# Solvent Suppression using TopSpin 3.x

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## Introduction

There are number of solvent suppression schemes used in NMR, and the technical details can become extensive. Here is a brief list [the two- (or more) letter code identifier in par and pp names]:

**presaturation** – often gives cleanest suppression, but removes exchangeable protons [**pr** or **ps**]
**noesy1d preset** – can provide cleaner baselines; used in many metabolomics studies [**pn**]
**purge preset** – a relatively new method of presaturation, often superior to standard preset [**purge**; **pp** is a purge pulse that is different]
**wet** – a prominent method used with mixed solvents (multiple-peak suppression); also reduces intensity of exchangeable protons [**wt** or **wet**]
**watergate** – various types exist, the basic requiring optimization but is high-quality [**wg**]
**3-9-19** – the most common wg variant; simple to optimize with no effect on exchangeable protons [**wg** or **19**]
**w5** – a relatively new wg variant similar to 3-9-19 [**w5**]
**excitation sculpting** – a high-quality method utilizing selective rf and gradients [**es**]

A significant issue with solvent suppression on Bruker spectrometers is which variants are available in the experiment you really need. **purge** may run great in a $^{1}$H 1d, but does not exist (currently) in tocsy or noesy 2Ds. All the following describe only how to obtain 1D $^{1}$H spectra. See cgf for more information about extension into 2D or other experiments. *Another issue is quantitative behavior. Presat, wet and watergate are good quantitatively (except for exchangeable protons with presat). Do not use noesy1d quantitatively. Until the shaped-rf is updated, do not use exct sculpting either.*

## A. *Initial Setup:*

1. Always start by acquiring a one-scan 1H spectrum.

   *It is not required, but best to run solvent suppression experiments on-resonance to the solvent peak. If you believe this is not optimal, find cgfry for further discussion.*

2. Put the solvent peak on-resonance by clicking  , left-click with the cursor in the middle of the solvent peak, then choose O1. Retake the one-scan 1H spectrum to verify that the peak is in the center of the spectrum.

   [Another, possibly simpler, method for going on resonance is to enter the shift of the solvent peak in the parameter **o1p**. This will not be as accurate, since it won't account for solution/temperature/etc variations in chemical shift.]

3. For many methods — watergate, wet, excitation sculpting — the above is sufficient. But for preset methods, it is best to optimize the **o1** (**o1p**) value by using the **gs** utility:

   a) **gs**↵
   b) click **offset**
   c) change **o1** by click on sliding scale above/below; wait 1 to 2 scans to see effect
   d) SAVE on best value; for most sequences here, **o1** (not **o2**, definitely not **o3**)

4. Copy parameter into a new expno using: **iexpno**

**B. *Presaturation:***

1. In the new expno, run **ased** and change the first parameter PULPROG to **zgpr** .
2. The critical new parameter is **PLW9**, which will perform a low-power cw pulse on-resonance. You can raise the power of this parameter to decrease the intensity of the residual signal, but setting it too high will damage the probe!

   **PLW9 ≤ 3 mWatts (≤ 0.003 in the 1st box on the ased screen)**
   **≥ 25 –dBW (value in 2nd box on the ased screen should ≥ 25)**

3. Run **rga** prior to doing **zg** .
4. Take new data with **ns = 4×i** and **ds = 2×j** (i,j = 1,2,4,8,…).
5. zgcppr and zgcpgppr are two variants using composite pulse. So, cgf's experience does not recommend these (but zgcpgppr is the better of the two).

**C. noesygppr1d *Presaturation:***

1. Do the same steps above, but read in the Bruker parameter set **watersup** . I.e., do

   **rpar WATERSUP all**

2. Change **o1** or **o1p** to match the value found in A.2.
3. Run **rga** prior to doing **zg** .
4. Take data with **ns = 8×i** and **ds = 4×j** (i,j = 1,2,4,8,…).
5. PLW9 again might be smaller than optimal. Same conditions apply as in B.2.

**D. purge *Presaturation:***

1. Do the same steps above, but read in the UWchem parameter set ***probe*_1Hpurge** . I.e., do

   **rpar *probe*_1Hpurge all**

2. Change **o1** or **o1p** to match the value found in A.2.
3. Run **rga** prior to doing **zg** .
4. Take data with **ns = 1×i** and **ds = 2×j** (i,j = 1,2,4,8,…).

**E. watergate 3-9-19 *suppression:***

1. Do the same steps above, but read in the Bruker parameter set **P3919GP** . I.e., do

   **rpar P3919GP all**

2. Change **o1** or **o1p** to match the value found in A.2.
3. Change **d19 = 180μs** . The spectrum will have "nulls" in peak intensities (excitation profile) at 1/(2×d19), so this is a critical parameter. 180μs works well at 500 MHz (nulls at ±5.5 ppm from spectrum center).
4. Run **rga** prior to doing **zg** .

5. Take data with **ns = 8×i** and **ds = 4×j** (i,j = 1,2,4,8,…).

**F. watergate w5 *suppression:***

1. Do the same steps above, but read in the Bruker parameter set **P3919GP** . I.e., do

   **rpar P3919GP all**

2. Run **ased** and change the first parameter PULPROG to zggpw5.
2. Change **o1** or **o1p** to match the value found in A.2.
3. Change **d19 = 180μs** [see comments in section E.3 above]
4. Run **rga** prior to doing **zg** .
5. Take data with **ns = 8×i** and **ds = 4×j** (i,j = 1,2,4,8,…).

**G. *excitation sculpting:***

1. Do the same steps above, but read in the Bruker parameter set **P3919GP** . I.e., do

   **rpar ZGESGP all**

2. Change **o1** or **o1p** to match the value found in A.2.
3. Have to figure out how to get away from the rectangular selection pulses (these will produce "weird" peak intensities rippling throughout the spectrum)**!!**
4. Run **rga** prior to doing **zg** .
5. Take data with **ns = 8×i** and **ds = 4×j** (i,j = 1,2,4,8,…).

**H. *Multiple-peak solvent suppression:***

1. Take a 1-scan proton spectrum as described in section A.
2. Integrate the solvent peaks to be suppressed in the proton spectrum, and **Save As… reg** : see section B of the notes at:

   http://www.chem.wisc.edu/~cic/nmr/Guides/Ba3vug/HW637/HW5_Av400-sel1DbyTopSpin.pdf

3. click on: **CREATE DATASETS**

   and choose either preset or wet toward the bottom of the list.