KJM 9250

XHDEPT, HETCOR and COLOC Experiments on the AVII-600

Version 7.3

Topspin 3.2 Windows 7 AVII600

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1.0 Introduction

^{13}C detected aw coded **XHDEPT, HETCOR and COLOC** parameter sets are set up with 2K acquired ^{13}C points and 128 to 256 ^{1}H increments. ^{1}H and ^{13}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 ^{1}H detected **HXDEPT**, **HETCO**R 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**

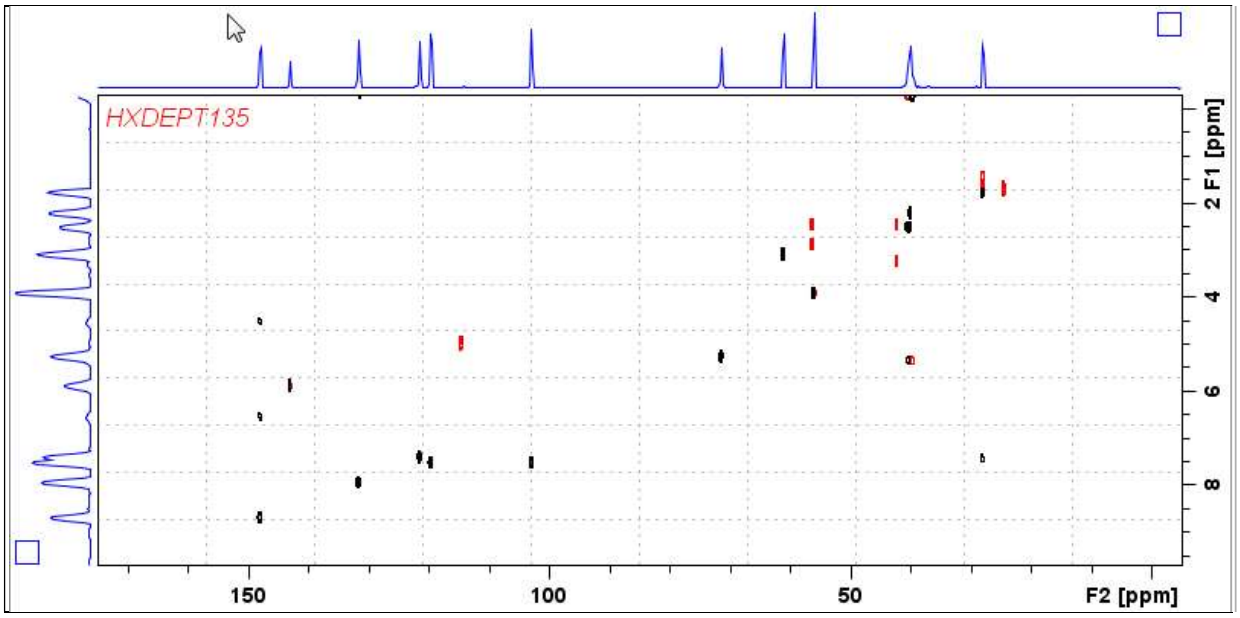
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)** in ppm.
Enter **O1P = ^{13}C**spectral window midpoint in ppm.
Enter **O2P = ^{1}H** spectral window midpoint in ppm.

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 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg 125-160 Hz).
p0 = p3* 0.5, 1.0 or 1.5 for **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



