KJM 9250

AVI-600 Homonuclear Decoupling Experiments

Version 7.3

Topspin 1.3 Windows XP AVI600

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1.0 Introduction

Homonuclear decoupling experiments can be performed using Bruker's **zghd** or **zghd.2** pulse programmes which incorporate homonuclear decoupling during FID acquisition, or during the FID acquisition and the interpulse delay period (**D1**), respectively.

Variants of Bruker's zghd pulse programme which incorporate excitation sculpturing (ES), continuous wave (CW) presaturation, or combined ES and CW presaturation on F1 have been created.

The hd power level can be *increased* (raised) by s*ubtracting* 3-12 db or decreased (attenuated) by *adding* 3-12 db *respectively* to the prosol Table linked **PL24** power level which is applied via F2.

The application of a decoupling radio frequency slightly increases the frequency of nearby signals. This effect is known as the Bloch-Seigert effect.

2.0 Homonuclear Decoupled Parameter Sets

The following **aw** coded **homonuclear decoupled** parameter sets are present on the AVI-600.

2.1	**awprotonhd**	*with hd during FID acquisition*
2.2	**awprotonhd.2**	*with hd during D1 + FID acquisition*
2.3	**awprotonhdpr**	*with pr during D1 + hd during FID acquisition*
2.4	**awprotoneshd**	*with ES peak suppression + hd during FID acquisition*
2.5	**awprotoneshdpr**	*with combined ES and pr + hd during FID acquisition*
2.6	**awprotoneshdpr**	*with two peaks suppressed + hd during FID acquisition*

2.1 awprotonhd spectrum with homonuclear decoupling at O2 during FID acquisition

Parameter set: **awprotonhd (+ getprosol)**
Pulse programme: **zghd**

Prior to setting up a **homonuclear decoupling** experiment determine the frequency in **Hz** of the signal to be decoupled in a standard ^{1}H NMR spectrum.

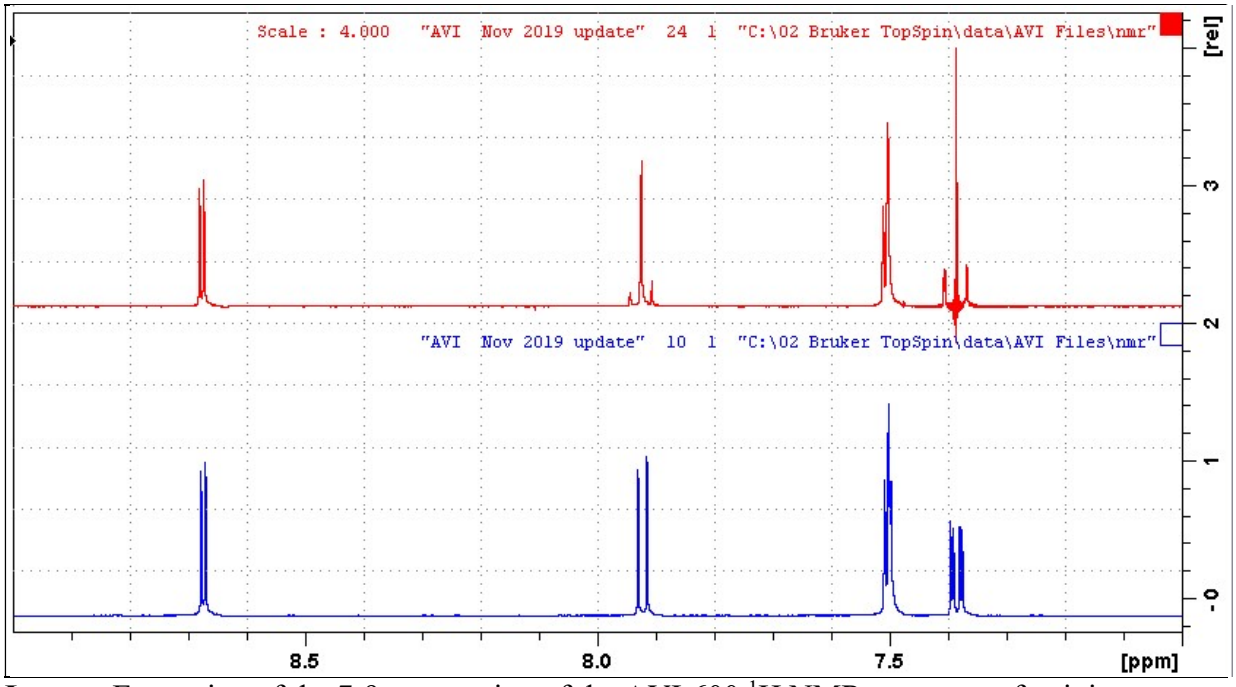
Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.
Type **eda** (enter) and adjust acquisition parameters as required.

NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
SW = 16 ppm, **O1** = 6 ppm, **TD** = 64 K points or other values of your choice.
D1 = repetition delay = 2.0, 3.0 sec or other time of your choice.

Type **ased** (enter) and review other parameters including the **PL24** power level.
Do not adjust the **PL1** power level.

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

Process with **EF or EFP** (applies **LB** = 0.1, 0.3 Hz or other values of your choice)
or FT (no line broadening factor applied).



Lower: Expansion of the 7-9 ppm region of the AVI-600 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during FID acquisition of the signal at 7.39 ppm. The signal at 7.93 ppm is collapsed to a singlet.

2.2 awprotonhd.2 spectrum with homonuclear decoupling during D1 and FID acquisition

Parameter set: **awprotonhd.2 (+ getprosol)**
Pulse programme: **zghd.2**

Prior to setting up a **homonuclear experiment** determine the frequency in **Hz** of the signal to be decoupled in a standard ^{1}H NMR spectrum.

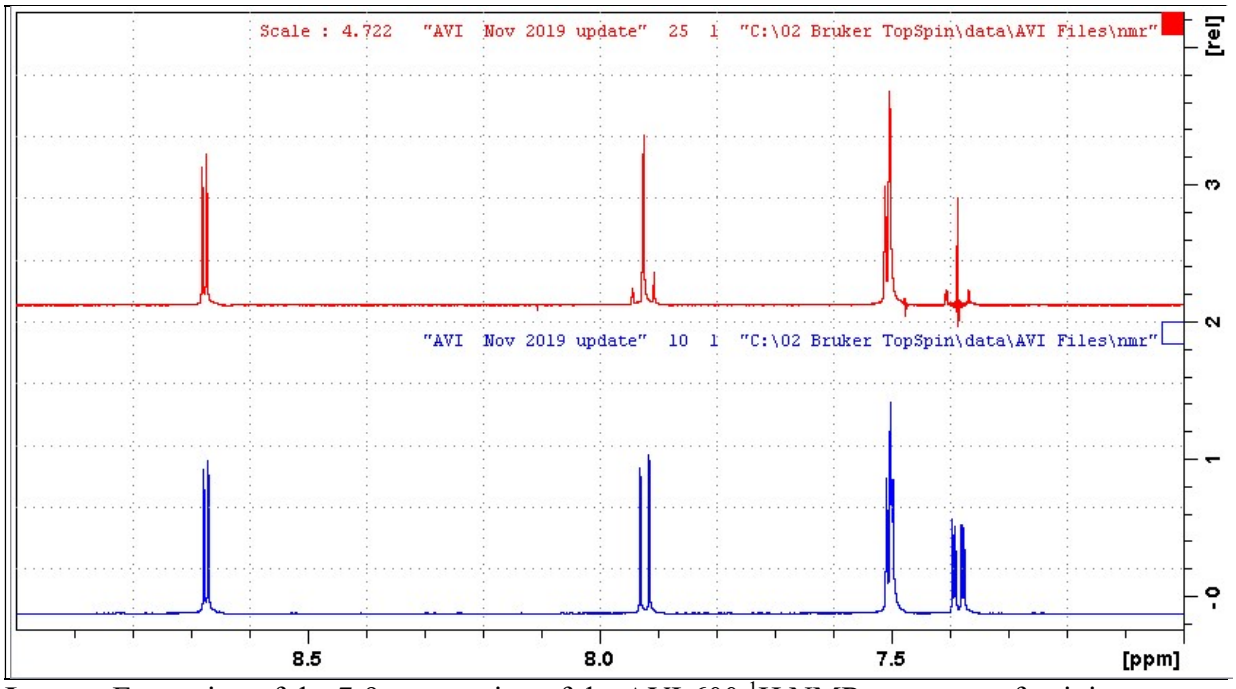
Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.
Type **eda** (enter) and adjust acquisition parameters as required.

NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
SW = 16 ppm, **O1** = 6 ppm, **TD** = 64 K points or other values of your choice.
D1 = repetition delay = 2.0, 3.0 sec or other time of your choice.

