KJM 9250

^{1}H NMR Spectra on the AVIIIHD-800

Version 1.0

Topspin 3.5
Windows 7

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1.0 Introduction

aw coded ^{1}H NMR parameter files generally use a 90^o pulse for maximum ^{1}H signal.

Best ^{1}H resolution is obtained using **FT** and **PK** (or **APK**) processing. **FT** processing does not apply a line broadening factor. **EF** or **EFP** processing applies a line broadening factor (**LB**).

Resolution enhancement uses negative **LB** values. Try **LB** = -1.0 to -2.5 Hz with **GB** = 0.33, and **GFP** processing. Remember to reset **LB** and **GB** to their normal values (0.1 to 0.3 and 0 respectively) after **GFP** processing.

1.1 Presaturation Experiments

Continuous wave or excitation sculptured (ES) can be used to presaturate ^{1}H NMR signals. The simplest of these techniques is continuous wave presaturation.

CW presaturation power levels (db settings) can be increased or decreased by subtracting or adding 3-12 db respectively. 6 db = a factor of 2.

The **ES** shaped pulse's excitation window can be decreased by doubling its shaped pulse time from 2000 usec to 4000 usec and halving its power by adding 6 db to that read in using the **getprosol** command.

2.0 ^{1}H NMR experiments

2.1 ^{1}H NMR with a 30, 45 or 90 degree pulse

2.2 ^{1}H NMR with CW presaturation

2.3 ^{1}H NMR with dual CW presaturation

2.4 ^{1}H NMR with ES peak suppression

2.5 ^{1}H NMR with combined ES + CW presaturation on F1

2.6 ^{1}H NMR with combined ES + CW presaturation on F1 and CW presaturation on F2

2.7 ^{1}H NMR with three peak ES + dual CW presaturation

2.1 ^{1}H NMR with a 30, 45 or 90 degree pulse

Parameter sets: **awproton30, awproton45, awproton90 (+ getprosol)**
Pulse programmes**: zg30, awzg45 or zg respectively**

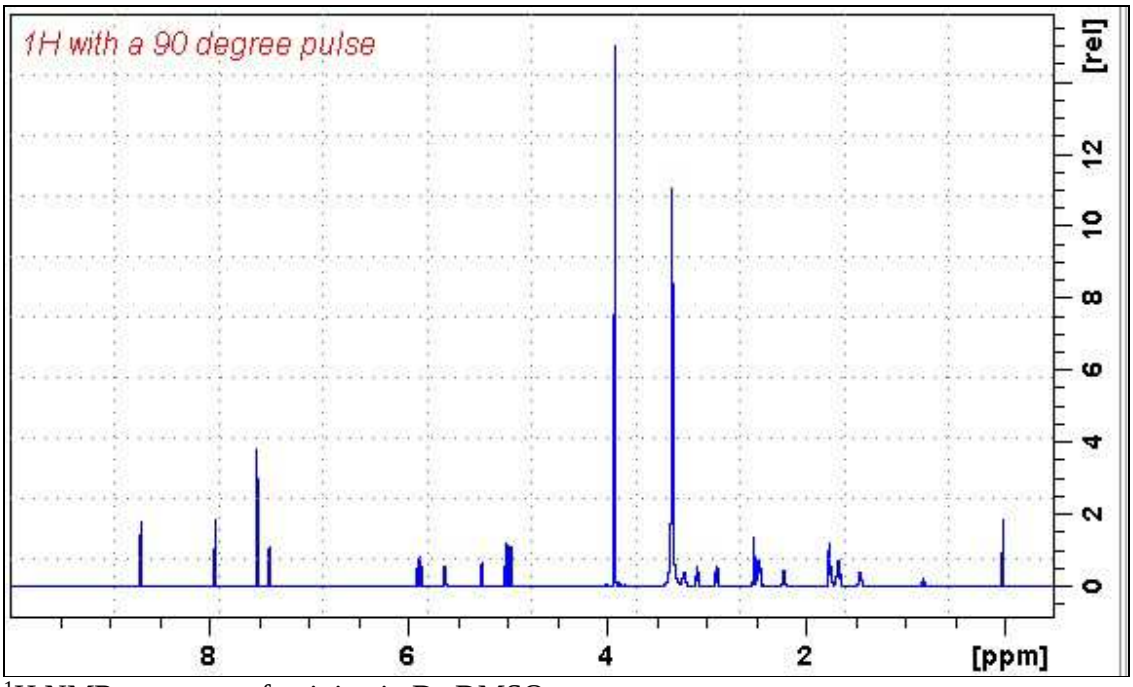
TD = 128 K, **SI** = 128 K
SW = 20 ppm, **O1P** = 7.93 ppm.

