KJM 5250 and KJM 9250

AVneo400 ^{15}N HSQC and HMBC Spectra on the AVneo400 Spectrometer.

Version 3.1
Topspin 4.3

AVneo400 ^{15}N f2 (f3 on the AVneo800) HSQC and HMBC Spectra.

(The f2 or f3 radio channels give rise to the F1 dimension in the 2 D spectra, the f1 radio channel give rise to the F2 dimension in the 2D spectra)

1.1 Introduction

aw coded ^{15}N **f2 HSQC, HSQC-DIPSI2** and **HMBC** parameter sets have been set up with 2048 (2K) points acquired across a **9 or 14 ppm ^{1}H** window and a **400 ppm ^{15}N window (SW))**.These settings were used to acquire 15N-HSQC and HMBC spectra ex an aromatic compound containing an NH and a quaternary N atom. Different ^{1}H and ^{15}N settings may (will) be required for other nitrogen containing compounds such as peptides.

1.2 Processing

^{15}N **f2 HSQC** and **HSQC-DIPSI2** experiments are phase sensitive experiments which should be phased **before** using the **abs1** and **abs2** commands.

The ^{15}N **f2 HMBC** experiment is an absolute value experiment. Phasing is not required.

2.0 Experiments and Parameter Sets

The following aw coded ^{15}N-^{1}H **f2 HSQC, HSQC-DIPS**I2 and **HMBC** parameter sets are available on the Neo-400 MHz spectrometer.

  2.1 ^{15}N **f2 HSQC**

  2.2 ^{15}N **f2 HSQC-DIPSI2**

  2.3 ^{15}N **f2 HMBC**

2.1 ^{1}H-^{15}N HSQC spectrum

Parameter set: **aw15nf2hsqc (+ get prosol)**
Pulse program: **hsqcetgpsi**

SW ^{1}H = **14 ppm** (or other suitable value).
SW ^{15}N = **400** ppm (or other suitable value).

TD ^{1}H = 2K, TD ^{15}N = 128-160 (your choice).
NS = multiple of 8, DS = 8 or 16.

Type **ased** (enter) and review other parameters used in the job.
O1P = ^{1}H spectral window midpoint = 6.5 ppm other value of your choice.
O2P = ^{15}N spectral window midpoint = 150 ppm other value of your choice.
D1 = repetition delay = 1-2 sec or other time of your choice.
CNST2 = ^1J ^{15}N-^{1}H coupling constant = **90 Hz** or other value of your choice.
ZGOPTNS = Not used.

Type **ased** (enter) and review parameters used in the job.
Check **D24 = 1/8J (~ 1.39 msec)** for CNST2 = 90 Hz.
   This value is not auto-calculated using Topspin's hsqcdiedetgpsisp.2 pp.
Check gradients and shaped pulses are OK.
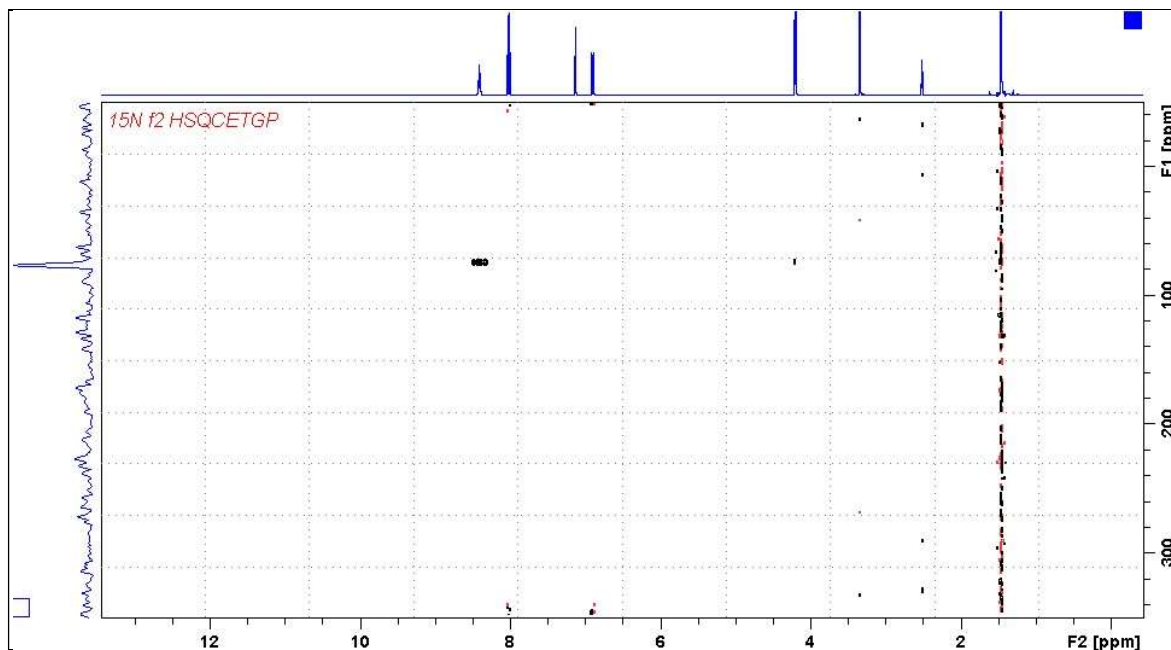
Set **receiver gain** using **RGA** *(Important!)*.

