

Multiple signal suppression with presaturation using wavemaker software



Helena Kovacs, Eriks Kupce
Bruker BioSpin
Switzerland



The wavemaker syntax in the pulse program:



The WaveMaker syntax is incorporated into the pulse program:

```
;sp6:wvm: cw(1 s, PL ; B1max = cnst6 Hz) cw(1 s ; B1max = cnst7 Hz) ss = 2 us
```

suppression of the multiplet frequencies in the peak list **on-resonance (o1p) suppression of H2O**

This creates a multiple-signal selective pulse for the pulse program entry: **p18:sp6:f1**
where cnst6 and cnst7 are given by the user, the rest is set automatically by wavemaker.

cnst6: suppression bandwidth/power for the **individual off-resonance signals**. Typically 5-20Hz.
cnst7: suppression bandwidth/power for **on-resonance H2O signal**. Typically 35-50Hz.

p18: 1sec / in microsec / length of the suppression pulse
ss: step size, yields the number of digital points in the waveform = p18/ss. Typically 500000-1 Mio.
The higher the number of signals to suppress, the more digital points are needed for high selectivity.

Note that B1max = 5 Hz (or similar) is per each multiplet component, so the total power will depend on the number of frequencies in the peaklist. For example power corresponding to 5 peaks is 5x5Hz = 25Hz. To obtain the power in dB, use the TopSpin command: *pulse 25Hz*.

In case you run into the shape size limitations
Error message: maximum allowed number of points exceeded
set NPmax = 1000000 in wvm_globals which can be found in *TS/exp/stan/nmr/wavemaker* directory. By default NPmax = 64k.

Pulse program noesygppr1d.wvm:



store the pulse program, noesygppr1d.wvm in the directory:
<topspin home>/exp/stan/nmr/lists/pp/user

```
"I3=d1/p18"
```

```
1 ze
2 30m
  d12 p10:f1
  4u BLKGRAD
3 p18:sp6:f1 ph29
  4u
  lo to 3 times I3
  50u UNBLKGRAD
  p16:gp1
  d16 p11:f1
  p1 ph1
  2u
  p1 ph2
  d8
  p0 ph3
  go=2 ph31
  30m mc #0 to 2 F0(zd)
exit
```

Parameters for the suppression pulse:

I3:=4 for example, if d1=4sec and p18=1 sec,
the multiple suppression pulse is repeated 4 times
sp6: total suppression power. If number of peaks in the peaklist is 5, sp6= 5 times cnst6
spnam6: noesygppr1d.wvm_sp6.wv created by the wavemaker on the flight

```
ph1=0 2
ph2=0 0 0 0 0 0 0 2 2 2 2 2 2 2 2
ph3=0 0 2 2 1 1 3 3
ph29=0
ph31=0 2 2 0 1 3 3 1 2 0 0 2 3 1 1 3
```

```
;sp6:wvm: cw(1 s, PL ; B1max = cnst6 Hz) cw(1 s, PL ; B1max = cnst7 Hz) ss = 2 us
```

Au program to copy the peaklist:



The command *copyPL* with the extension *exp.no* converts the TopSpin peaklist, peaklist.xml, into WaveMaker format, PL_list, in the working directory.