D1 = 1.5 sec or other time of your choice.
NS = any number, **DS =** 2, 4 or 8.

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

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

Process with **FT** (no line broadening) or **EFP** (applies **LB**).



^{1}H NMR spectrum of quinine in D_6-DMSO.

2.2 ^{1}H NMR with CW presaturation

Parameter set: **awprotonpr (+ getprosol)**
Pulse programme: **zgpr**

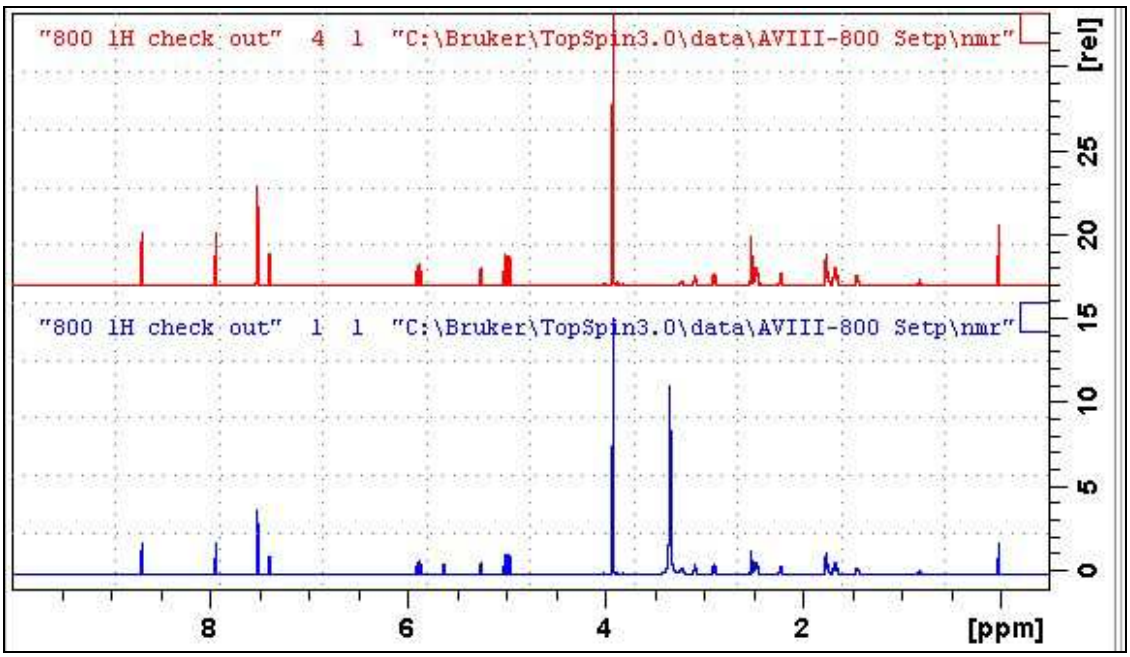
TD = 128 K, **SI** = 128 K.
SW = 20 ppm.

O1 = frequency in Hz of the F1 signal to be presaturated
= spectral window mid-point. Check **SW** is wide enough.
PL9 = **F1** presaturation power applied during **D1**.
D1 = 2 sec or other time of your choice.

Type **ased** (enter) and review parameters used in the job.
Add (or subtract) 3-12 db to **PLW9** to decrease (or increase) the presaturation power.
6 db = a factor of 2. A larger attenuation setting decreases the power level.

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

Process with **EFP** (applies **LB**).



Lower: ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: ^{1}H NMR spectrum with CW presaturation of the HOD line at 3.37 ppm.

2.3 ^{1}H NMR with dual CW presaturation

Parameter set: **awprotonprf1prf2 (+ getprosol)**
Pulse programme: **awprotonprf1prf2**

TD = 128 K, **SI** = 128 K.
SW = 20 ppm.

