UNIVERSITY OF CAMBRIDGE
Department of Chemistry

(Heteronuclear) Decoupling
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greenimpact Silver Award

Athena SWAN Silver Award

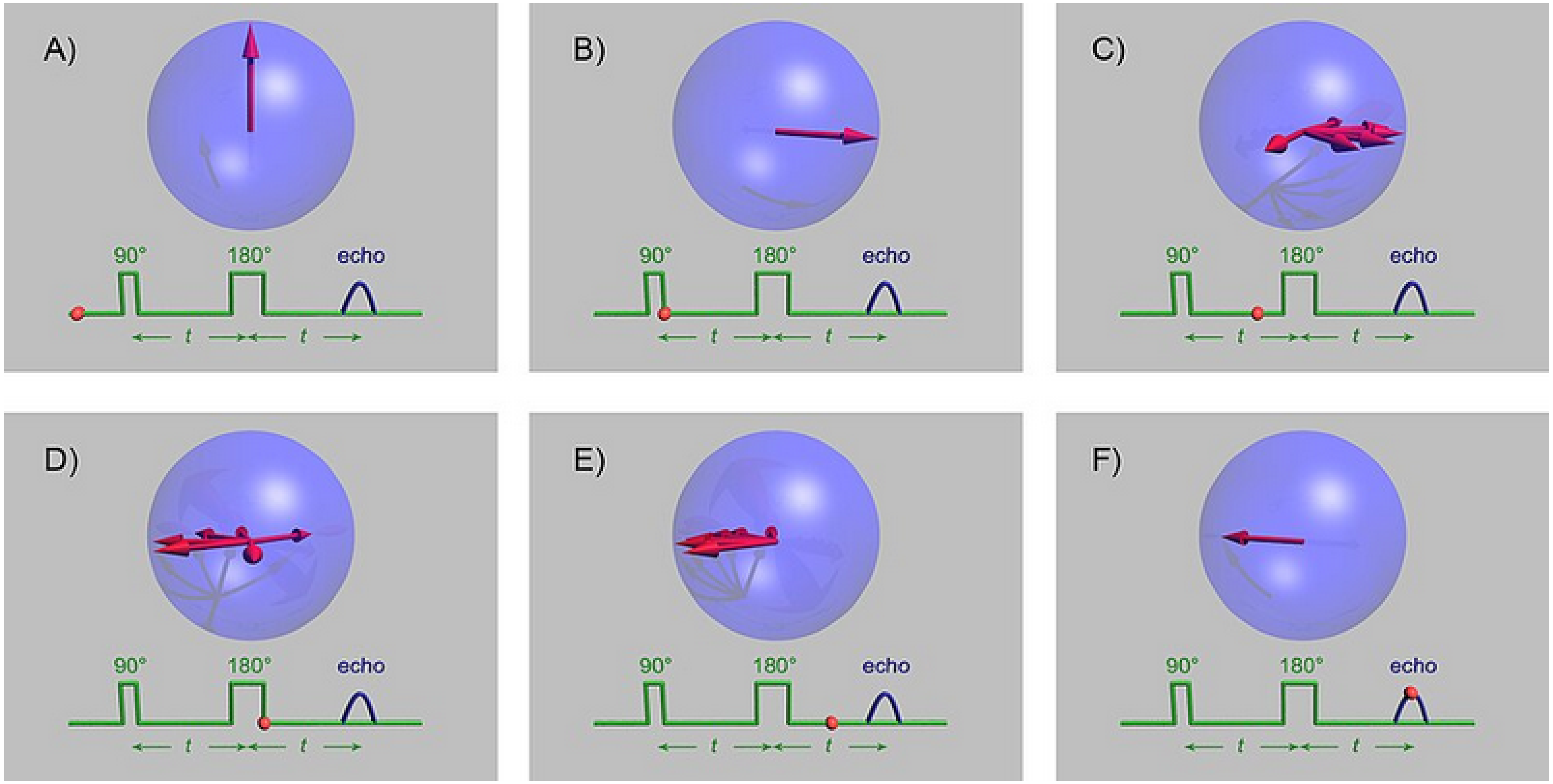
Outline

- Basic theory
  - Inversion elements, supercycles
- Imperfections
- Overview of common schemes
- Modifying setup
- BUSS
- Hardware / heating limitations
- 2H decoupling

What is decoupling?

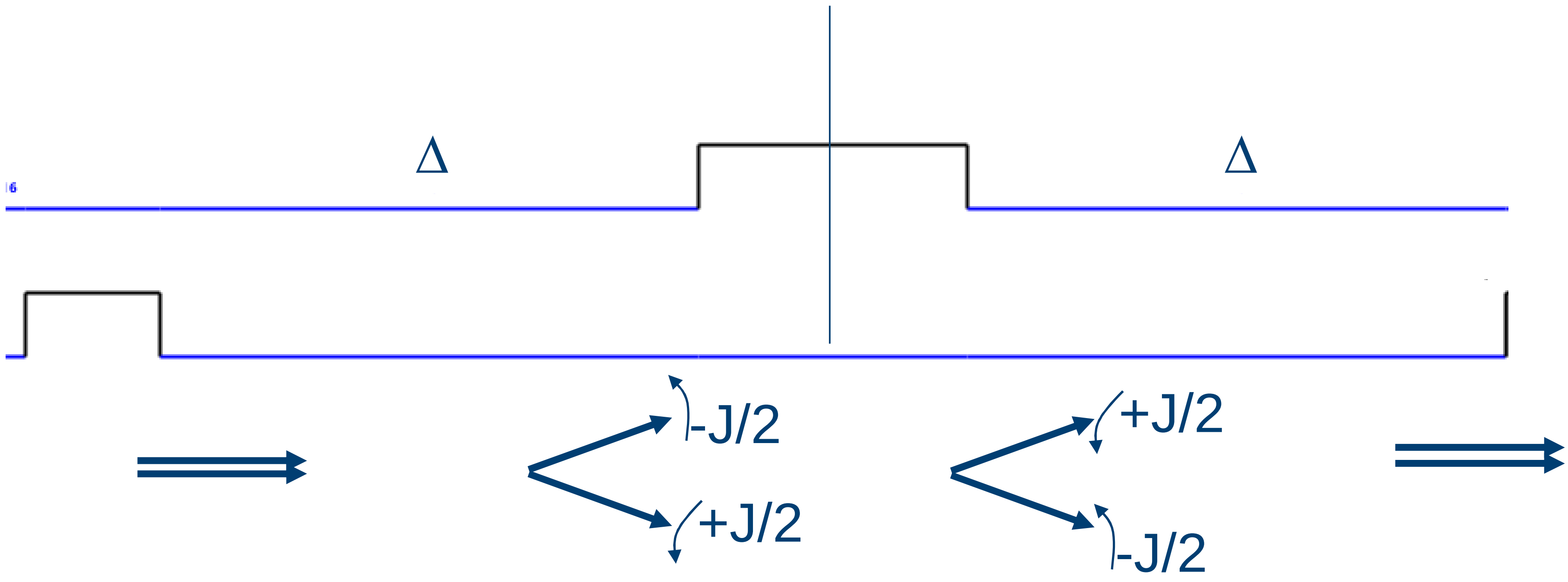
https://en.wikipedia.org/wiki/Spin_echo

- Spin echo:



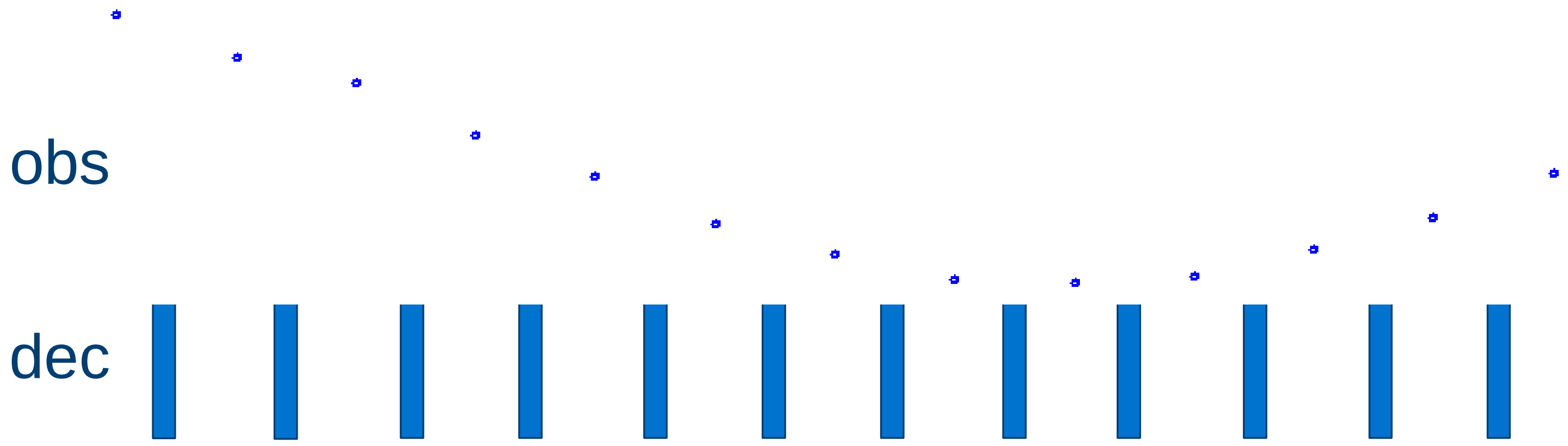
What is decoupling?

- We can remove the effect of heteronuclear coupling over a period, by inserting 180 degree (inversion) pulse in the centre:

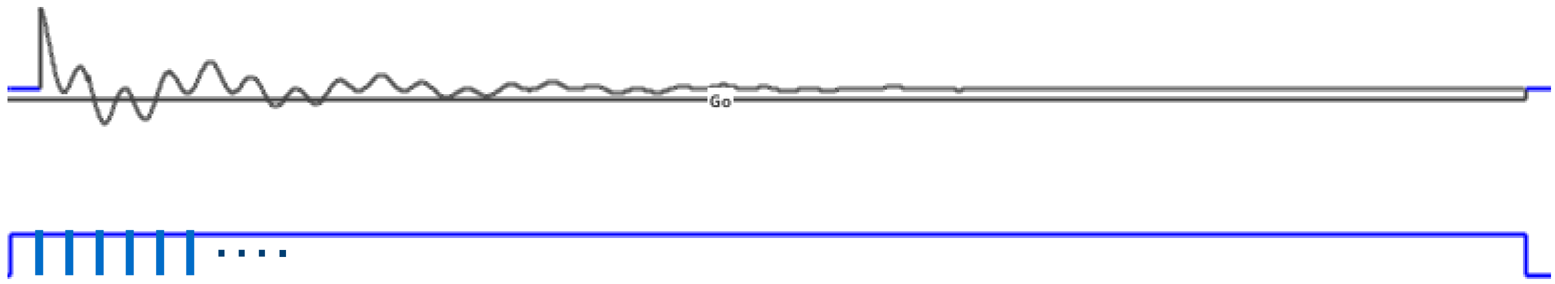


What is decoupling?

