KJM 9250
AVIIIHD-800 Homonuclear Decoupling Experiments

Version 5.0

Topspin 3.5
Windows 7

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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 FD acquisition, or during both 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 Decoupling Experiments

The following **aw** coded **homonuclear decoupled** parameter sets are installed on the AVIIIHD-800. Identical **uio** coded versions of these parameter sets have also been saved

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 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.

This experiment runs with **DIGMOD = digital**

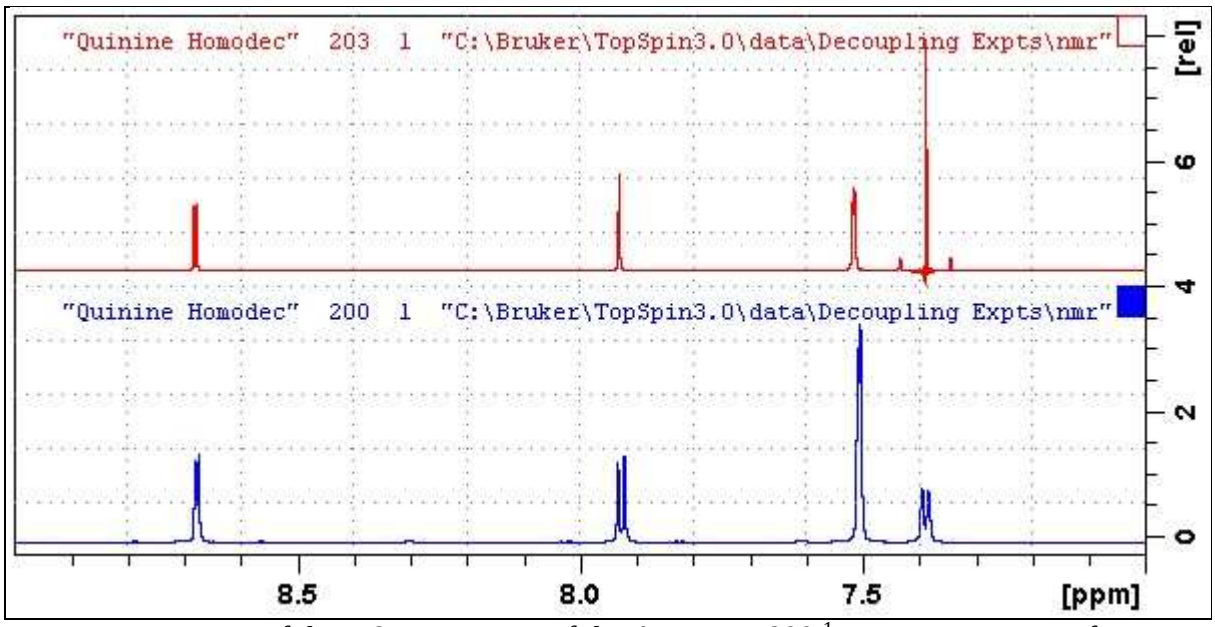
Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.

Type **eda** (enter) and adjust acquisition parameters as required.
SW = 16 ppm, **O1** = 6 ppm, **TD** = 64 K points or other values of your choice.
NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
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 or PL2** 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 AVIIIHD-800 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during FID acquisition of the signal at 7.49 ppm. The signal at 7.93 ppm is collapsed to a singlet.

2.2 awprotonhd.2 with homonuclear decoupling during d1 and FID acquisition

parameter set: **awprotonhd.2 (+ getprosol)**
pulse programme: **zghd.2**

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.