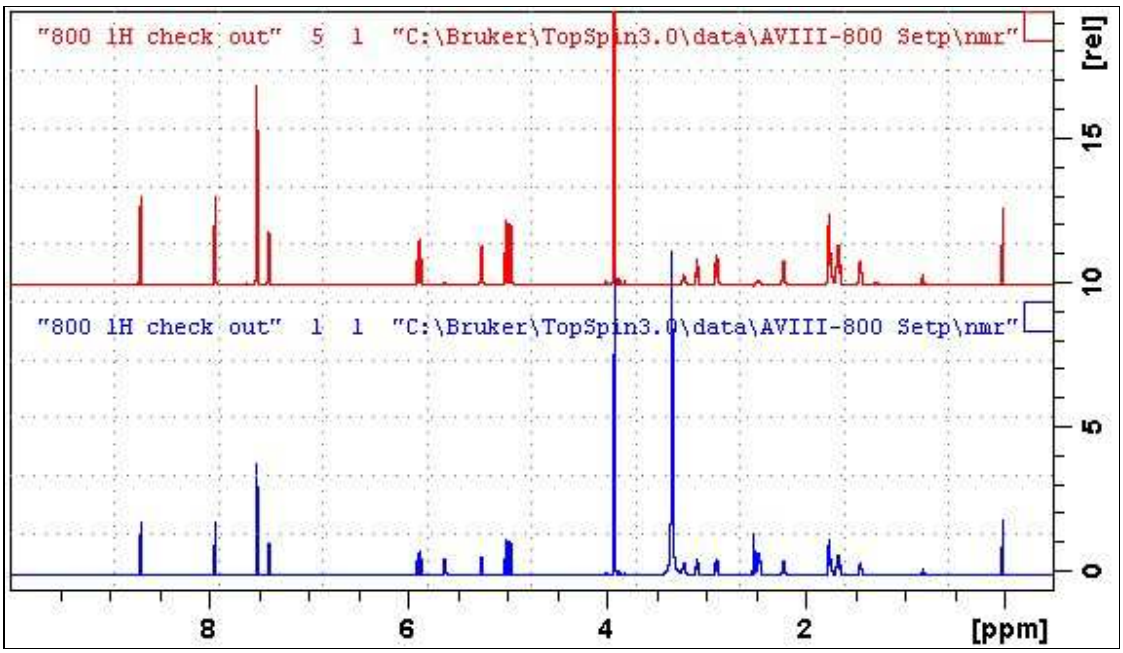
O1 = frequency in Hz of the F1 signal to be presaturated
= spectral window mid-point. Check **SW** is wide enough.
O2 = frequency in Hz of the F2 signal to be presaturated.

PL9 = F1 presaturation power applied during **D1**.
PL21 = F2 presaturation power applied during **D1**.
D1 = 2 sec or other time of your choice.

Type **ased** (enter) and review parameters used in the job.
Add (or subtract) 3-12 db to **PL9** and/or **PL21** to decrease (or increase) the presaturation power. 6 db = a factor of 2. A <u>larger</u> attenuation setting <u>decreases</u> the power level.

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

Process with **EFP** (applies **LB**).



Lower: ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: ^{1}H NMR spectrum with CW presaturation of the HOD (3.37 ppm) and DMSO (2.5 ppm) lines.