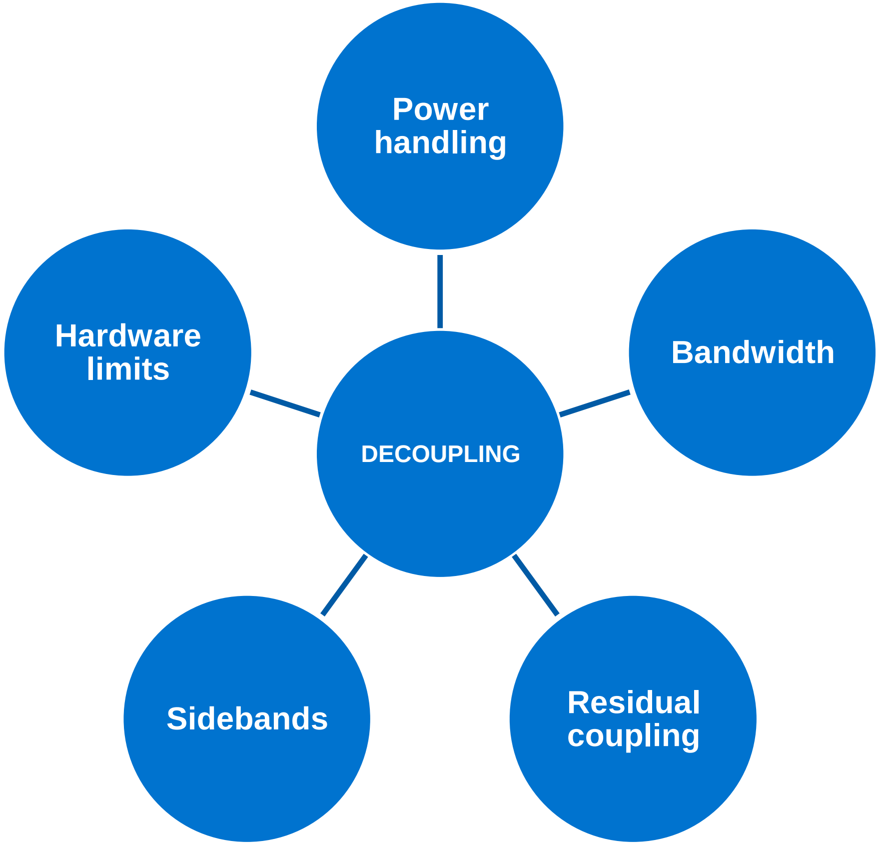
- Apply 180 degree pulse half way between each sampling point:



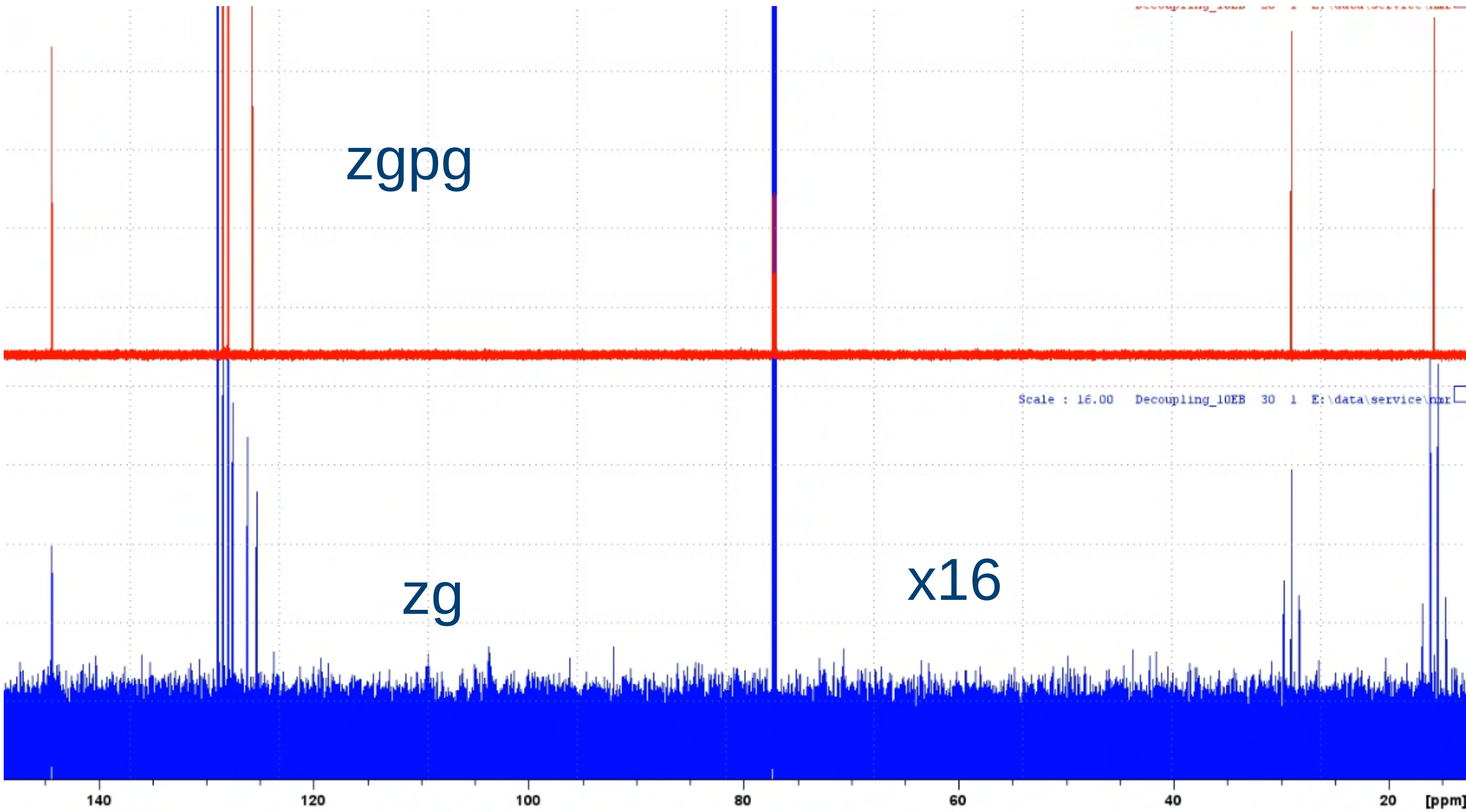
- Or: just apply a continuous sequence of 180 degree pulses…



Evaluating decoupling



Why decoupling?



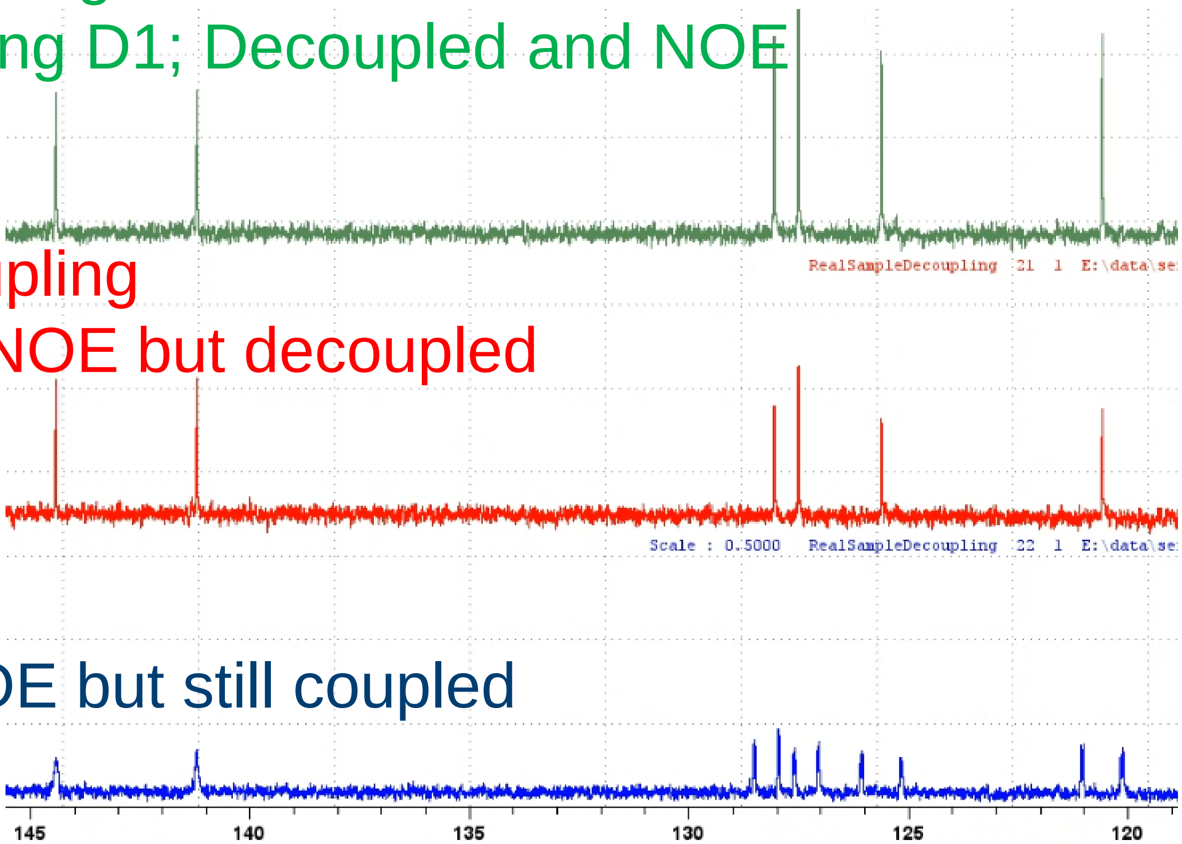
Gated decoupling

- When do we need to apply decoupling?