Process with: **SI(F2) = 2K SI(F1) = 512 or 1K**
             WDW(F1) = WDW(F2) = QSINE
             SSB(F2) = SSB(F1) = 2
             xfb, abs1 and abs2

^{15}N f2 HSQC spectrum of an aromatic NH containing compound.

2.2 ¹H-¹⁵N HSQC-DIPSI2 spectrum

Parameter sets: **aw15nf2hsqc-dipsi2 (+ getprosol)**
Pulse programme: **hsqcdietgpsi**

SW ¹H = 14 ppm (or other suitable value).
SW ¹⁵N = 400 ppm (or other suitable value).
TD ¹H = 2K, **TD ¹⁵N** = 128-160 (your choice).
NS = multiple of 8 or 16, **DS** = 16.

O1P = ¹H spectral window midpoint = 6.5 ppm other value of your choice.
O2P = ¹⁵N spectral window midpoint = 150 ppm other value of your choice.
D1 = repetition delay = **1.0 sec** or other time of your choice.
CNST2 = ^1J ¹⁵N-¹H coupling constant = **90 Hz** or other value of your choice.
ZGOPTNS = Not used.

Type **ased** (enter) and review parameters used in the job.
Check **D24** = 1/8J (~ 1.39 msec for CNST2 = 90 Hz).
   This values is not auto-calculated using Topspin's hsqcdietgpsi pp.
Check gradients and shaped pulses are OK.
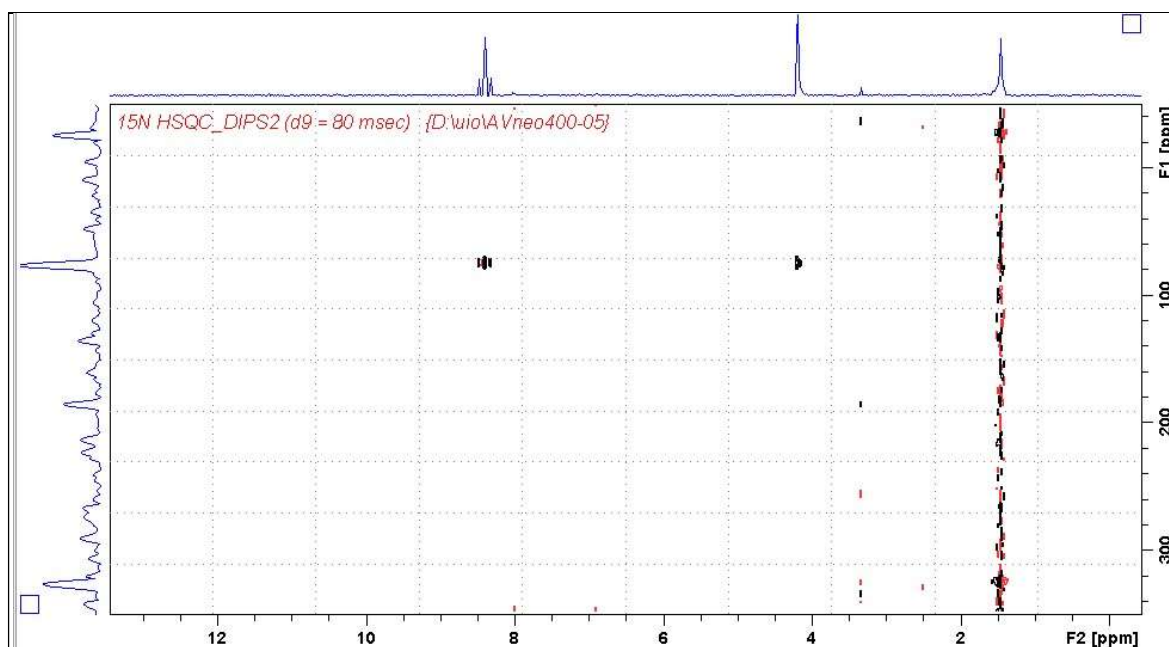
Set **receiver gain** using **RGA** *(Important!).*