2.4 ^{1}H NMR with ES peak suppression

Parameter sets: **awprotones (+ getprosol)**
Pulse programmes: **zgesgp**

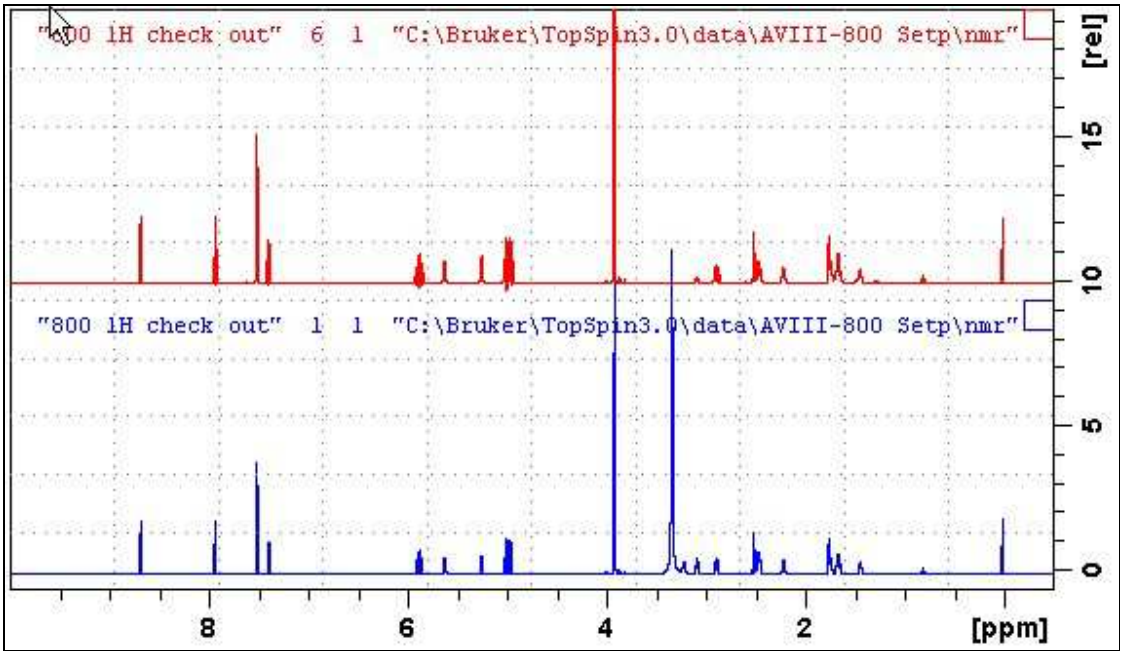
TD = 128 K, **SI** = 128 K.
SW = 20 ppm.

O1 = frequency in Hz of the F1 signal to be ES suppressed
= spectral window mid-point. Check **SW** is wide enough.
D1 = 2 sec or other time of your choice.

Type **ased** (enter) and review parameters used in the job. Verify gradients are OK.
Check **P12** = 2000 usec, **SPNAM1** = **squa100.1000**.

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

Process with **EFP** (applies **LB**).



Lower: ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: ^{1}H NMR spectrum with ES suppression of the HOD line at 3.37 ppm.

2.5 ^{1}H NMR with combined ES + CW presaturation on F1

Parameter set: **awprotonespr (+ getprosol)**
Pulse programmes: **awprotonespr**

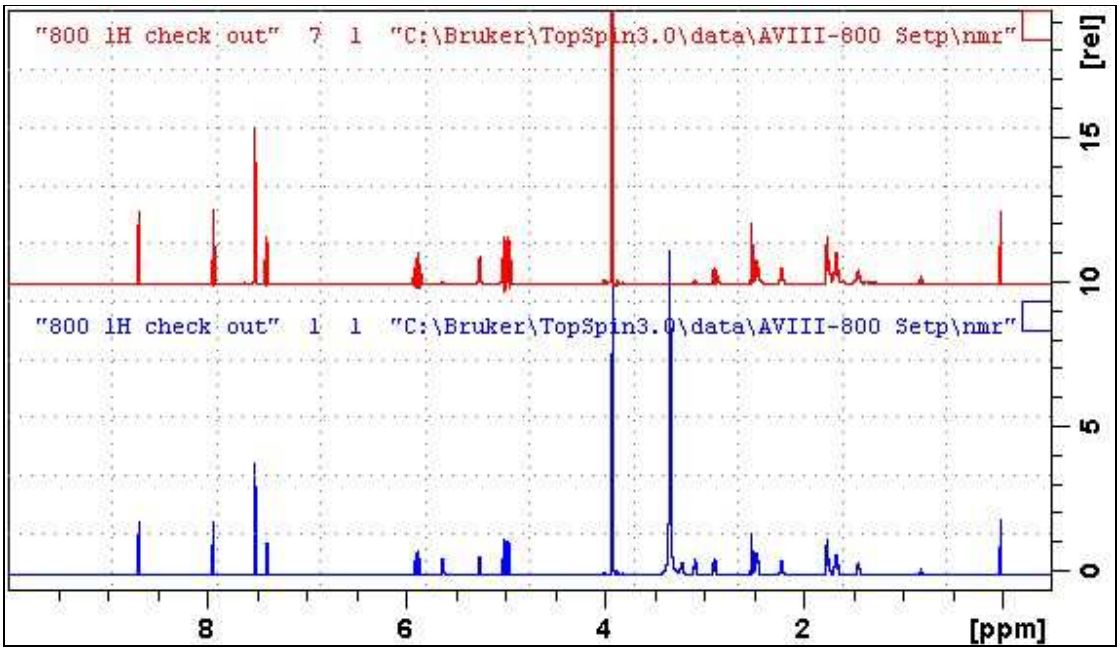
TD = 128 K, **SI** = 128 K .
SW = 20 ppm.