Power-gated decoupling
Reduced power during D1; Decoupled and NOE
zgpg

Inverse-gated decoupling
During D1 only; No NOE but decoupled
zgig

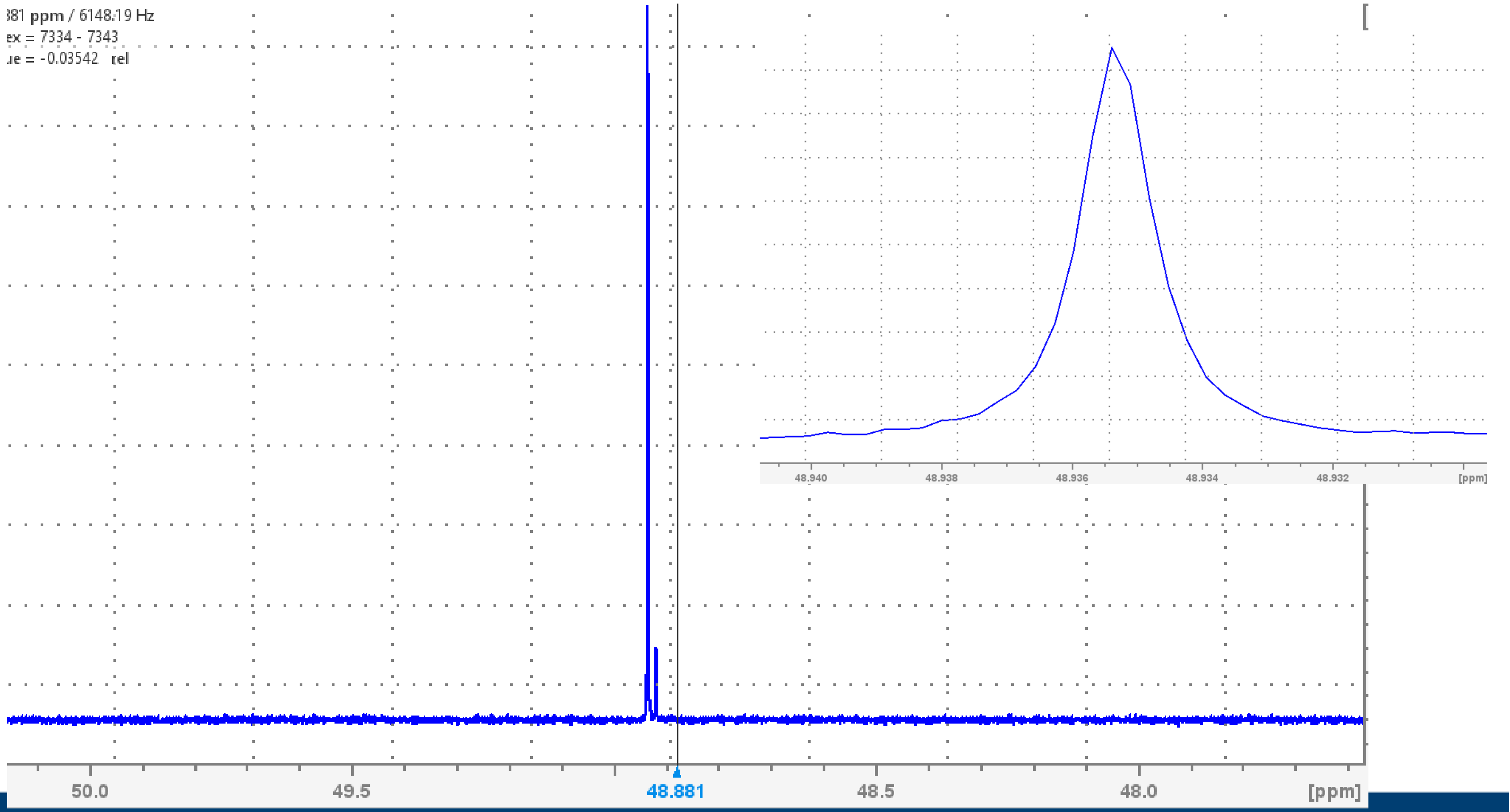
Gated decoupling
During D1 only; NOE but still coupled
zggd



CW decoupling works

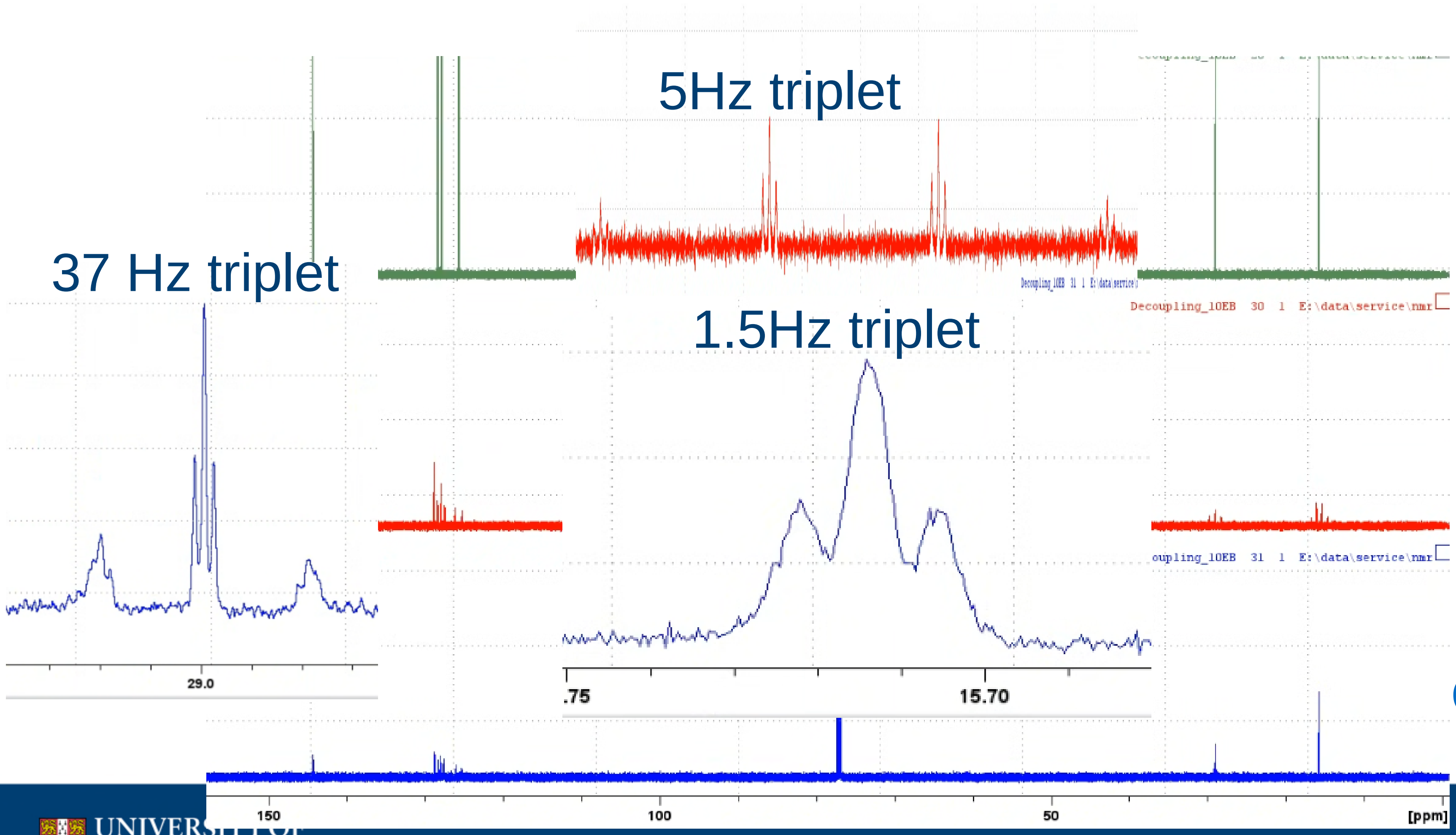
- 13C methanol

Peak[ppm]= 48.9354, Width[Hz/ppm]= 0.162/ 0.0013,



CW decoupling works… sort of

- 10% EB: If we set the decoupler offset on res for methyl protons for example:



Units

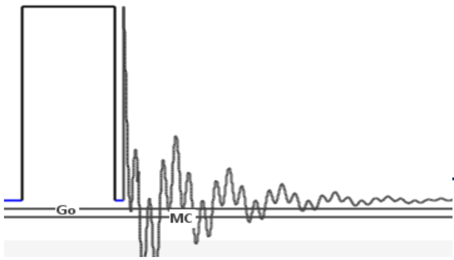
- **Amplitude / RF field strength / B1 / B2**
- Voltage
- RF field strength = 1/360
  - Eg 10us 90 = 40us 360 = 25kHz

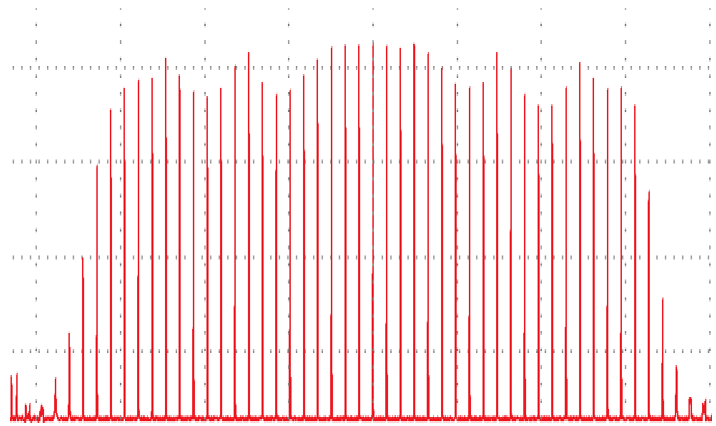
Units

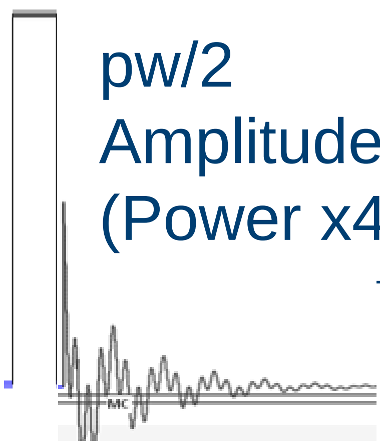
- **Power: PLW / PLdB**
- Wattage – $\propto$ to **square** of voltage
- **Pulse length *2 == Power /4**
- dB – **Attenuation** on Bruker systems
  - dB1 – dB2 = 10 log(PLW2/PLW1)
  - +6.02dB means factor 2 longer pulse
- “-dBW” = -10 log (PLW)
- Decoupling limits: integral power / time