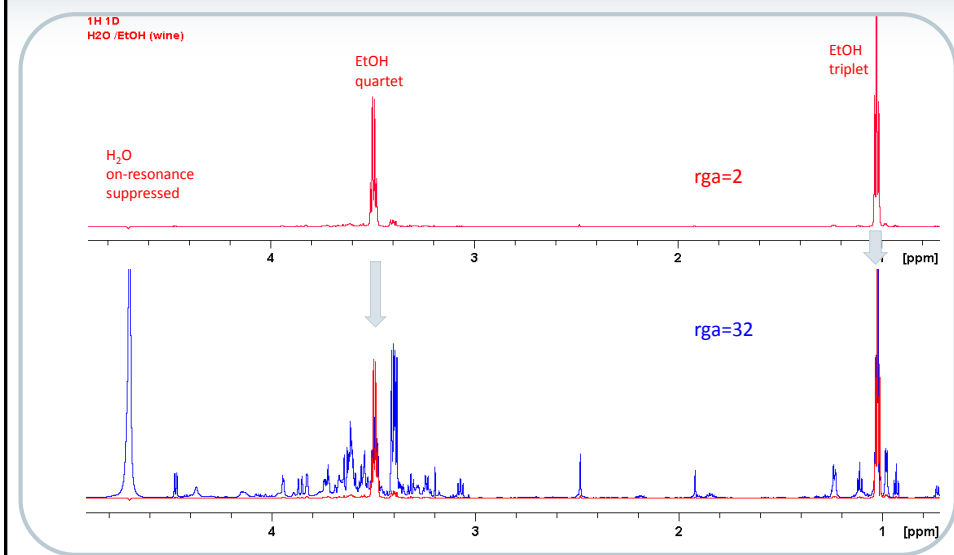
The au-program *copyPL* should be stored in the directory:
<topspin home>/exp/stan/nmr/au/scr/user

```
char sourcefile[256], targetfile[256];

sprintf(targetfile, "%s/%s/%d/PL.xml", disk, name, expno);
if(i_argc < 3) GETINT("Enter peaklist EXPNO:", expno)
else expno=atoi(i_argv[2]);
DATASET(name, expno, 1, disk, user);
sprintf(sourcefile, "%s/peaklist.xml", PROCPATH(0));
if ( (i1 = dircp (sourcefile,targetfile)) < 0 ) Proc_err (DEF_ERR_OPT, dircp_err(i1));
QUIT
```

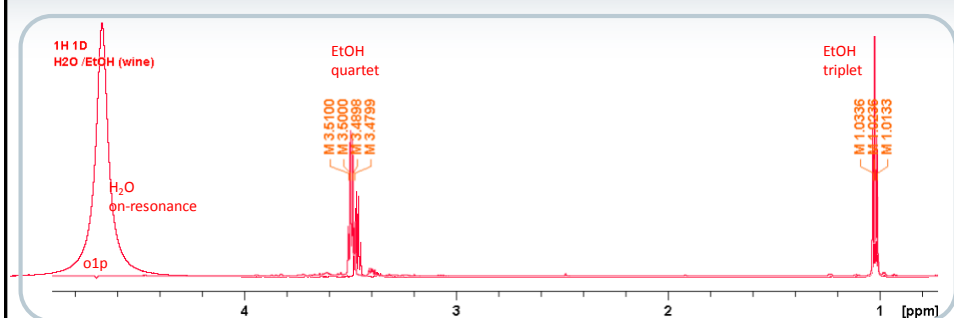
Example 1. H₂O/ ethanol

suppression of the H₂O broad, on-resonance, signal and 7 off-resonance ethanol, sharp multiplet components



Example 1, step 1. set-up H₂O/ EtOH suppression

suppression of the H₂O broad, on-resonance, signal and 7 off-resonance ethanol, sharp multiplet components

