
KJM 9250

$^{1}$H NMR spectra on the AVI-600 and AVII-600

Version 5.0

Topspin 3.5 Windows 7
Topspin 1.3 Windows XP


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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 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 spectra with a 30, 45 or 90 degree pulse**

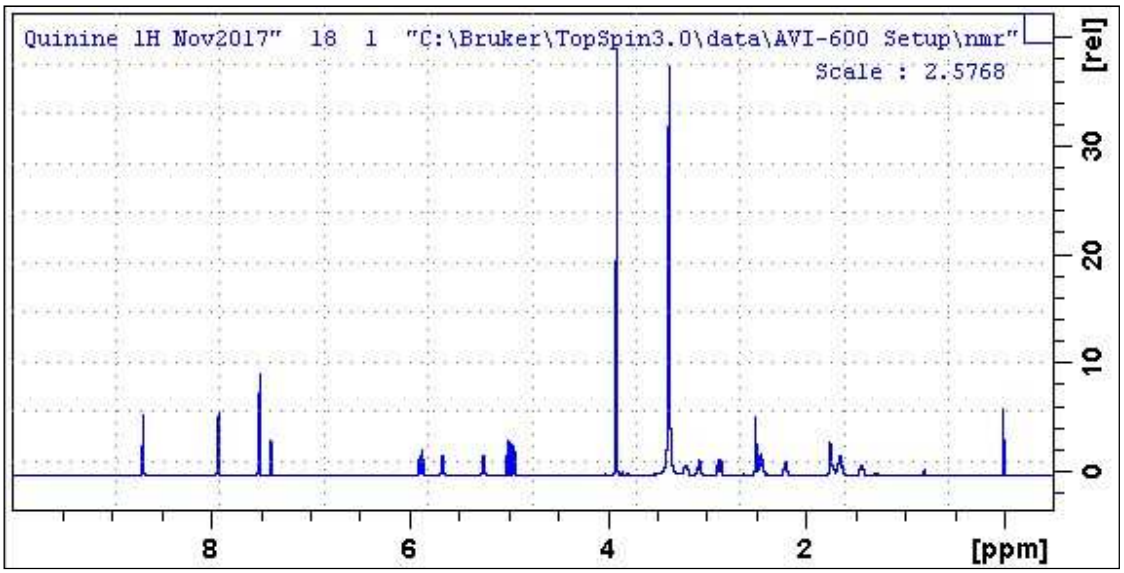
Parameter sets: **awproton30, awproton45, awproton90 (+ getprosol)**
Pulse programmes**: zg30, awzg45 or zg respectively**

**TD** = 64 K, **SI** = 64 K
**SW** = 16 ppm, **O1P** = 7.0 ppm.
**D1** = 1.5 sec or other time of your choice.
**NS** = any number, **DS =** 2, 4, 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**).



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

## 2.2 $^{1}$H NMR spectrum with CW presaturation

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

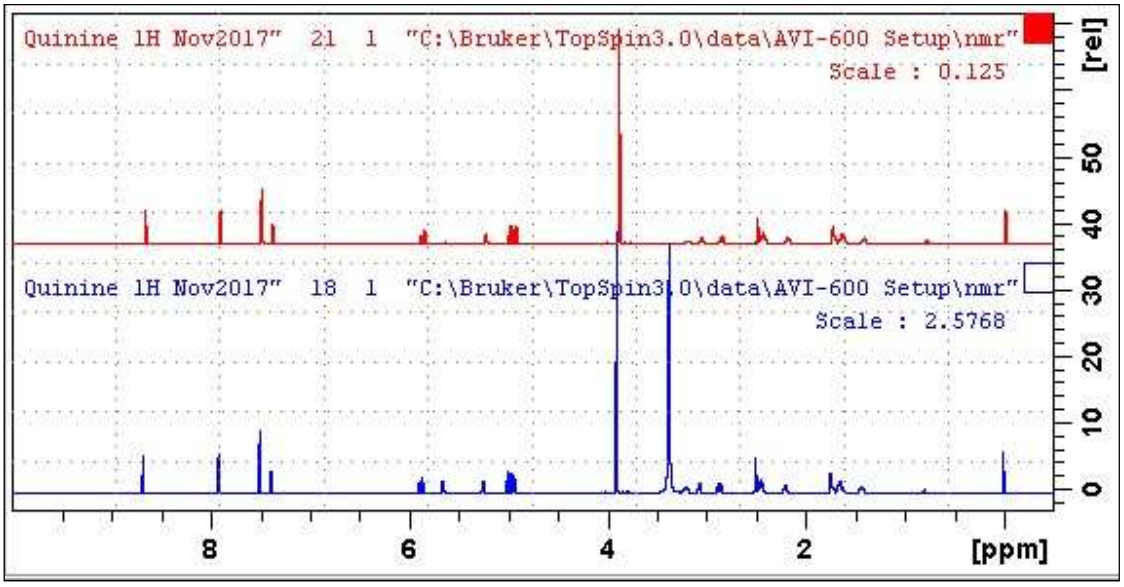
**TD** = 32 K or 64K , **SI** = 32 K or 64 K.
**SW** = 18 ppm.