O1 = frequency in Hz of the F1 signal to be combined ES + CW presaturated.
= spectral window mid-point. Check SW is wide enough.
PL9 = F1 presaturation power applied during **D1**.
D1 = **2 sec** or other time of your choice.

Type **ased** (enter) and review parameters used in the job. Verify gradients are OK.
Check **P12** = **2000 usec**, **SPNAM1** = **squa100.1000**.

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

Process with **EFP** (applies **LB**).



Lower: ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: ^{1}H NMR with combined ES + CW presaturation of the HOD line at 3.37 ppm.

2.6 ^{1}H NMR with combined ES+CW presaturation on F1 + CW presaturation on F2

Parameter set: **awprotonesprf1prf2 (+ getprosol)**
Pulse programmes: **awprotonesprf1prf2**

TD =128 K, **SI** = 128 K.
SW = 20 ppm.

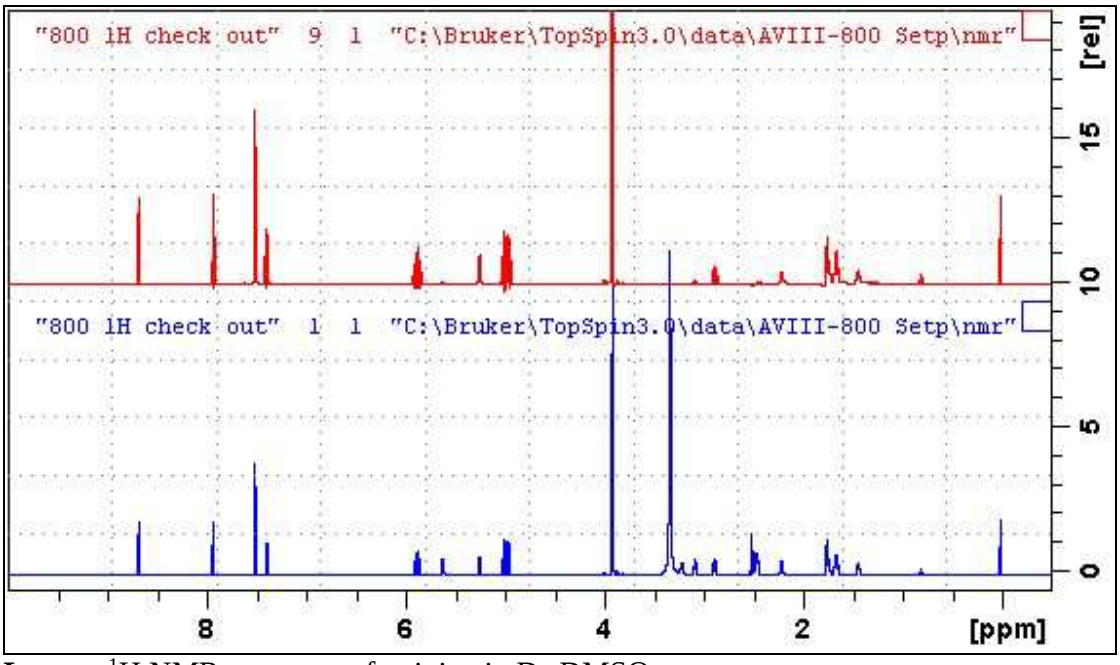
O1 = frequency in Hz of the F1 signal to be combined ES + CW suppressed
= spectral window mid-point. Check SW is wide enough.
O2 = frequency in Hz of the F2 signal to be CW presaturated.

PL9 = F1 presaturation power applied during **D1**.
PL21 = F2 presaturation power applied during **D1**.
D1 = 2 sec or other time of your choice.