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

2.2 HXDEPTQF

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

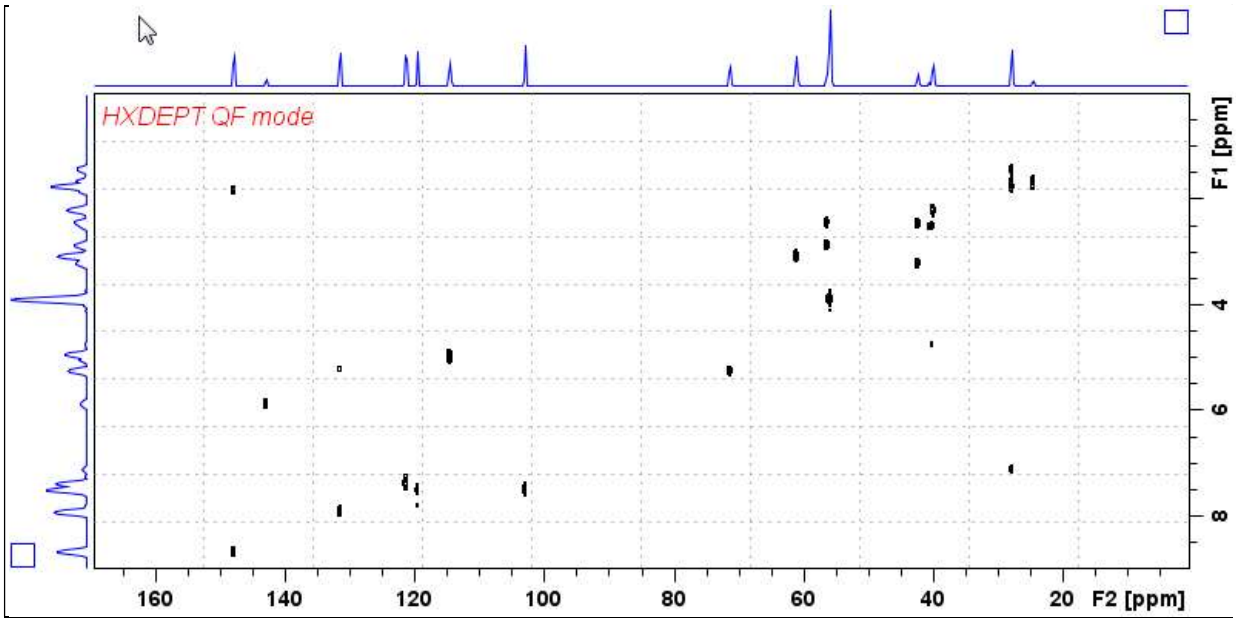
Type **eda** (enter) and enter **SW (^{1}H)** and **SW (^{13}C)**in ppm.
Enter **O1P = ^{13}C**spectral window midpoint in ppm.
Enter **O2P = ^{1}H** spectral window midpoint in ppm.

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 = ^{1}J coupling constant = **145 Hz** or other value of your choice (eg 125-160 Hz).
p0 = 45 degree 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



AVII-600 **HXDEPTQF** spectrum of quinine in D_6-DMSO.

2.3 HETCOR spectrum

Parameter set: **awhetcor (+ getprosol)**
Pulse programme: **hxcoqf**

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

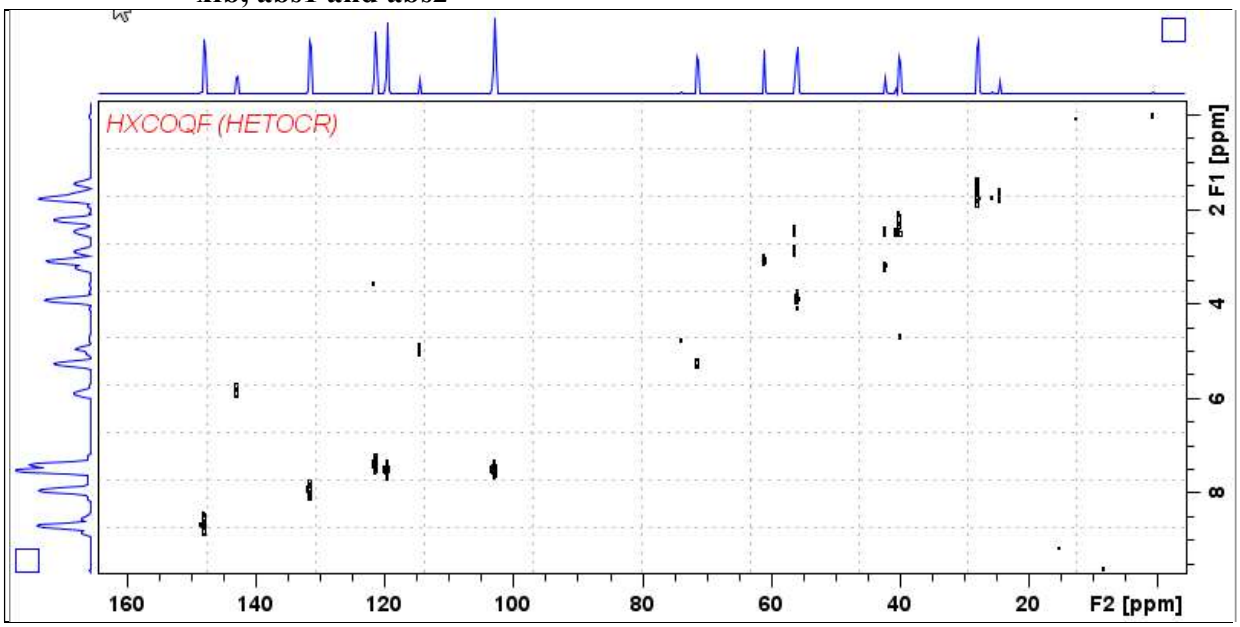
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 8, 16 (multiple of 4 or 8 recommended), **DS** = 8 or 16.
D1 = repetition delay = **1.5 sec** or other time of your choice.