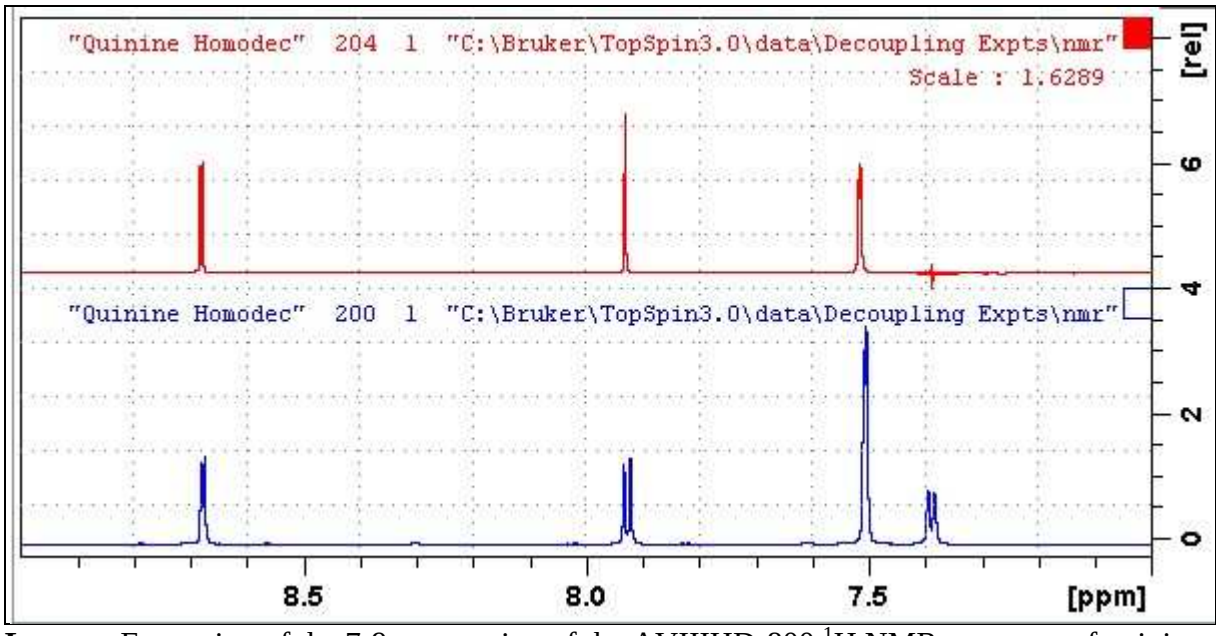
This experiment runs with **DIGMOD = digital**

Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.

Type **eda** (enter) and adjust acquisition parameters as required.
SW = 16 ppm, **O1** = 6 ppm, **TD** = 64 K points or other values of your choice.
NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
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 or PL2** 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 AVIIIHD-800 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during **D1** and FID acquisition of the signal at 7.49 ppm. The signal at 7.93 ppm is collapsed to a singlet.

2.3 awprotonhdpr with CW presaturation and homonuclear decoupling during FID acquisition