Type **ased** (enter) and review other parameters including the **PL24** power level.
Do not adjust the **PL1** power level.

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

Process with **EF or EFP** (applies **LB** = 0.1, 0.3 Hz or other values of your choice)
or FT (no line broadening factor applied).



Lower: Expansion of the 7-9 ppm region of the AVI-600 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during **D1** and **FID** acquisition of the signal at 7.39 ppm. The signal at 7.93 ppm is collapsed to a singlet.

2.3 awprotonhdpr spectrum with CW presaturation and homonuclear decoupling during FID acquisition

Parameter set: **awprotonhdpr (+ getprosol)**
Pulse programme: **awzghdpr**

Prior to setting up a **homonuclear experiment** determine the frequencies in **Hz** of the signals to be presaturated **(O1)** and decoupled (**O2**) respectively in a standard ^{1}H NMR spectrum.

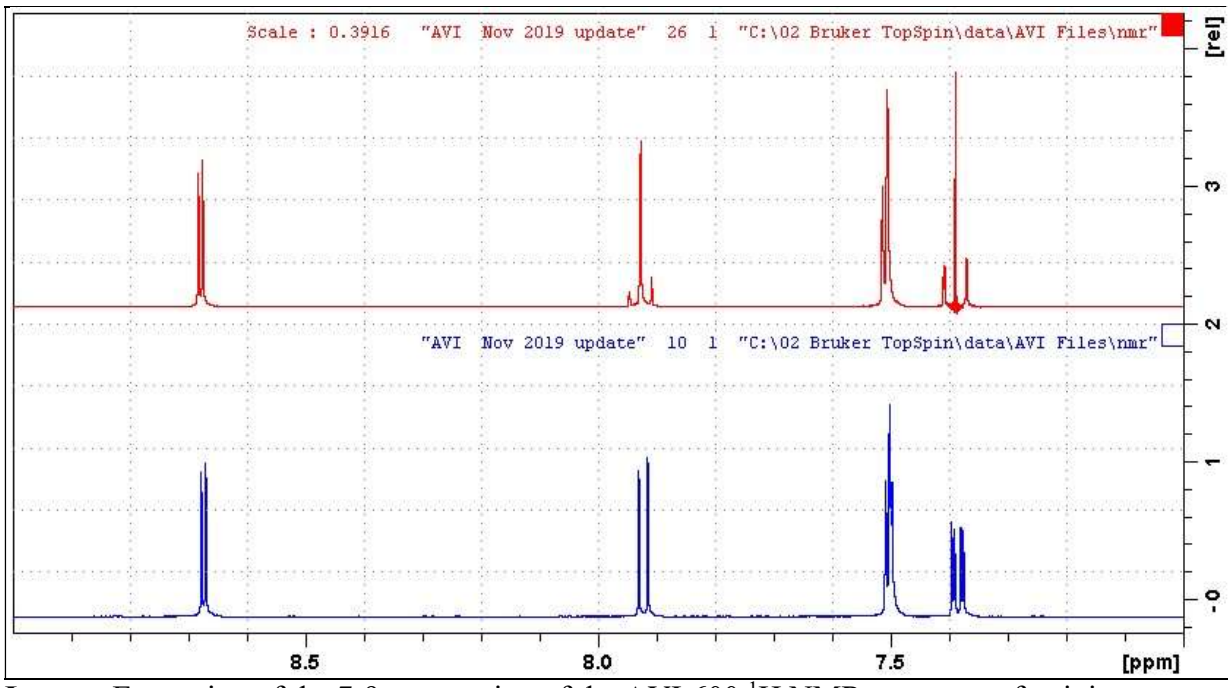
Type **O1** (enter) and enter the frequency in Hz of the signal to be presaturated.
O1 will be set as the spectrum's midpoint.
Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.

Type **eda** (enter) and adjust acquisition parameters as required.
NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
SW = 16 ppm, **TD** = 64 K points or other values of your choice.
D1 = repetition delay = 2.0, 3.0 sec or other time of your choice.

Type **ased** (return) and review other parameters including the **PL24** hd and **PL9** presaturation power levels.

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

Process with **EF or EFP** (applies **LB** = 0.1, 0.3 Hz or other values of your choice)
or FT (no line broadening factor applied).



