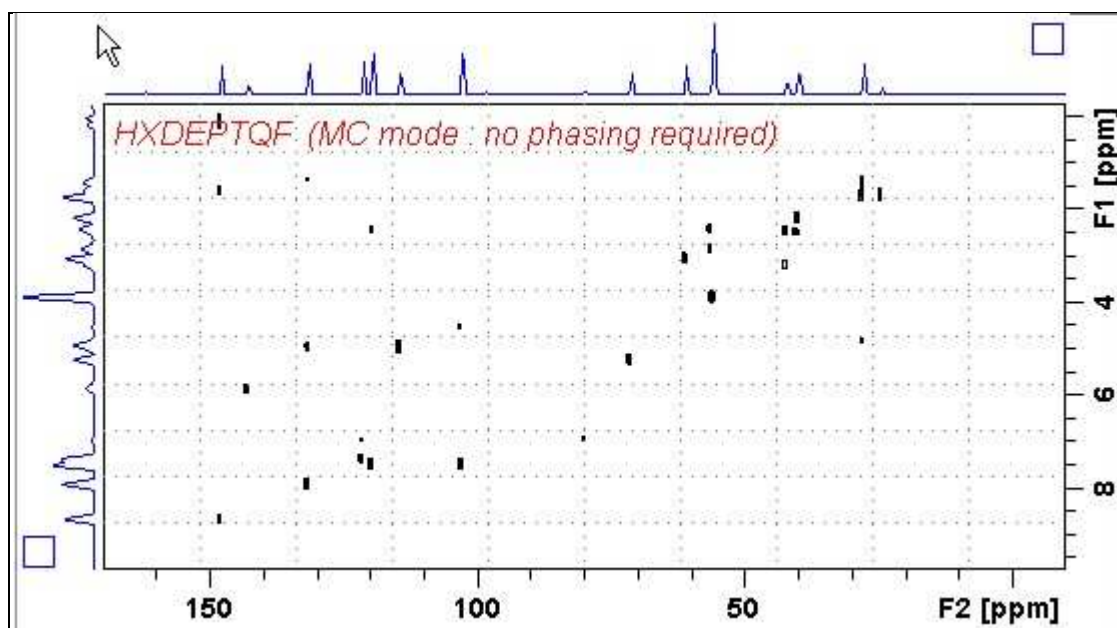
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

**xfb, abs1 and abs2**



800 MHz **HXDEPTQF** spectrum of quinine in D<sub>6</sub>-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 (<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.

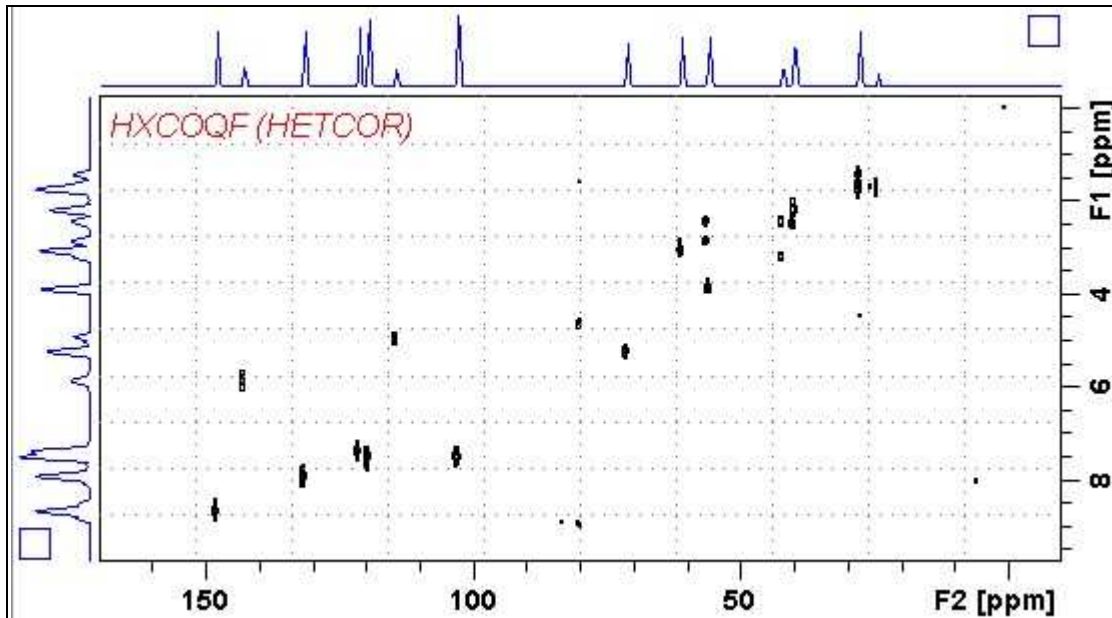
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