parameter set: **awprotonhdpr (+ getprosol)**
pulse programme: **awzghdpr**

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

This experiment runs with **DIGMOD = digital.**

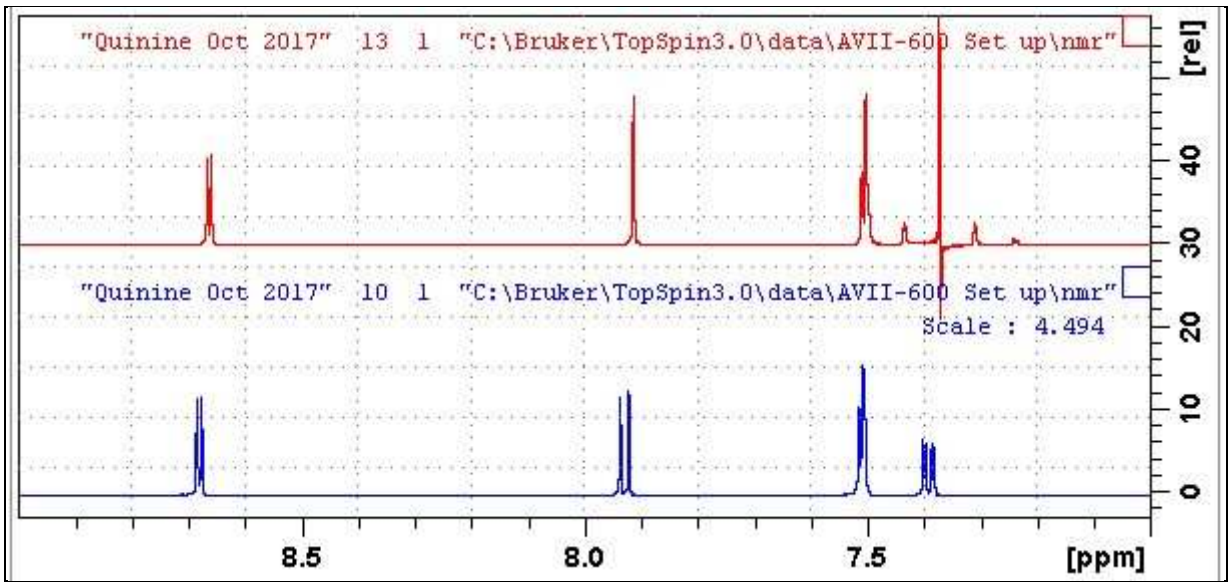
Type **O1** (enter) and enter the frequency in Hz of the signal to be presaturated.
O1 will be set as the spectrum's midpoint.
Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.

Type **eda** (enter) and adjust acquisition parameters as required.
SW = 16 ppm, **TD** = 64 K points or other values of your choice.
NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
D1 = repetition delay = 2.0, 3.0 sec or other time of your choice.
PL9 = presatuation power level, applied during **D1**.

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 AVIIIHD-800 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during FID acquisition of the signal at 7.49 ppm. CW presaturation was applied during **d1** to the HOD signal at 3.38 ppm. The signal at 7.93 ppm is collapsed to a singlet.

2.4 awprotoneshd 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.

This experiment runs with **DIGMOD = digital**.

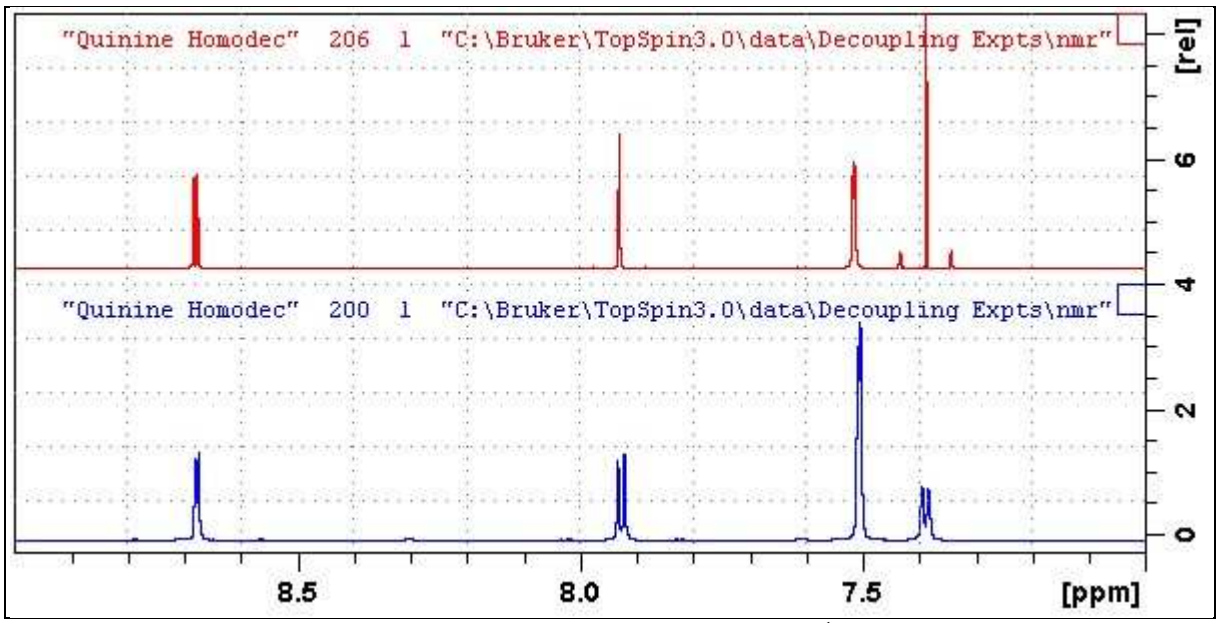
Type **O1** (enter) and enter the frequency in Hz of the signal to be presaturated.
O1 will be set as the spectrum's midpoint.
Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.