P1 [µsec]	11.210		F1 channel - high power pulse
PLW1 [W, dB]	8.2	-9.14	F1 channel - power level for pulse (default)

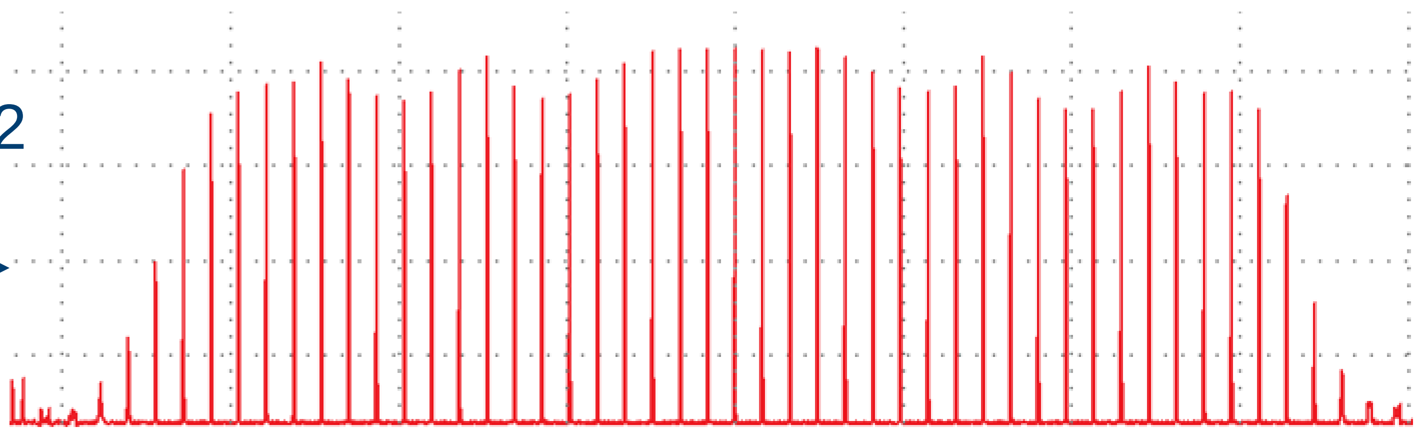
Scaling of pulses







pw/2
Amplitude x2
(Power x4)



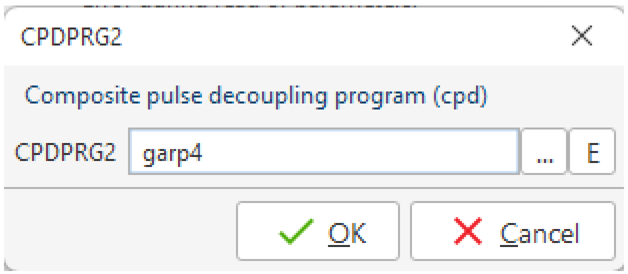
Bandwidth x2

Scaling of pulses

- For a given shape (inc adiabatic!), to double the bandwidth:
  - Double the RF field strength
  - Ie 4x the RF power. -6.02dB attenuation
  - Half the pulse length
- For adiabatic shapes:
  - Make a new shape with double the sweep
  - Keep same length
  - Need only double the RF power
  - (you can sort of do this for arbitrary shapes)

Implementation

- Bruker: “CPD program”




```
1 pcpd*0.339:0
  pcpd*0.613:180
  pcpd*2.864:0
  pcpd*2.981:180
  pcpd*0.770:0
  pcpd*0.691:180
```

```
  pcpd*0.593:180
  jump to 1
```

- Bruker: pulse program:

```
2 30m do:f2
  10u pl13:f2
  d11 cpd2:f2
  DELTA
  4u do:f2
  10u pl12:f2
  100m cpd2:f2
  p1 ph1
  go=2 ph31
  30m do:f2 pl13:f2 mc #0 to 2 F0(zd)
```

Hardware limitations

- Power corrupts!
- Limitation is something like average input power over each scan
- Cryoprobes: typical pulses (assumes 1s D1)

	5 mm 600 MHz TCI H&F-C/N-D CryoProbe™	
^{1}H		
hard pulse [3] (max. length 1ms)	8.0 µs	
hard pulse for lossy samples	Power level corresponding to 8.0 µs pulse for non-lossy sample	
trim pulse p28 [4]	1 ms @ 8 µs 2 ms @ 10 µs	
TOCSY spin lock [5]	200 ms @ 25 µs 400 ms @ 35 µs	
ROESY spin lock	Up to CW for power level corresponding to a 80 µs pulse	
WALTZ65 decoupling during ^{13}C-detection	Up to CW for power level corresponding to a 80 µs pulse	==3125Hz
DIPSI2-decoupling in triple resonance	400 ms @ 35 µs	==7143Hz
^{13}C		
GARP4 decoupling [7]	250 ms @ 55 µs (> 165 ppm bandwidth)	==4545Hz

Prodigy Cryoprobes

- Much less robust the He-cooled
- No comparable method of monitoring coil
- => stick to published limits!

Hardware limits: RT probes

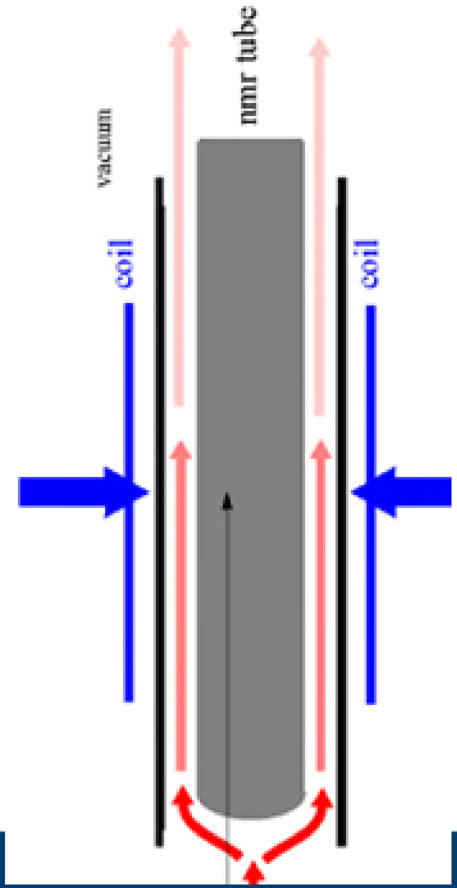
- Much less well documented…
- However: CW limit (5mm rt probes): **5W (pref. 1W)**

13C		
GARP decoupling [7)]	100 msec @ 55 µsec	100 msec @ 55 µsec

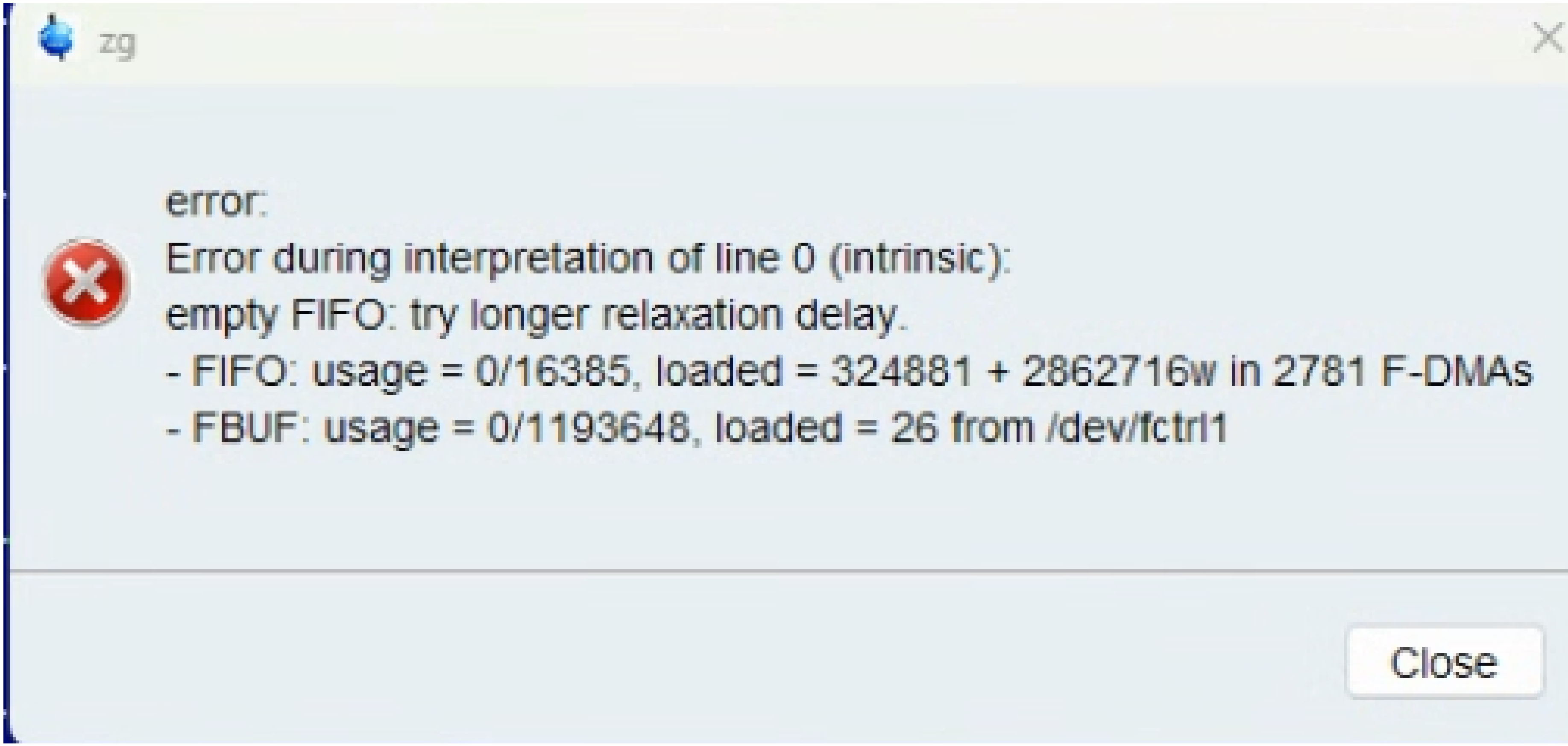
>5W@500MHz, ~10W@800MHz

Salty samples

- In cryoprobes coil is thermally insulated from sample
- E-field of pulse interacts with conductive samples
- Increased pulse length
- Absorption of energy by sample=> heating
- => small diameter tubes
- => lower power decoupling?