**xfb, abs1 and abs2**



800 MHz **HETCOR** spectrum of quinine in D<sub>6</sub>-DMSO.

## 2.4 HETCORLR spectrum

Parameter sets: **awhetcorlr** (+ **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>n</sup>J 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.

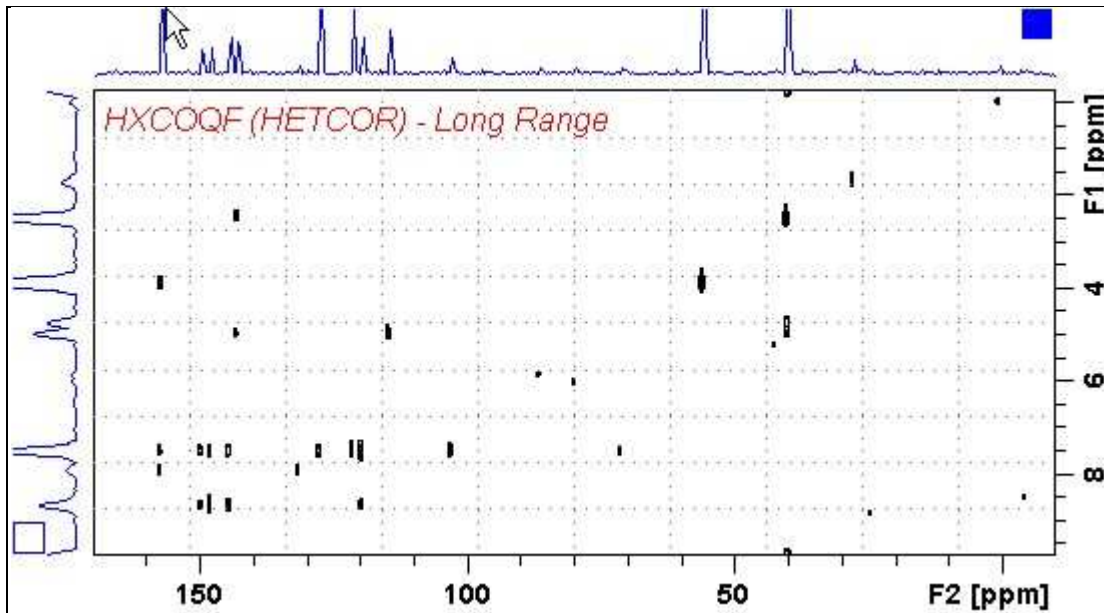
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

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



800 MHz **HETCORLR** spectrum of quinine in D<sub>6</sub>-DMSO optimized for <sup>n</sup>J = 10 Hz (**D2** = 50 msec, **D3** = 33 msec).

## 2.5.1 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 msec or other delay for <sup>n</sup>J evolution [D6= 1000/(2\* <sup>n</sup>J) msec].