**O1** = frequency in Hz of the F1 signal to be presaturated.
= spectral window midpoint. 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 **PL9** 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:** 600 MHz $^{1}$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 spectrum with dual CW presaturation

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

**TD** = 64 K, **SI** = 64 K.
**SW** = 18 ppm.

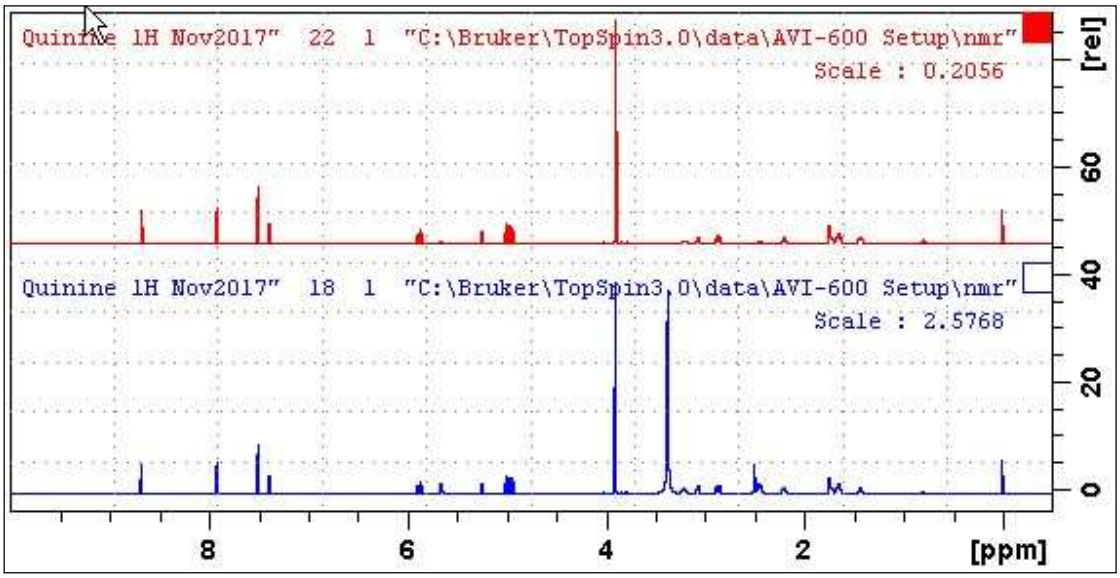
**O1** = frequency in Hz of the F1 signal to be presaturated.
= spectral window midpoint. Check **SW** is wide enough.
**O2** = frequency in Hz of the F2 signal to be presaturated.

**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 **PL2**1 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:** 600 MHz $^{1}$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 spectrum with ES peak suppression

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

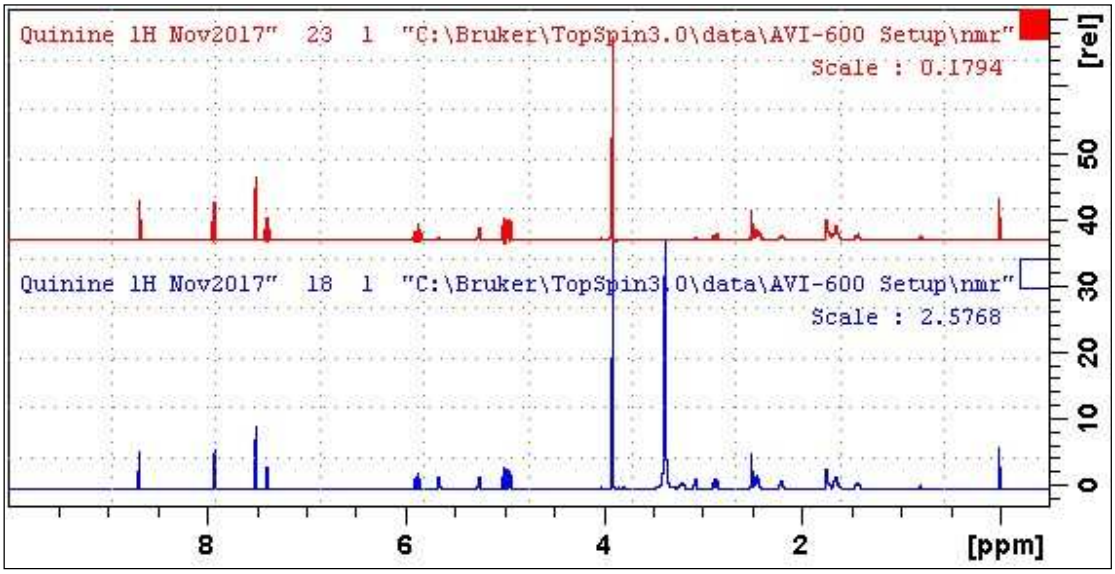
**TD** = 64 K, **SI** = 64 K.
**SW** = 18 ppm.