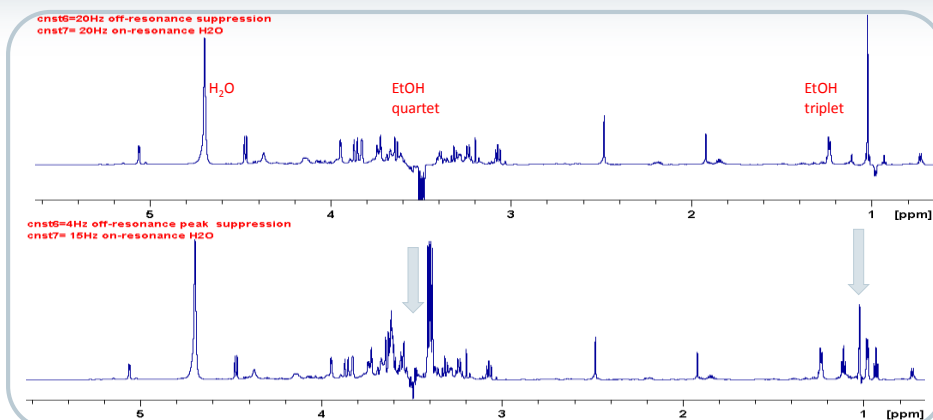


1. record a 1D spectrum
2. set o1p on-resonance for H₂O
3. pick peaks, each multiplet component separately (EtOH quartet and triplet = 7 peaks)
4. set-up a new experiment
5. convert peaklist with TopSpin command: `copyPL + exp.no of the peaklist experiment`
6. set cns6 = 20Hz (off-resonance EtOH multiplet component suppression)
7. set cns7 = 20Hz (on-resonance H₂O suppression)
8. create multiple selective pulse with the command: `wvm -a (pop-up information) or wvm -q (quiet)`
9. record a spectrum
10. optimize cns6 and cns7, increase receiver gain

Example 1, step 2. optimize H₂O/ EtOH suppression



suppression of the H₂O broad, on-resonance, signal and
7 off-resonance ethanol, sharp multiplet components

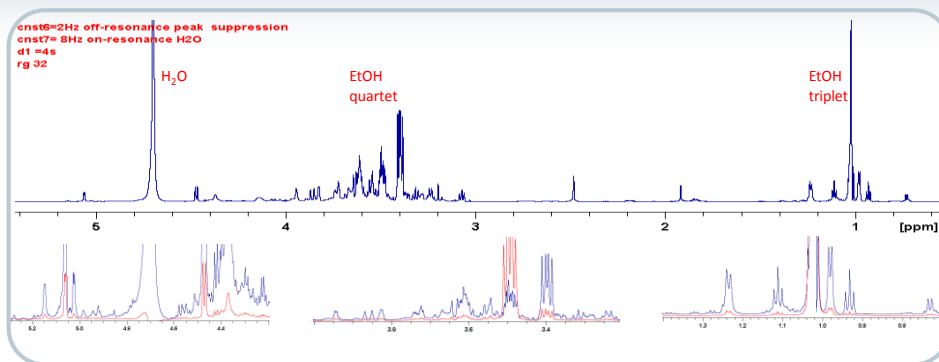


1. set-up a new experiment
2. change cns6 and cns7, increase receiver gain, if possible
3. convert peaklist with TopSpin commando: copyPL + exp.no where the peaklist is
4. create multiple selective pulse with the command: wvm -a (pop-up information) or wvm -q (quiet)
5. record a spectrum
6. repeat

Example 1. optimized H₂O/ EtOH suppression



suppression of the H₂O broad, on-resonance, signal and
7 off-resonance ethanol, sharp multiplet components

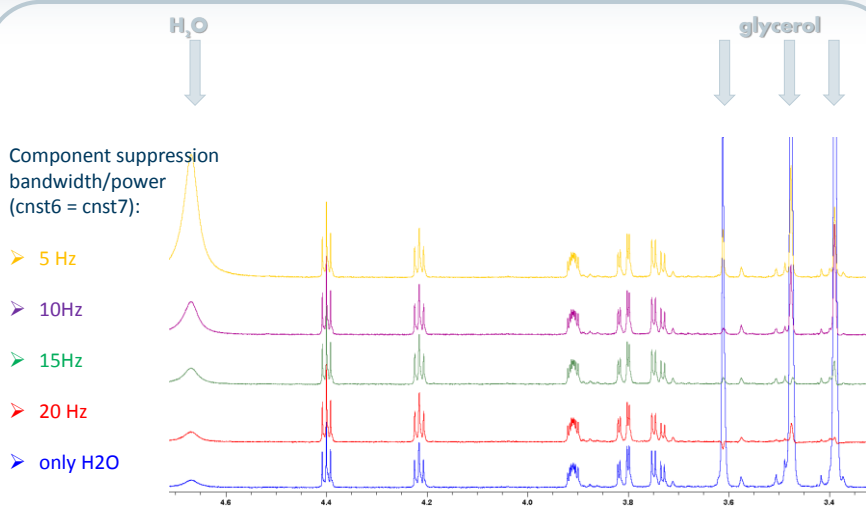


Remarks

- the goal is to be able to increase RG so that all weak signals become visible
- suppression should not bleach out signals close to the suppressed frequencies
- negative intensity indicates too strong suppression
- suppressed signals do not need to disappear, their intensity should be in the same range as the solvent peaks