Hardware limitations – shaped pulses



Hardware limitations – shaped pulses

- On AVIIIHD (and older) spectrometers, waveform memory is a limitation
- Exact limitations depend on the exact spectrometer, but 3 cases:
- **1) shapes with <75ns per time point have to fit into the FIFO buffer.**
    - This buffer is small and you can't do decoupling in this regime.
- **2) shapes with ~ <3us/point: everything must fit into waveform memory**
    - Limit is total number of time slices
    - Shorter time slice means shorter max dec period
- **3) shapes with ~ >3us/point : no limit unless complex pulse sequence**
    - May sometimes need to make the time slices longer

Explicit decoupling allows longer aq..

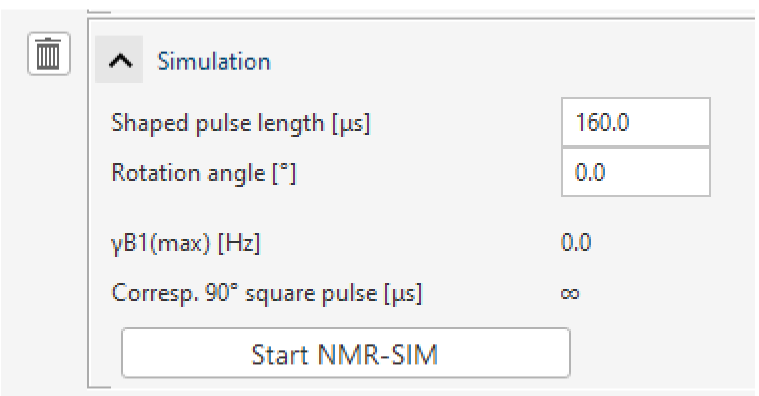
```
"l31=(nsdone+ds)%4+1"

d1

p1 ph1

ACQ_START(ph30,ph31)

2u DWELL_GEN:f1

3 (p63*0.5:sp14 ph21):f2

  lo to 3 times l31

4 (p63:sp31 ph21):f2

  (p63:sp31 ph23):f2

…

  lo to 4 times l1
```

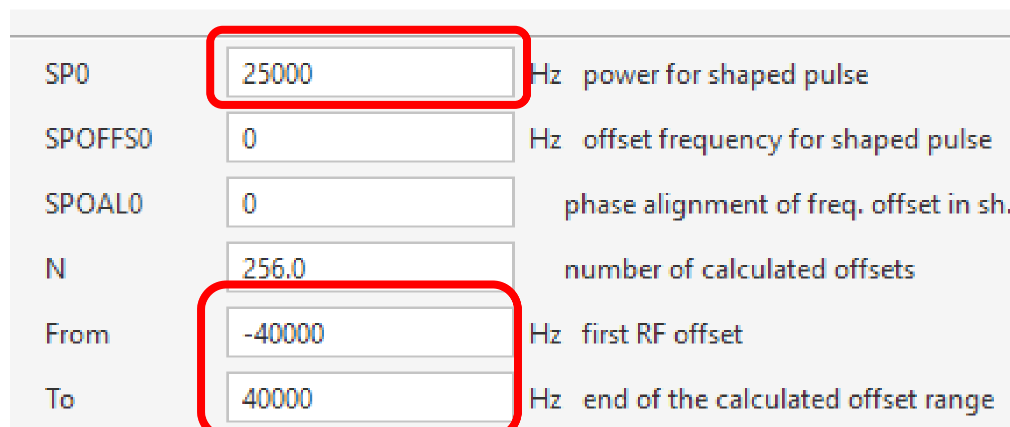
Phases needed for P5M4:
(360) Means in units of degrees!

```
ph22=(360) 60
ph23=(360) 150
ph24=(360) 180
ph25=(360) 240
ph26=(360) 330
```

Notes on simulations

- These are done using stdisp/nmrsim
- These are approximations – experimental performance perhaps worse
- But: useful visualisation.
- Trick: to get 360deg pulse simulation to work, set flip angle to zero
- Then set power and calculation range manually

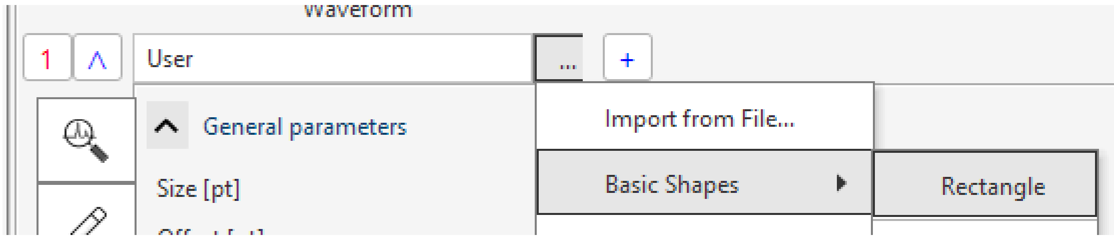




Basics of stdisp/nmrsim calcaulations

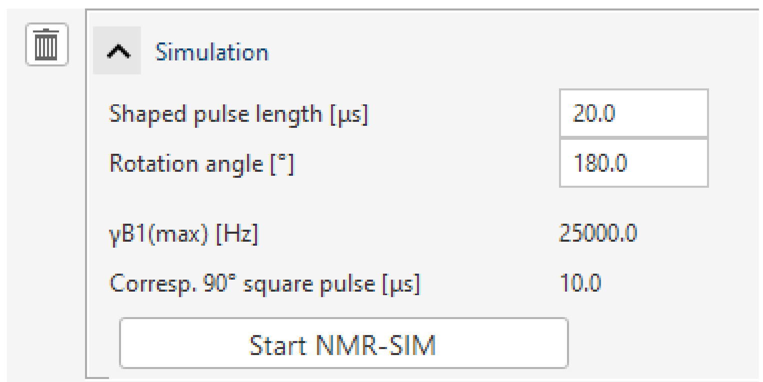
- Open a shape file:

- or Create a new shape:

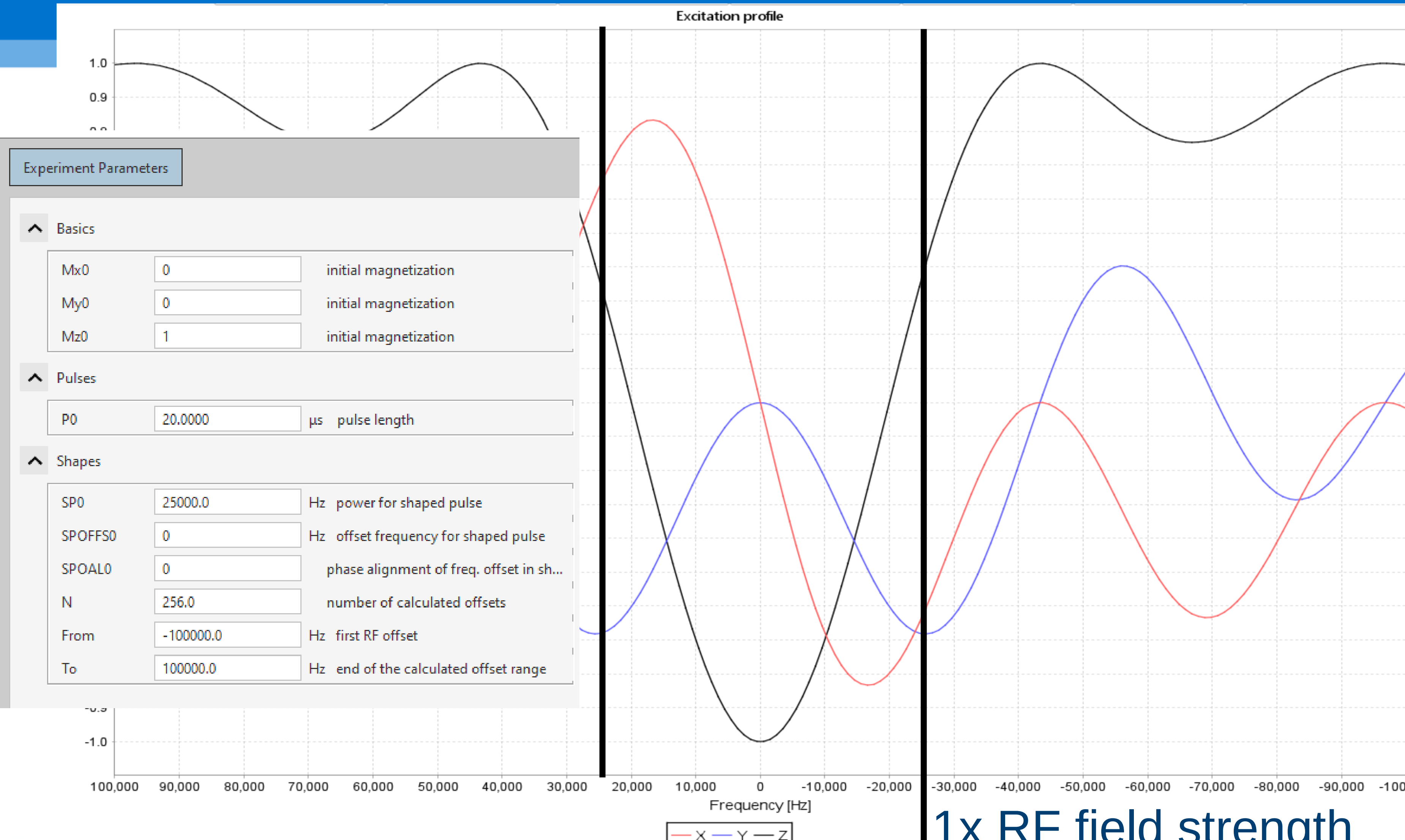


- Simulate:

- Set length and flip angle:

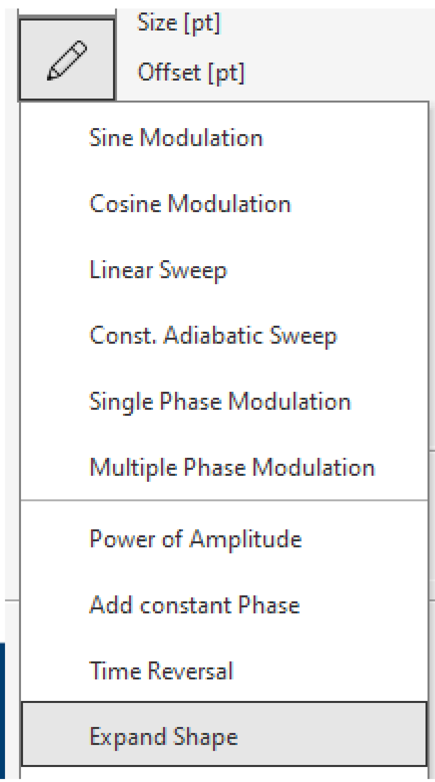


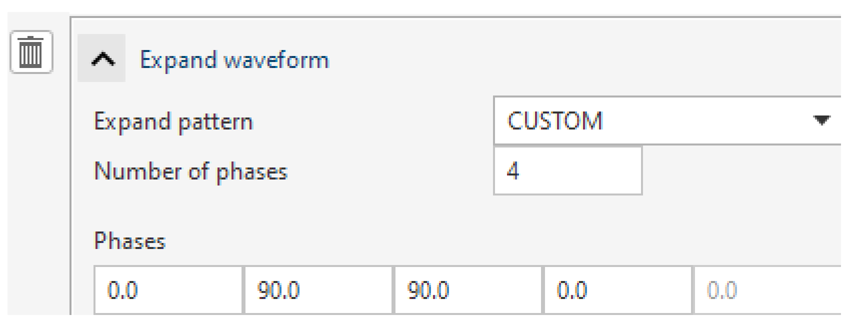
Example: hard 180



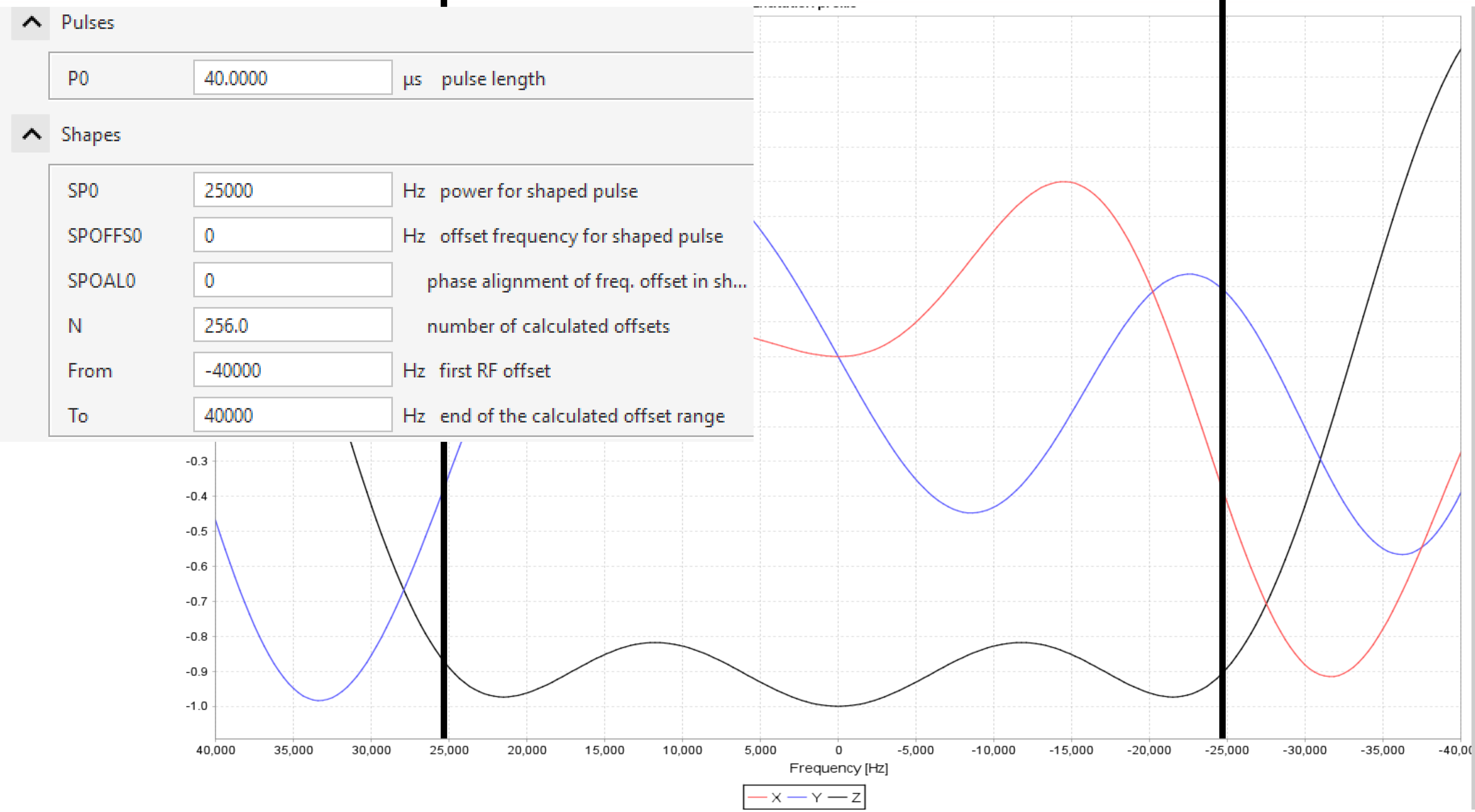
Broadband decoupling step 1 – composite pulse

- First problem: simple 180 is poor inversion element.
- Solution: “composite pulse” (Levitt et al 1980)
- Eg: $90_x180_y90_x$