Lower: Expansion of the 7-9 ppm region of the AVI-600 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during FID acquisition of the signal at 7.39 ppm. ES was applied to the HOD signal at 3.38 ppm. The signal at 7.93 ppm is collapsed to a singlet.

2.4 awprotoneshd spectrum with ES peak suppression and homonuclear decoupling during FID acquisition

Parameter set: **awprotoneshd (+ getprosol)**
Pulse programme: **awzgeshd**

Prior to setting up a **homonuclear decoupling** experiment determine the frequencies in **Hz** of the signals to be **ES** suppressed **(O1)** and decoupled (**O2**) respectively in a standard ^{1}H NMR spectrum.

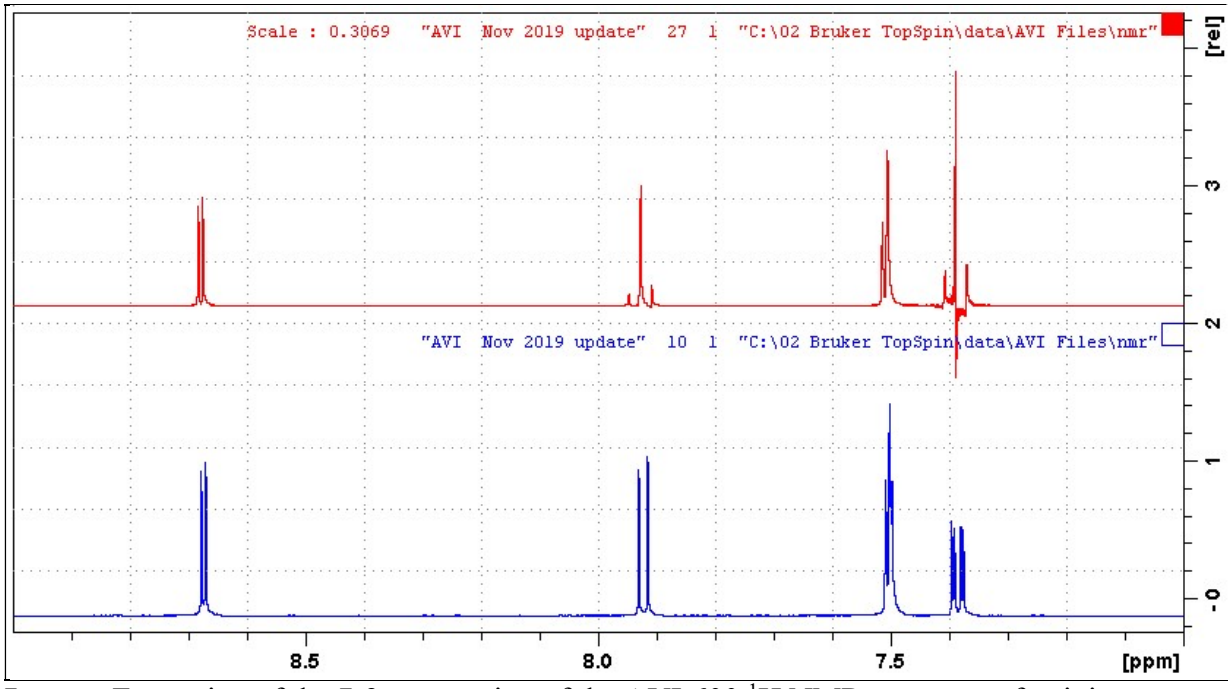
Type **O1** (enter) and enter the frequency in Hz of the signal to be presaturated.
O1 will be set as the spectrum's midpoint.
Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.

Type **eda** (enter) and adjust acquisition parameters as required.
NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
SW = 16 ppm, **TD** = 64 K points or other values of your choice.
D1 = repetition delay = 2.0, 3.0 sec or other time of your choice.

Type **ased** (enter) and review other parameters including the **PL24** hd power level.
Check that a **2000 usec P12:sp1 squa100.1000** ES pulse is used and **SMSQ10.100** gradients are set to 31% (GPZ1) and 11% (GPZ2).

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

Process with **EF or EFP** (applies **LB** = 0.1, 0.3 Hz or other values of your choice)
or **FT** (no line broadening factor applied).



Lower: Expansion of the 7-9 ppm region of the AVI-600 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during FID acquisition of the signal at 7.39 ppm. ES was applied to the HOD signal at 3.38 ppm. The signal at 7.93 ppm is collapsed to a singlet.