Process with: **SI(F2) = 2K SI(F1) = 512 or 1K**
                WDW(F1) = WDW(F2) = QSINE
                SSB(F2) = SSB(F1) = 2
                xfb, abs1 and abs2

¹⁵N f2 HSQC-DIPSI2 spectrum of an aromatic NH containing compound.

^{15}N F2 HMBC spectrum

Parameter sets: **aw15nf2hmbc+ getprosol)**
Pulse programme: **hmbcfgpndqf**

Type **eda** (enter) and review the following default parameters
SW ^{1}H = 9 ppm, SW ^{15}N = 400 ppm (or other suitable values).
TD ^{1}H = 2K, TD ^{15}N = 128-160 (your choice).
NS = multiple of 8 or 16, **DS** = 16.

O1P = ^{1}H spectral window midpoint = 4.79 ppm other value of your choice.
O2P = ^{15}N spectral window midpoint = 100 ppm other value of your choice.
D1 = repetition delay = **1.0 sec** or other time of your choice.
CNST13 = 5 Hz (long range coupling constant).
ZGOPTNS = Not used.
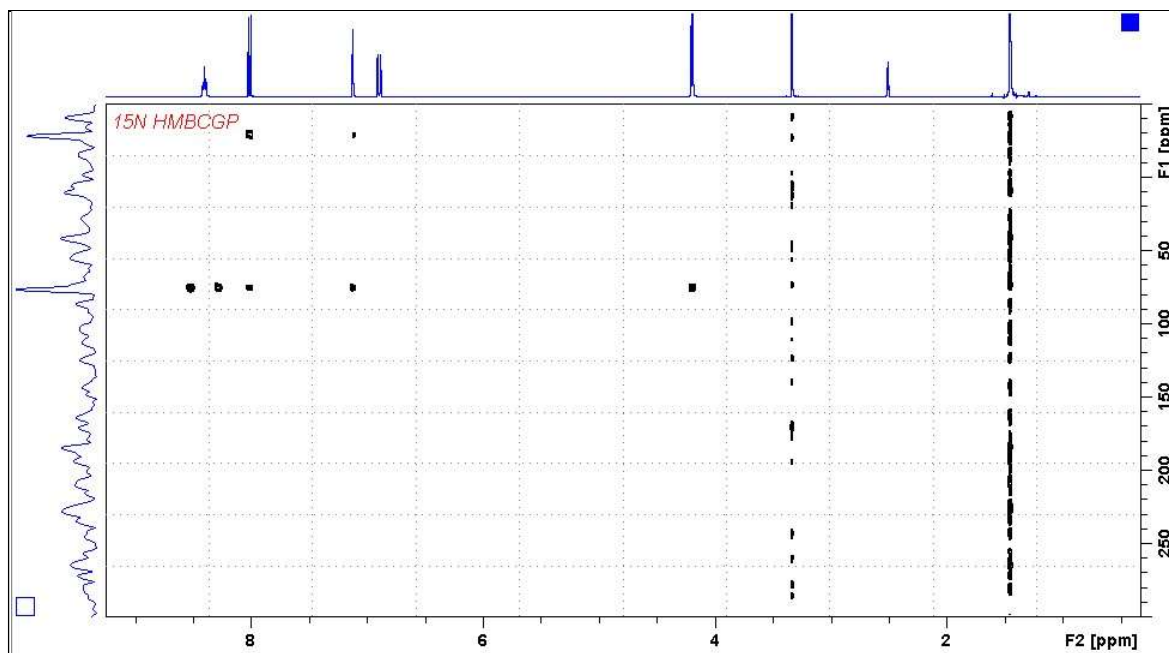
Check gradient settings.

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

Process with: **SI(F2) = 2K SI(F1) = 512 or 1K**
   WDW(F1) = WDW(F2) = SINE
   SSB(F2) = SSB(F1) = 0
   xfb and abs1 + abs2

^{15}**N f2 HMBC** spectrum of an aromatic NH and quaternary N containing compound.