CNST2 = ^{1}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



AVII-600 **HETCOR** spectrum of quinine in D_6-DMSO.

2.4 COLOC spectrum

Parameter sets: **awcoloc (+ getprosol)**
Pulse programme: **colocqf**

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

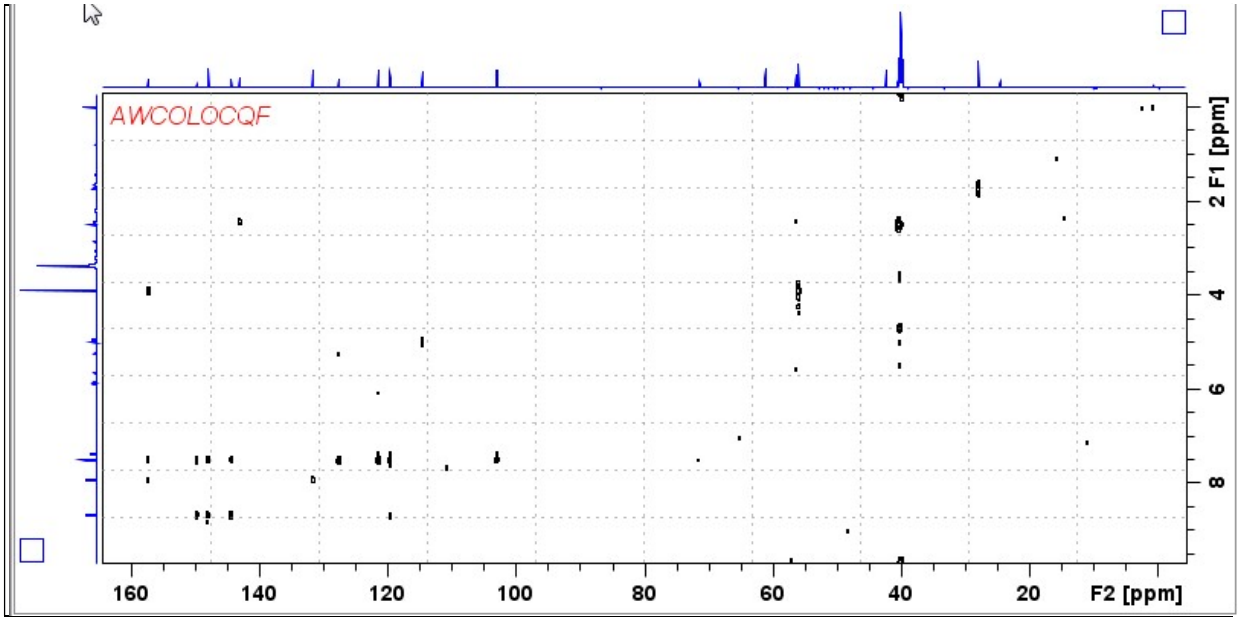
TD(F2) = 1K or 2K, **TD(F1)** = 128-256 (your choice).
NS = 8, 16 (multiple of 4 or 8 recommended), **DS** = 8 or 16.

D1 = repetition delay =**1.5 sec** or other time of your choice.
D6 = 50-80 msec or other delay for ^{n}J evolution.
D18 = 30 msec or other delay for ^{n}J evolution.
Parameter set **D6** and **D18** delay values are those for ^{n}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



AVII-600 **COLOC** spectrum of quinine in D_6-DMSO optimized for ^{n}J = ~10 Hz