Type **ased** (enter) and review parameters used in the job. Verify gradients are OK.
Check **P40** = 2000 usec, **SPNAM10** = **squa100.1000.**

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

Process with **EFP** (applies **LB**).



Lower: ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: ^{1}H NMR with combined ES + CW presaturation of the HOD line (3.37 ppm) on F1 and the DMSO line (2.5 ppm) on F2.

2.7 ^{1}H NMR with three peak ES+ dual CW presaturation

Parameter set: **awprotonesprf1prf2 (+ getprosol)**
Pulse programmes: **awprotonesprf1prf2**

TD = 128 K, **SI** = 128 K.
SW = 20 ppm.

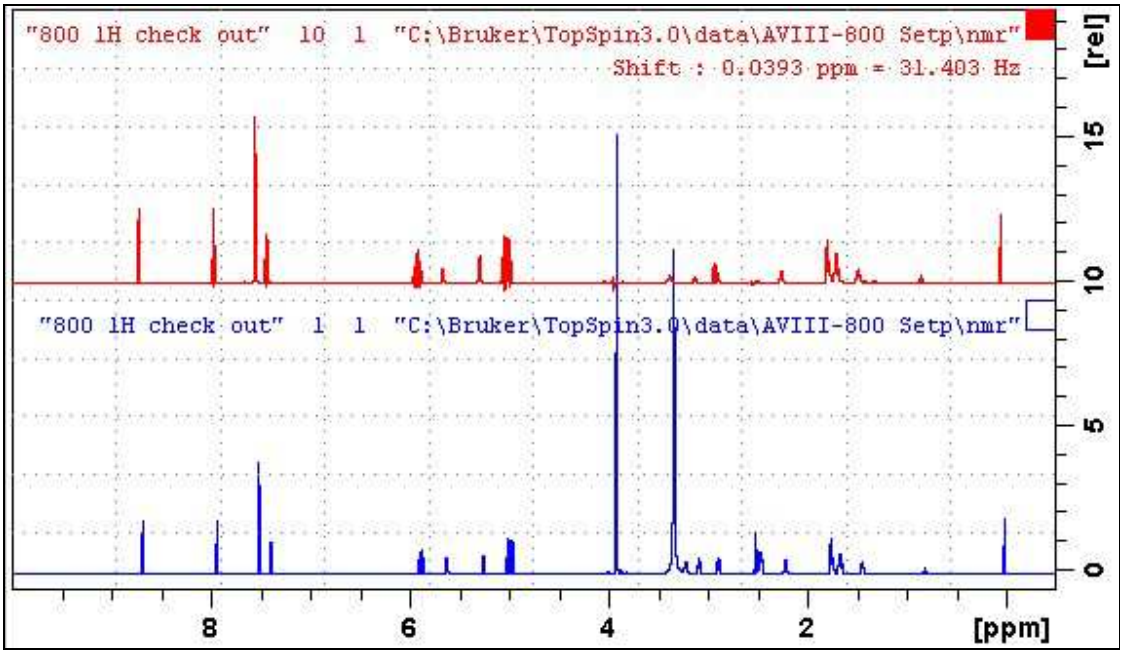
O1 = frequency in Hz of the F1 signal to be CW suppressed
= spectral window mid-point. Check SW is wide enough.
O1* = frequency in Hz of the F1 signal to be ES suppressed.
SPOFFS10 = **(O1*-O1)** Hz. **ES offset** from **O1** maybe a positive of negative value.
O2 = frequency in Hz of the F2 signal to be CW presaturated

PL9 = F1 presaturation power applied during **D1** (typically around 55 db).
PL21 = F2 presaturation power applied during **D1** (typically around 55 db).
D1 = 2 sec or other time of your choice.

Type **ased** (enter) and review parameters used in the job. Verify gradients are OK.
Check **P40** = **2000 usec**, **SPNAM10** = **squa100.1000.**

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

Process with **EFP** (applies **LB**).



Lower: ^{1}H NMR spectrum of quinine in D_6-DMSO.
Upper: ^{1}H NMR with CW presaturation on F1 of quinine's OCH_3 signal (3.89 ppm), offset ES suppression of the HOD line (3.37 ppm) and CW presaturation on F2 of the DMSO signal (2.5 ppm).