2.5 awprotoneshdpr spectrum with combined ES and CW presaturation and homonuclear decoupling during FID acquisition

Parameter set: **awprotoneshdpr (+ getprosol)**
Pulse programme: **awzgeshdpr**

Prior to setting up a **homonuclear decoupling** experiment determine the frequencies in **Hz** of the signals to be combined **ES** and **pr** suppressed **(O1)** and decoupled (**O2**) respectively in a standard ^{1}H NMR spectrum.

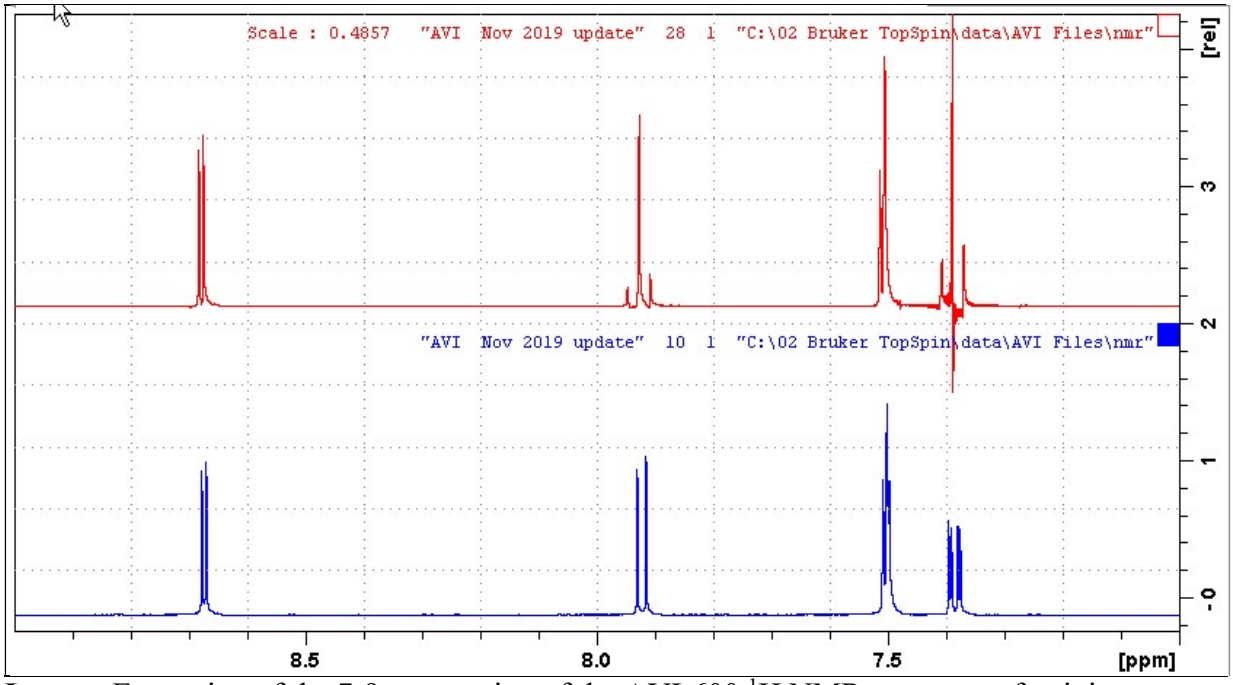
Type **O1** (enter) and enter the frequency in Hz of the signal to be presaturated.
O1 will be set as the spectrum's midpoint.
Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.

Type **eda** (enter) and adjust acquisition parameters as required.
NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
SW = 16 ppm, **TD** = 64 K points or other values of your choice.
D1 = repetition delay = 2.0, 3.0 sec or other time of your choice.

Type **ased** (enter) and review parameters including the **PL24** hd and **PL9** pr power levels. Check that P12 = 2000 usec, spnam1 = squa100.1000 and **SMSQ10.100** gradients are set to 31% (GPZ1) and 11% (GPZ2).

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

Process with **EF or EFP** (applies **LB** = 0.1, 0.3 Hz or other values of your choice)
or FT (no line broadening factor applied).



Lower: Expansion of the 7-9 ppm region of the AVI-600 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during FID acquisition of the signal at 7.39 ppm. ES was applied to the HOD signal at 3.38 ppm. The signal at 7.93 ppm is collapsed to a singlet.