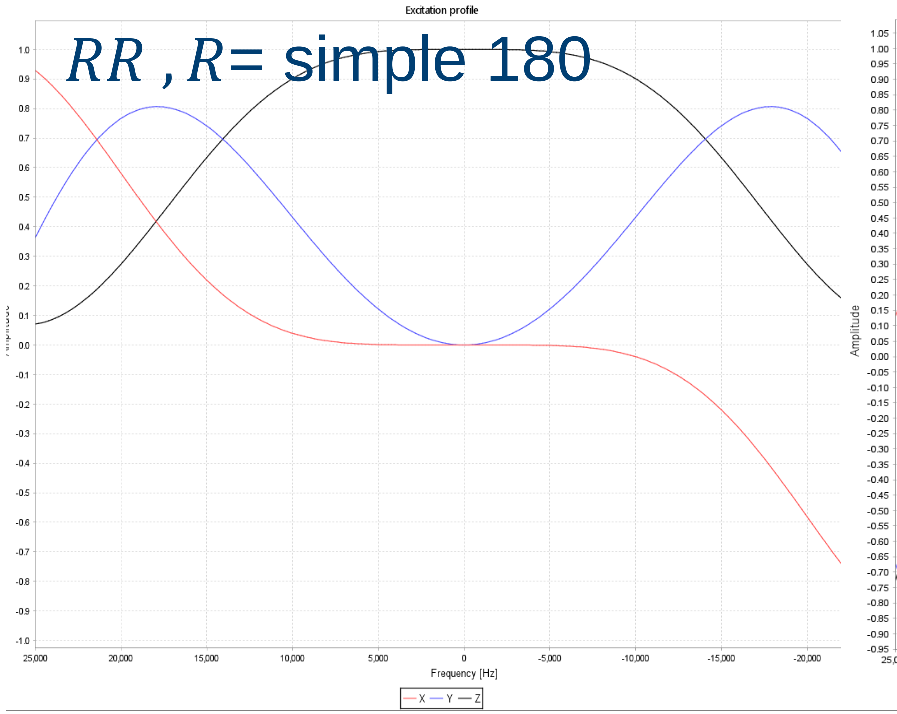


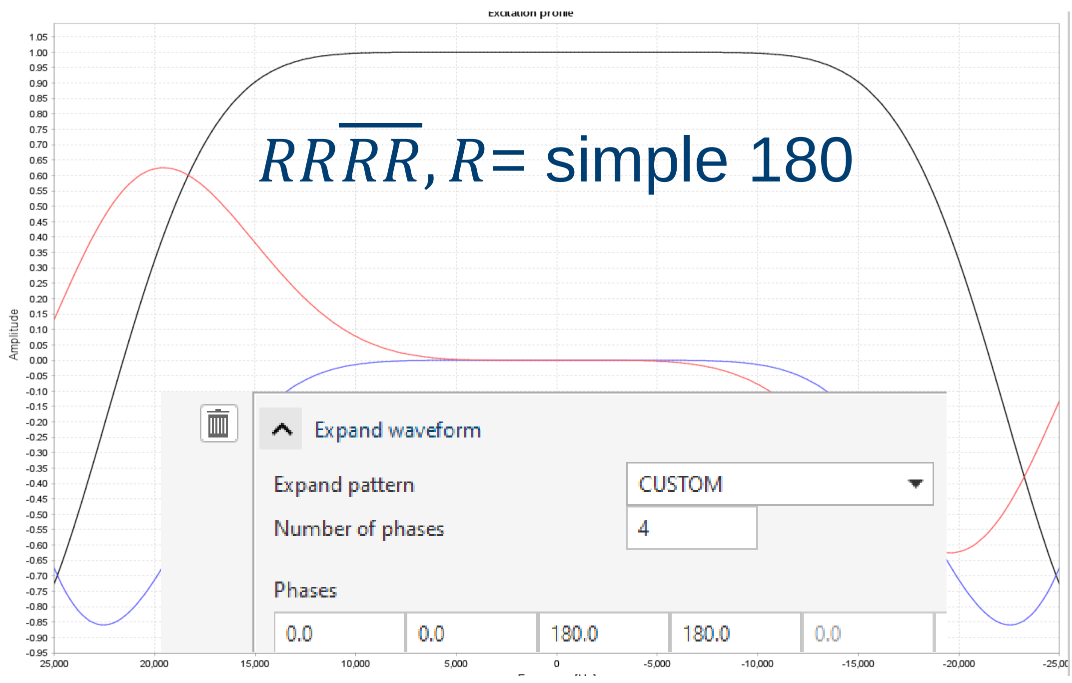
Composite pulse inversion profile



Broadband decoupling step 2 – supercycle $RR\overline{RR}$ - MLEV4

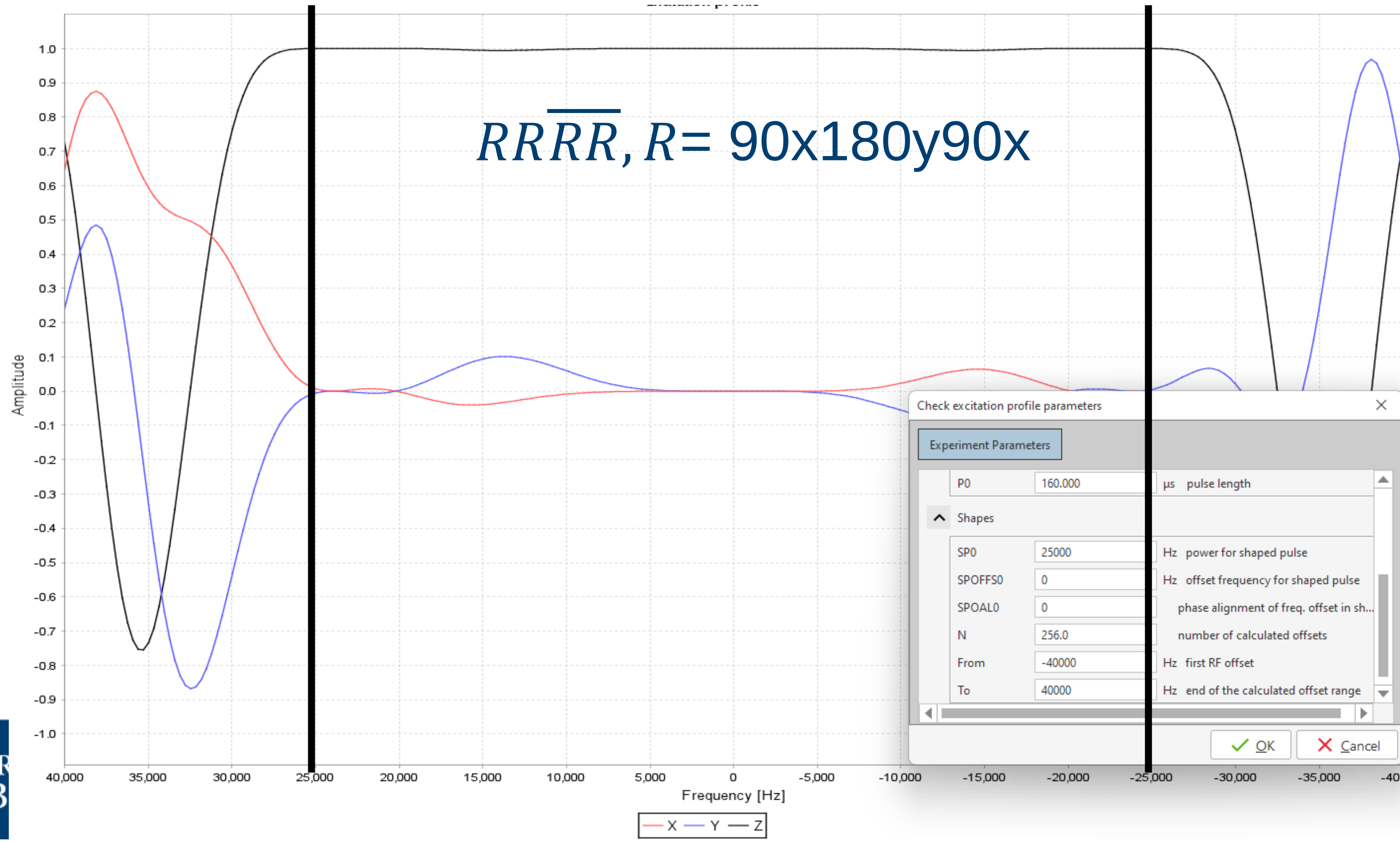
- R is the inversion element , $\overline{R}$ means 180 degree phase shift
- Ideally this should act like an exact 360 ie do nothing





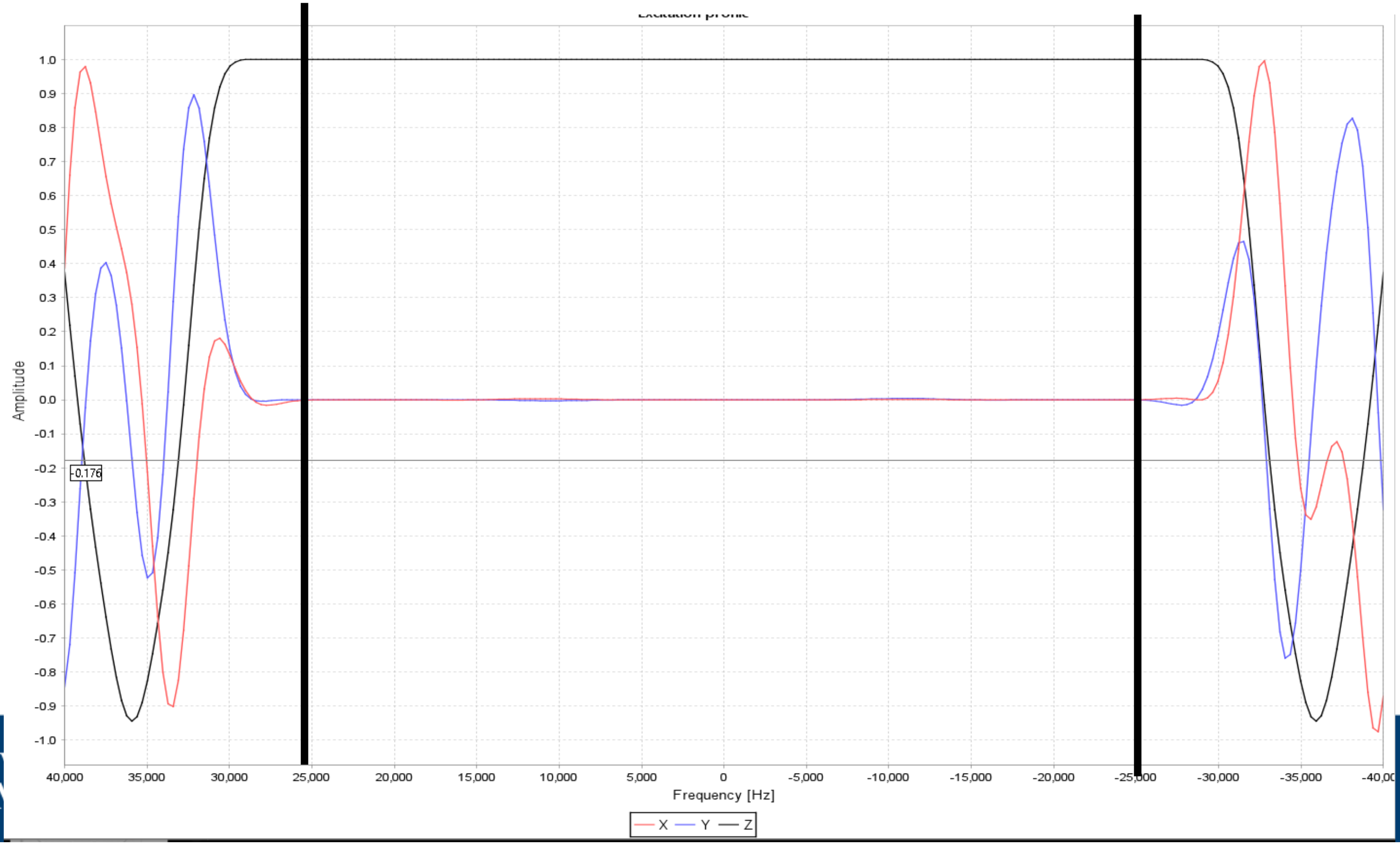
Composite pulse with supercycle

- Save the 90x180y90x as a shape and open it
- Apply the MLEV4 expansion



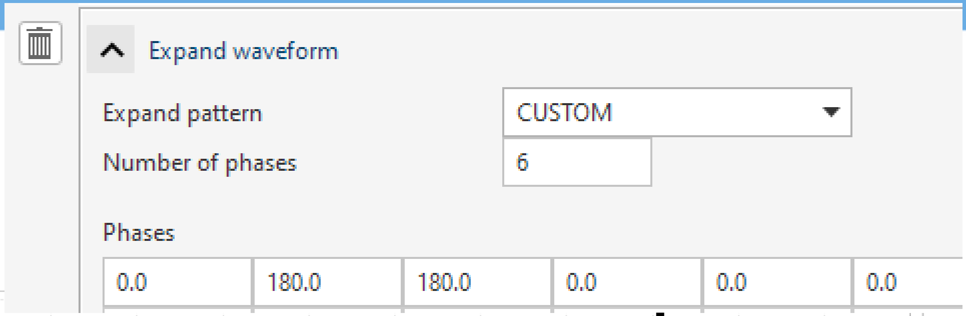
Broadband decoupling step 3 – cyclic permutation

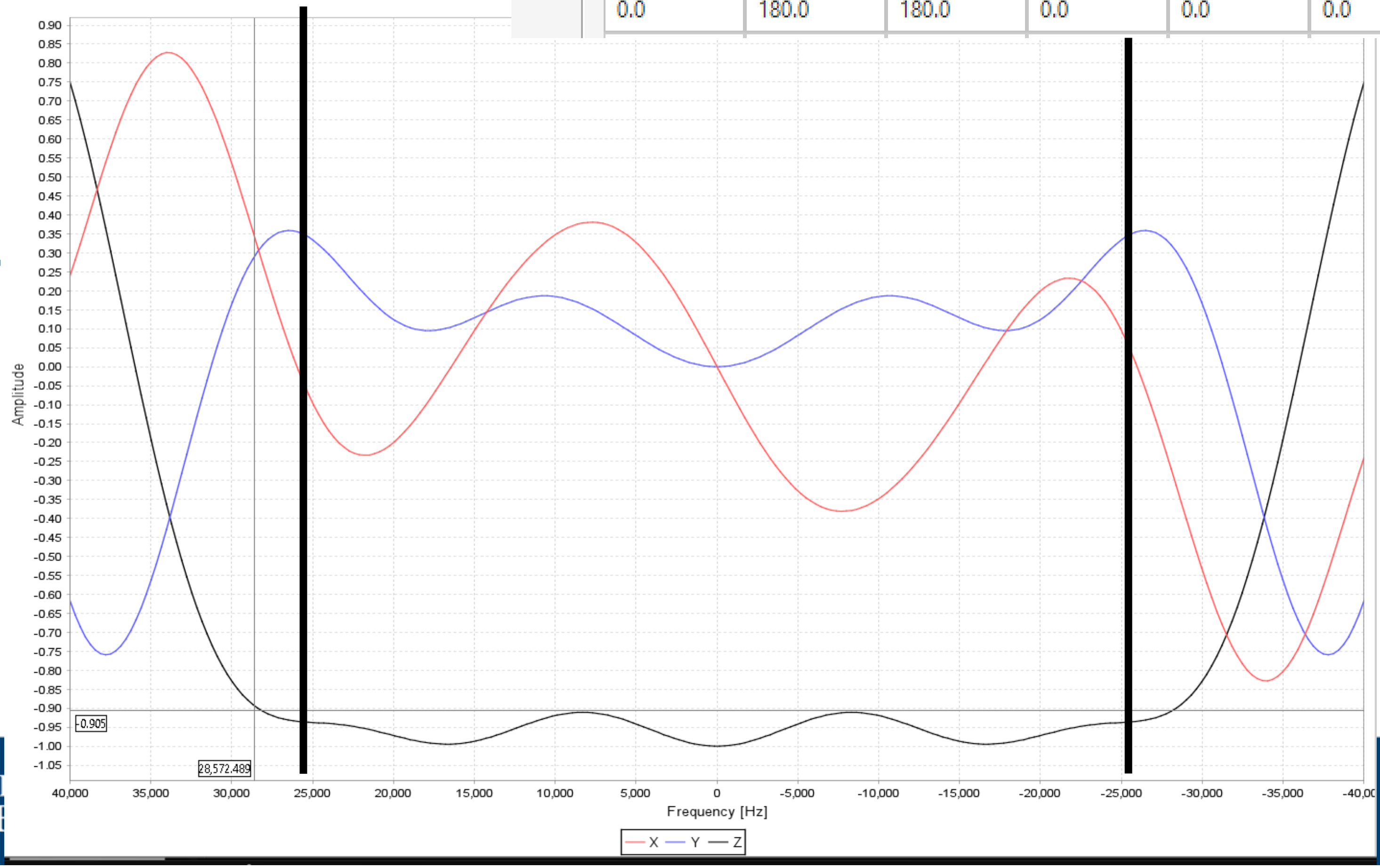
- We can take an inversion element off the end of the cycle and add to beginning, repeat this and concatenate.
- MLEV-16: $RR\bar{R}\bar{R}\ \bar{R}RR\bar{R}\ \bar{R}\bar{R}RR\ R\bar{R}\bar{R}R$