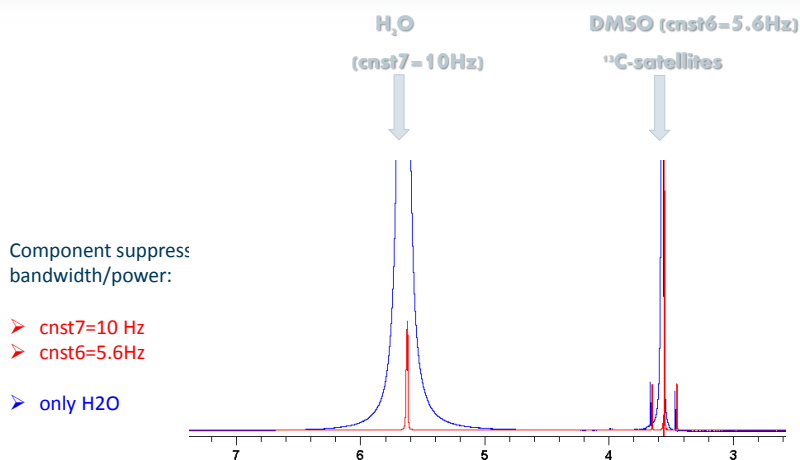
Example 2. suppression of peaks of similar intensity

H₂O/40% glycerol
suppression of 4 peaks of similar intensity



Example 3. suppression of peaks of different intensity

H₂O/DMSO
suppression of 2 peaks



Example 4. add soft decoupling of ^{13}C -satellites



$\text{H}_2\text{O}/\text{DMSO}$

suppression of 2 peaks and decoupling of ^{13}C -satellites with cw

➤ no ^{13}C -satellite decoupling

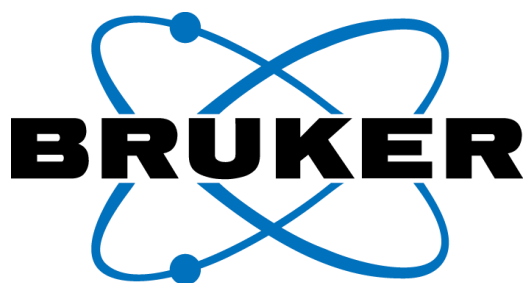
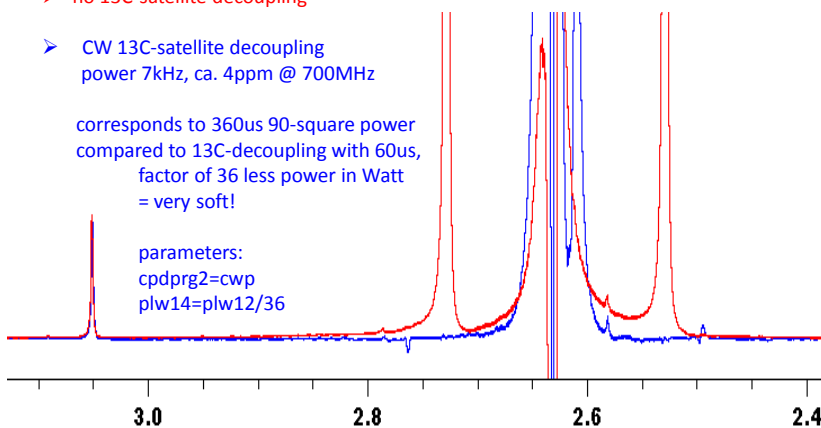
➤ CW ^{13}C -satellite decoupling
power 7kHz, ca. 4ppm @ 700MHz

corresponds to 360us 90-square power
compared to ^{13}C -decoupling with 60us,
factor of 36 less power in Watt
= very soft!

parameters:

cpdprg2=cwp

plw14=plw12/36



Innovation with Integrity

Thank you