2.6 awprotoneshdpr spectrum with two peak suppression and homonuclear decoupling during FID acquisition

Parameter set: **awprotoneshdpr (+ getprosol)**
Pulse programme: **awzgeshdpr**

Prior to setting up a two peak suppressed **homonuclear decoupling** experiment determine the frequencies in **Hz** of the signals to CW presaturated (**O1**), ES suppressed **(O1***) and decoupled (**O2**) respectively, in a standard ^{1}H NMR spectrum.

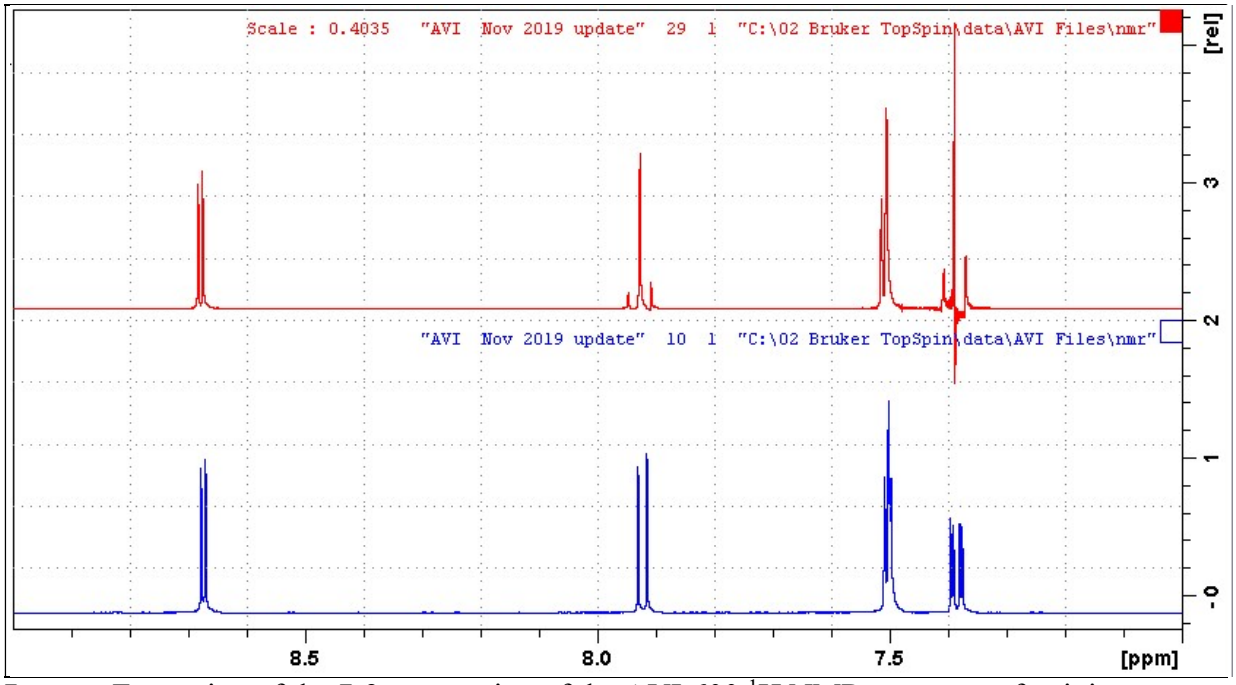
Type **O1** (enter) and enter the frequency in Hz of the signal to be CW presaturated during d1.
O1 will be set as the spectrum's midpoint.
Type **SPOFFS1 (**enter) and enter the frequency in Hz of the signal to be ES suppressed.
as **O1*-O1**. *This offset value may be a positive or negative value.*
Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.

Type **eda** (enter) and adjust acquisition parameters as required.
NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
SW = 16 ppm, **TD** = 64 K points or other values of your choice.
D1 = repetition delay = 2.0, 3.0 sec or other time of your choice.

Type **ased** (enter) and review parameters including the **PL24** hd and **PL9** pr power levels.
Check that a **2000 usec P12:sp1 squa100.1000** ES pulse is used and **SMSQ10.100** gradients are set to 31% (GPZ1) and 11% (GPZ2).

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

Process with **EF or EFP** (applies **LB** = 0.1, 0.3 Hz or other values of your choice)
or FT (no line broadening factor applied).



Lower: Expansion of the 7-9 ppm region of the AVI-600 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during FID acquisition of the signal at 7.39 ppm. ES was applied to the quinine OCH_3 signal at 3.90 ppm. CW presaturation was applied to the HOD signal at 3.38 ppm. The signal at 7.93 ppm is collapsed to a singlet.