**D18** = 30 msec or other delay for <sup>n</sup>J evolution [D18= 1000/(3\* <sup>n</sup>J) msec].

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

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

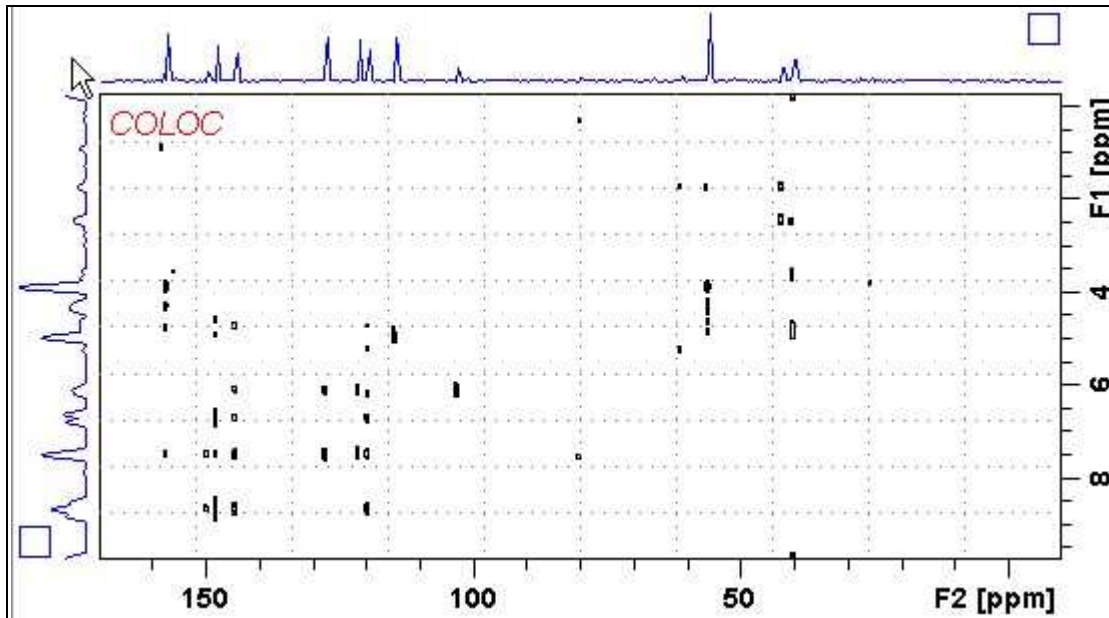
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

**xfb, abs1 and abs2**



800 MHz **COLOC** spectrum of quinine in D<sub>6</sub>-DMSO optimized for <sup>n</sup>J = ~10 Hz (**D6** = 50 msec, **D18** = 30 msec).

## 2.5.2 AWCOLORCQF spectrum

Parameter set: **awcolocl**r (+ **getprosol**)

Pulse programme: **awcolocqf**

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

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

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

Enter **O2P** =  $^1\text{H}$  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.

**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**

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

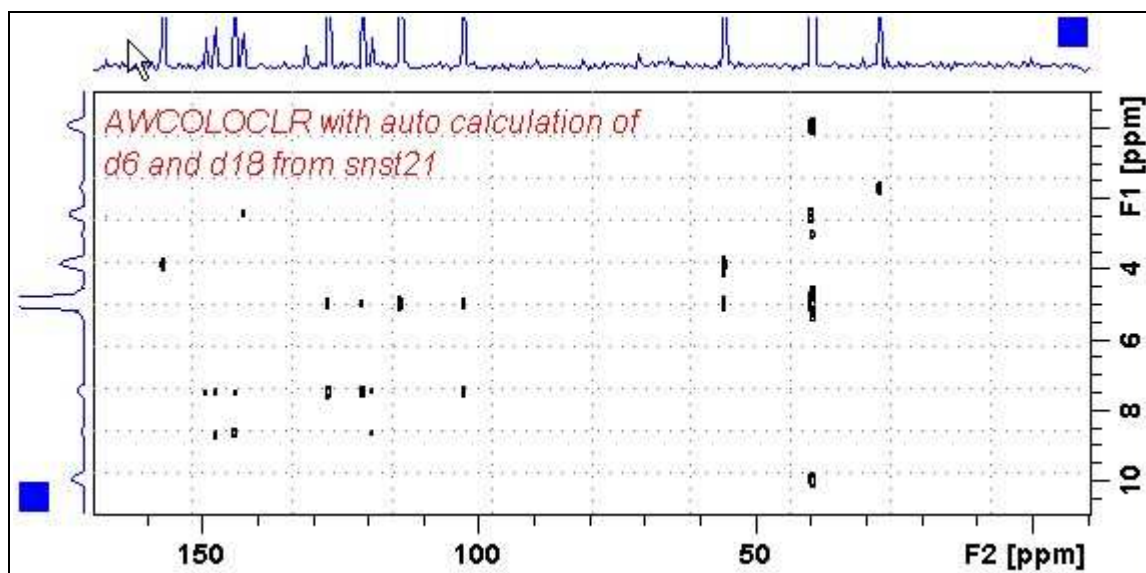
Set **receiver gain** using **RGA** (*Important!*).

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

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

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

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



800 MHz AWCOLORCQF spectrum of quinine in  $\text{D}_6$ -DMSO with **D6** and **D18** auto calculated from **CNST21** =  $J_{LR}$  10 Hz. (**D6** = 50 msec, **D18** = 33 msec).