Type **eda** (enter) and adjust acquisition parameters as required..
SW = 16 ppm, **TD** = 64 K points or other values of your choice.
NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8
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 **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 AVIIIHD-800 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during FID acquisition of the signal at 7.49 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 with combined ES + 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 **CW** suppressed **(O1**) and decoupled (**O2**) respectively in a standard ^{1}H NMR spectrum.

This experiment runs with **DIGMOD = digital**

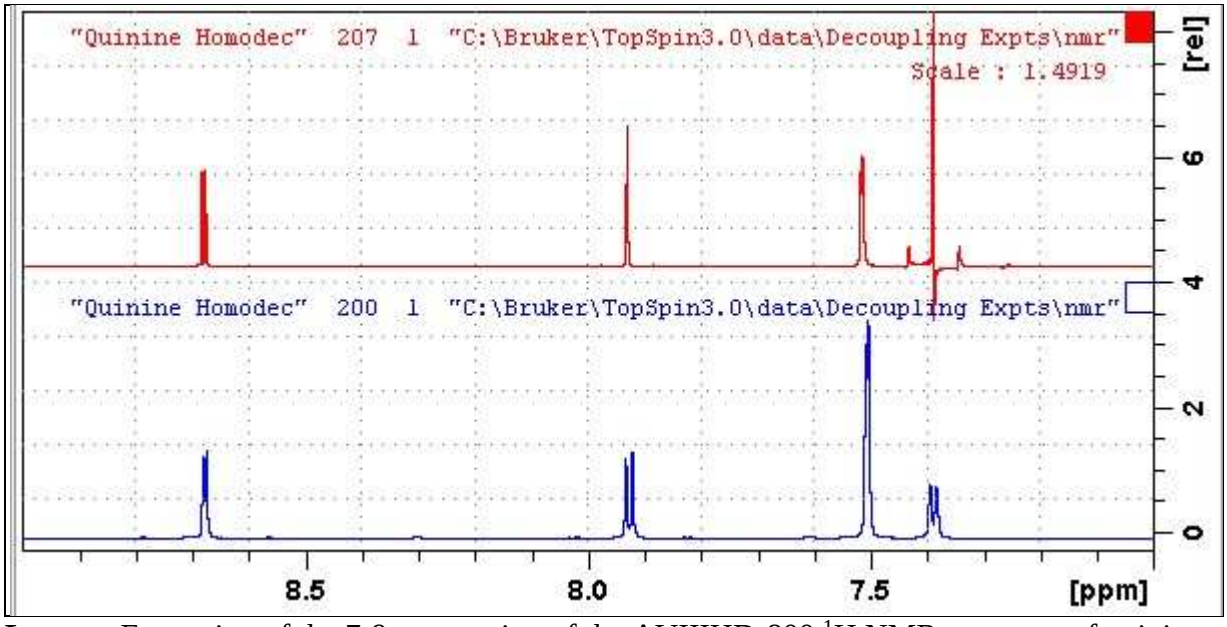
Type **O1** (enter) and enter the frequency in Hz of the signal to be presaturated.
O1 will be set as the spectrum's midpoint.
Type **O2** (enter) and enter the frequency in Hz of the signal to be decoupled.