**O1** = frequency in Hz of the F1 signal to be ES suppressed.
= spectral window midpoint 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:** 600 MHz $^{1}$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 and CW presaturation on F1

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

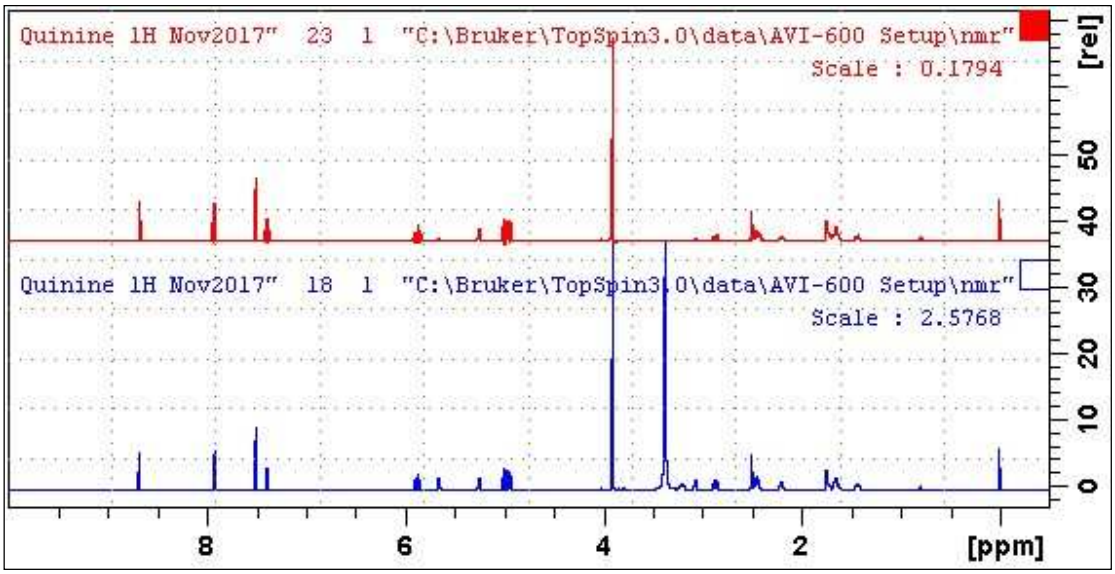
**TD** = 64 K, **SI** = 64 K.
**SW** = 18 ppm.

**O1** = frequency in Hz of the F1 signal to be ES suppressed.
= spectral window midpoint. 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:** 600 MHz $^{1}$H NMR spectrum of quinine in $D_6$-DMSO.
**Upper:** $^{1}$H NMR spectrum with combined ES and CW presaturation of the HOD line at 3.37 ppm.

