

Adiabatic decoupling for $^1\text{H}\{^{19}\text{F}\}$

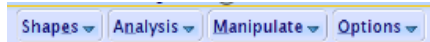
- [best: get **zghfigqn.adia.UW** from us] Use pulse sequence (pp) **zghfigqn.adiabatic**. Copy to new file since it has to be changed.
- [best: get **zghfigqn.adia.UW** from us] In the new pp file change: **sp15** to **sp31** and **p15** to **p63** for channel F2. Double check that this is correct for your probe using the Relations.info file located in folder /opt/topspin3x/exp/stan/nmr/lists/pp. Our relations file as of 2015Oct12 reads as follows:

```
;SH[12](F2) default+triple+triple2+ triple_na      sp31:f2 – shaped pulse 180 degree
                                                    (adiabatic decoupling)
```


```
;SHPW[12](F2) default+triple+triple2      p63:f2 channel - 180 degree shaped pulse
                                                    (adiabatic decoupling)
```

- Note: **p112** arguments (on F2) in pp are from composite pulse decoupling and are not used for adiabatic decoupling. They likely can be removed from the pp.
- For the following steps, there must be a 90° pulse calibration in edprosol for ^{19}F on the “decouple” channel. If one is not in your edprosol, it may be sufficient to copy in the calibration from the “observe” channel. Calculations of the adiabatic shapes rely on this decouple pw and power.
- Open shapetool (**stdisp**).

- From the flow bar:



choose: shapes → adiabatic shapes → smoothed chirp .

- Fill in all required parameters: size of shape, total sweep-width, length of pulse and % smoothing.
- One can also open a similar shape through  and change parameters.
- Create 3 pulses using shapetool:

```
crp32,1.5,20.2; crp48,1.5,20.2 and crp64,1.5,20.2 .
```

These read as:

Chirp adiabatic pulse

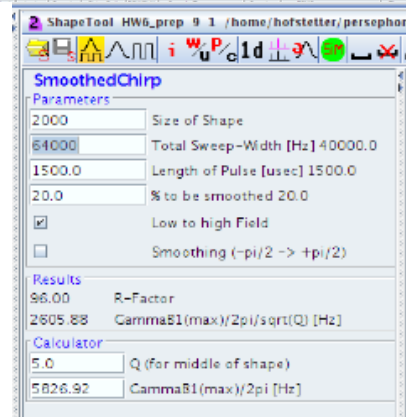
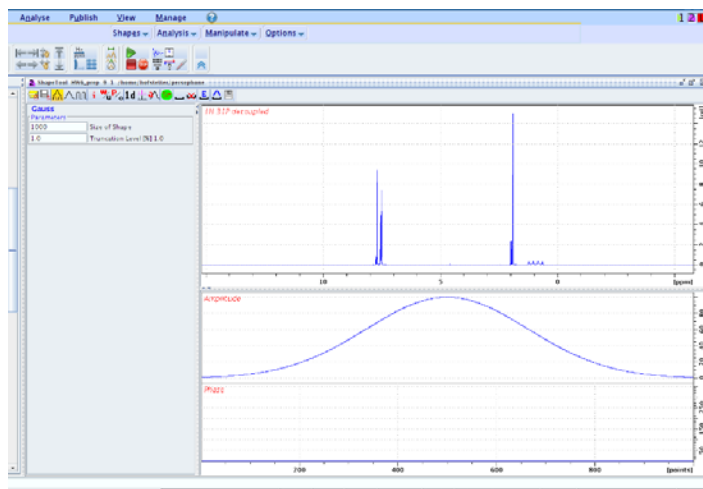
xx kHz – bandwidth in kHz

yy ms – length of pulse in ms

zz – % smoothing

.n – size of shape as $n \times 1000$ points

- Save under the above names in the /user folder.
- *Always(!)* do an **nmr_save** in TopSpin before editing the prosol table.




- Add adiabatic pulses to prosol table (type **edprosol** to open table).

Choose “observe” ^1H and “decouple” ^{19}F as nucleus from dropdown menu and click on the shape pulse tab. The adiabatic pulse needs to be added in position 12 according to the Relations.info file.

The screenshot shows the 'edprosol' software window. At the top, there are dropdown menus for 'Observe' (set to ^1H) and 'Decouple' (set to ^{19}F). Below these are fields for 'Observe Comment' and 'Decouple Comment'. The main area is a table with columns for 'Observe' and 'Decouple' pulses. The table contains 20 rows of pulse parameters. Row 12 is highlighted and contains an 'adiabatic decoupling' pulse with a pulse length of 1500 μs and a power level of 4.0057 W.

	Observe	Decouple			
	Filename	Filename			
	PuW[μs]	PuW[μs]			
	Pw[W]	Pw[W]			
	#				
selective excitation	Gaus1_270.1000	selective excitation			0
select. inversion/refocussing	Gaus1_180r.1000	select. inversion/refocussing			1
bandsel. excitation	Q5.1000				2
bandsel. inv./refoc.	Q3.1000				3
off-resonance presat. (p-power)	Squa100.1000				4
90° flip back (H ₂ O)	Squa100.1000				5
2nd 90° flip back (H ₂ O)	Sinc1.1000				6
90° WET	Sinc1.1000				7
120° NH region	Pc9_4_120.1000				8
180° NH region I	Ranob.1000				9
90° NH region I	Pc9_4_90.1000				10
90° NH region I timerev.	Pc9_4_90.1000				11
180° NH region II	Reburp.1000	adiabatic decoupling	Crp64.1.5.20.2	1500.00	4.0057
90° NH region II	Eburp2.1000				13
90° NH region II timerev.	Eburp2tr.1000				14
180° broadband	Bp720.50.20.1				15
cleanex 90° (H ₂ O)	Gaus1_90.1000				16
cleanex 180° (H ₂ O)	Gaus1_180r.1000				17
z-spoil (adiabatic)	Crp80.20.20.10				18
180° H1' (max.)	Reburp.1000				19
					20

- Click on the dots  next to the 2nd column (“decouple” filename) and choose the shaped pulse you made. Add the pulse description “adiabatic decoupling” to the first column in the popup. In the 3rd column (PuW [μs]) add 1500 μs as pulse length. The power level (Pw [W]) will be calculated.
- Save the pulse description in the first column by clicking Edit → Save Pulse Descriptions.
- Then save the pulses using File → Save. This requires the administrator password. If it asks for ^{19}F or Generic, do not check Generic!
- Load a standard $^1\text{H}\{^{19}\text{F}\}$ parameter set (e.g., zghfigqn30.2) and change the pp to zghfigqn.adia.UW. Check ased and make sure that the adiabatic pulses and power levels are correctly imported.
- Run spectrum.