Type **eda** (enter) and adjust acquisition parameters as required.
SW = 16 ppm, **TD** = 64 K points or other values of your choice.
NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
D1 = repetition delay = 2.0, 3.0 sec or other time of your choice.
PL 9 = CW presaturation power level applied during **D1**.

Type **ased** (enter) and review parameters including the **PL24** hd and **PL9** presaturation power levels. Check **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 AVIIIHD-800 ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: Homonuclear decoupling during FID acquisition of the signal at 7.49 ppm. Combined ES + CW presaturation was applied to the HOD signal at 3.38 ppm. The signal at 7.93 ppm is collapsed to a singlet.

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

parameter set: aw**protoneshdpr (+ 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.

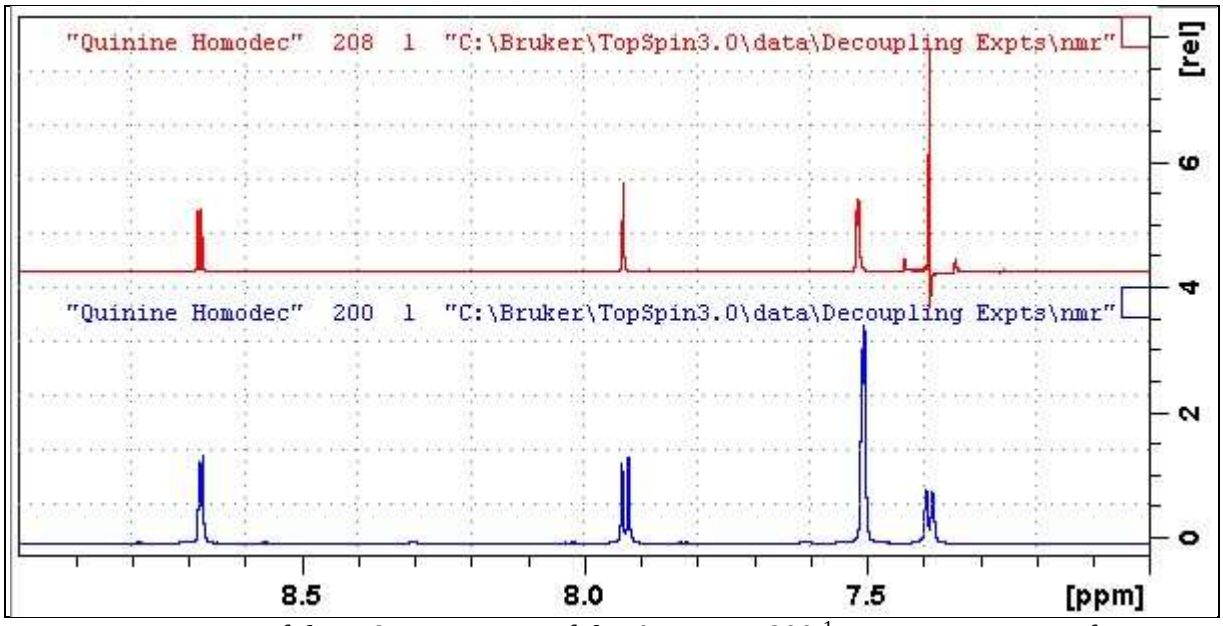
This experiment runs with **DIGMOD = digital**

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.
SW = 16 ppm, **TD** = 64 K points or other values of your choice.
NS = multiple of 2, 4 or 8, **DS** = 2, 4 or 8.
D1 = repetition delay = 2.0, 3.0 sec or other time of your choice.
PL 9 = CW presaturation power level applied during **D1**.

Type **ased** (enter) and review other parameters including **SPOFFS1** and the **PL24** hd and **PL9** presatursatton power levels. Check **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 AVIIIHD-800 ^{1}H NMR spectrum of quinine in D_6-DMSO.

Upper: Homonuclear decoupling during FID acquisition of the signal at 7.49 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.