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

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

**TD** =64 K, **SI** = 64 K.
**SW** = 18 ppm.

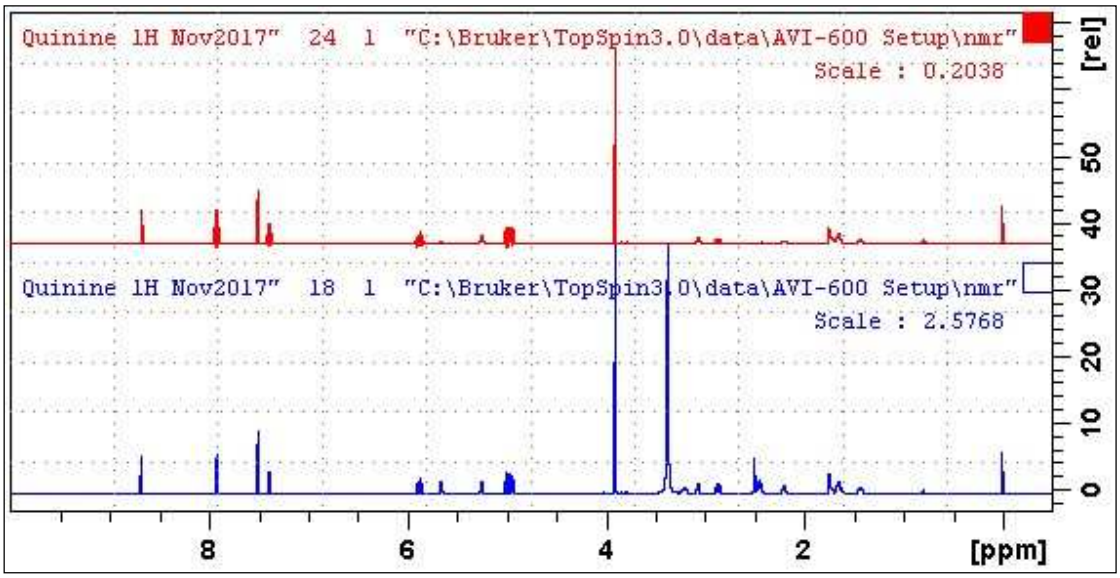
**O1** = frequency in Hz of the F1 signal to be combined ES + CW suppressed
= spectral window mid-point. Check SW is wide enough..
**O2** = frequency in Hz of the F2 signal to be CW presaturated.

**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:** 600 MHz $^{1}$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 spectrum with three peak ES + dual CW presaturation

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

**TD** = 64 K, **SI** = 64 K.
**SW** = 20 ppm.

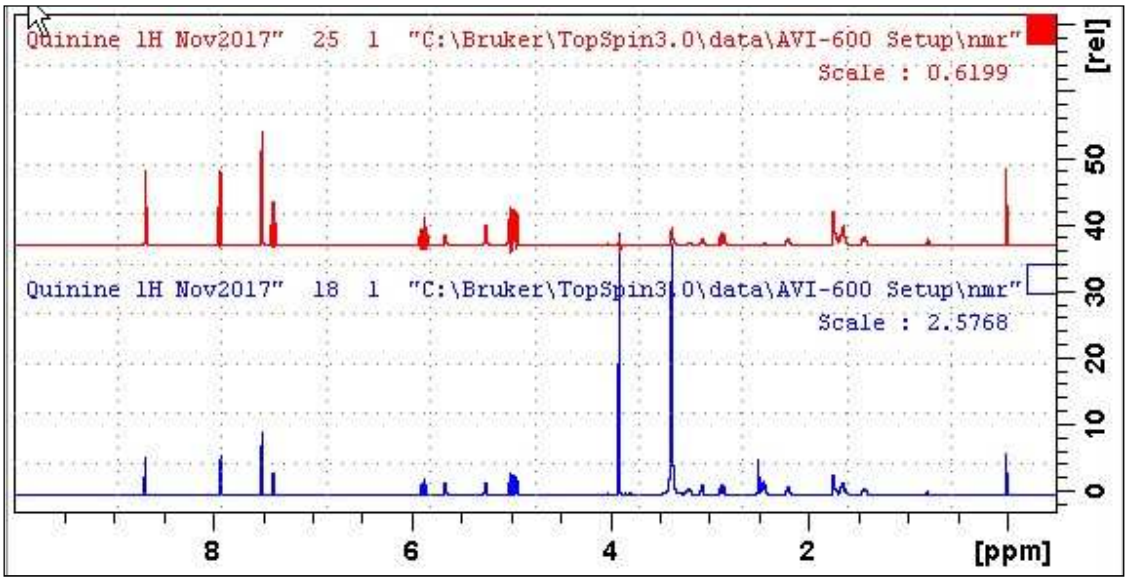
**O1** = frequency in Hz of the F1 signal to be CW suppressed.
= spectral window midpoint. Check SW is wide enough.
**O1*** = frequency in Hz of the F1 signal to be ES suppressed
**SPOFFS10** = **(O1*-O1)** Hz (may be a positive of negative value).
**O2** = frequency in Hz of the F2 signal to be CW presaturated.

**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:** 600 MHz $^{1}$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).