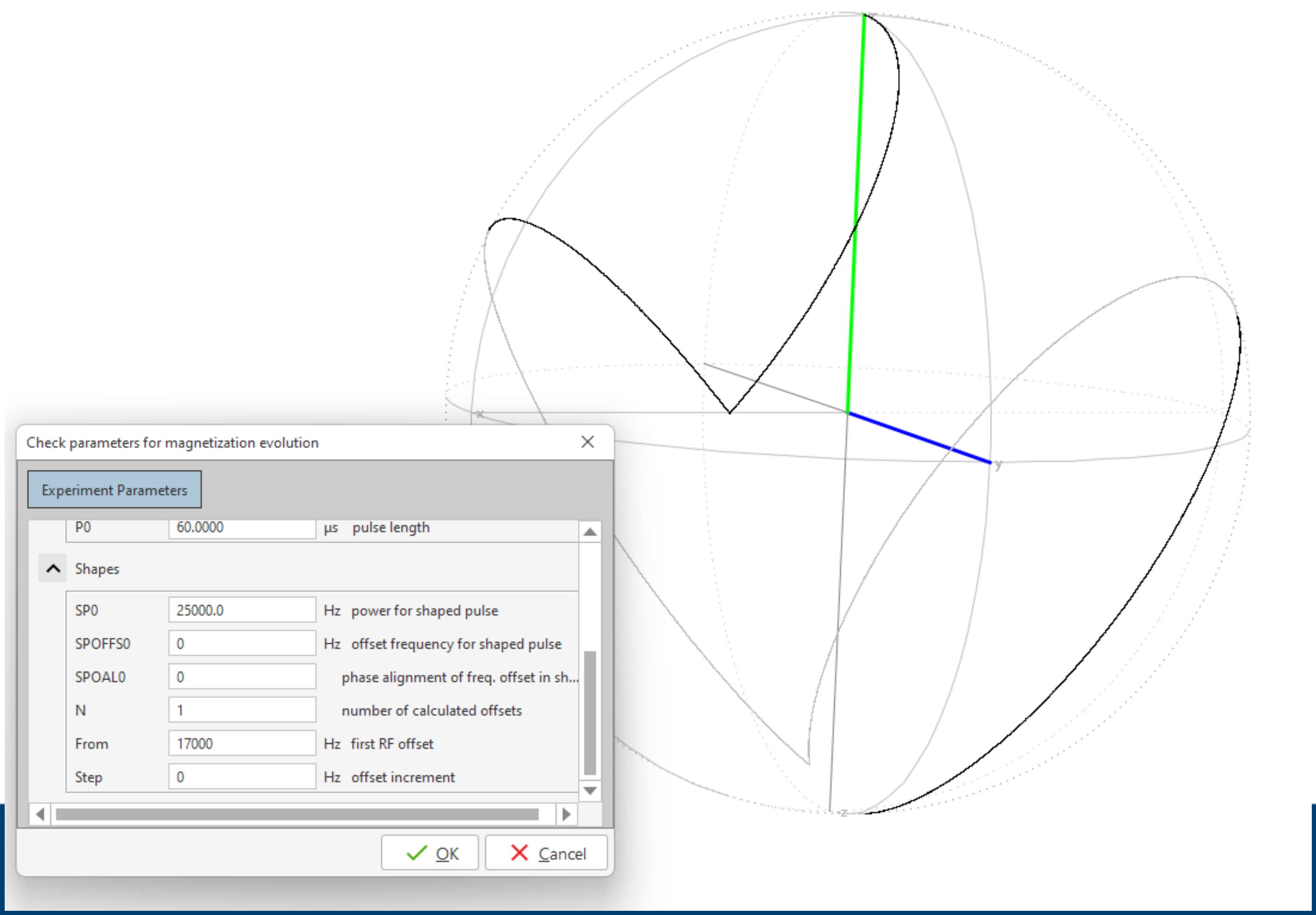
Next step: better composite pulse and supercycle

- Replace 90x180y90x
- Better: 90x180-x270x !
- $1\bar{2}3$
- WALTZ





Time evolution of 90x180-x270x



New supercycle: permute 90 degree pulse

- $1\bar{2}3\ 1\bar{2}3\ \bar{1}2\bar{3}\ \bar{1}2\bar{3}$ - WALTZ-4 this should be better than MLEV-4

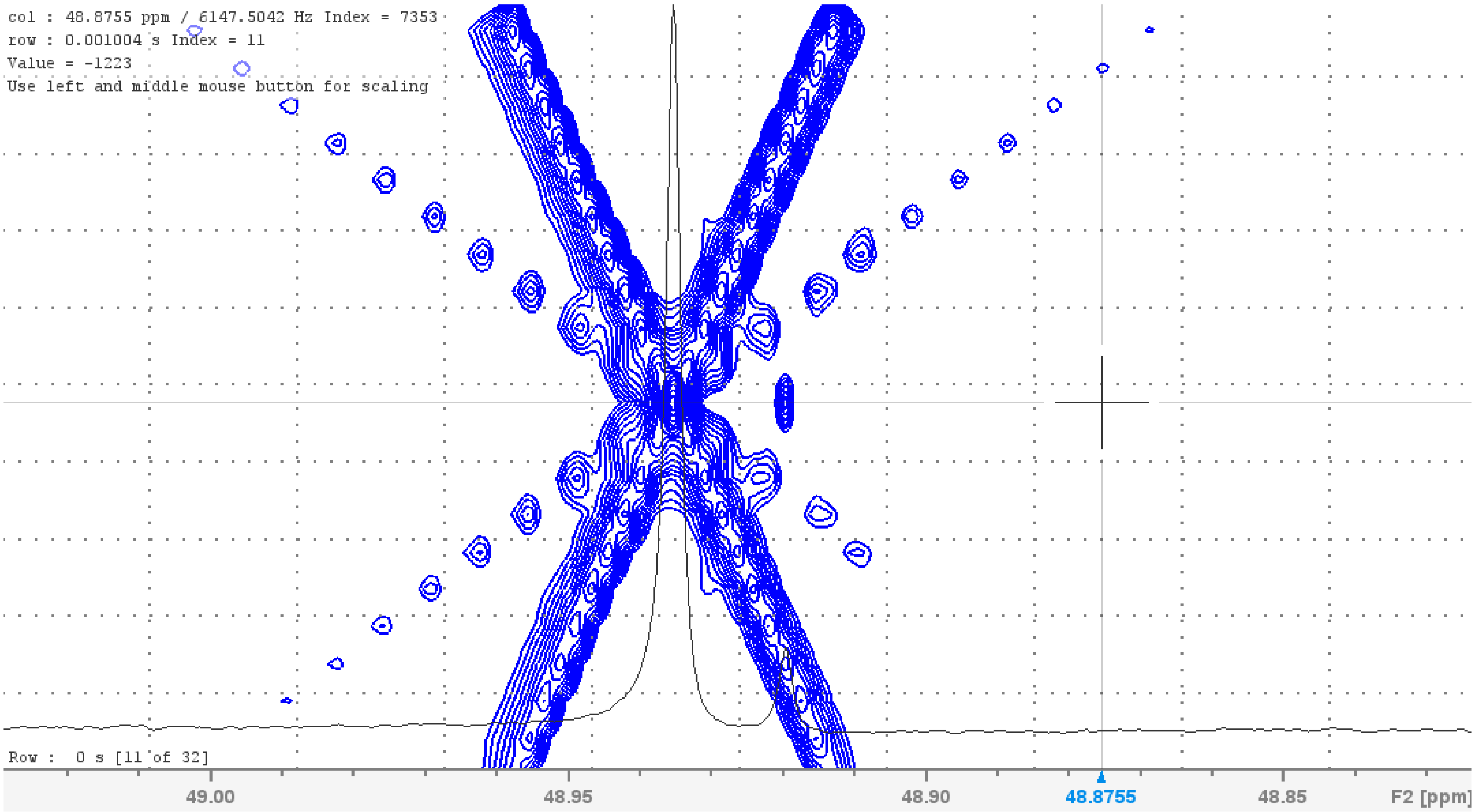
- $\bar{2}4\bar{2}3\bar{1}\ 2\bar{4}2\bar{3}1\ 2\bar{4}2\bar{3}1\ \bar{2}4\bar{2}3\bar{1}$ - WALTZ-8 $K\overline{KK}K$

- $\bar{3}4\bar{2}3\bar{1}2\bar{4}2\bar{3}\ 3\bar{4}2\bar{3}1\bar{2}4\bar{2}3\ 3\bar{4}2\bar{3}1\bar{2}4\bar{2}3\ \bar{3}4\bar{2}3\bar{1}2\bar{4}2\bar{3}$ $=$ $Q\overline{QQ}Q$ = WALTZ-16

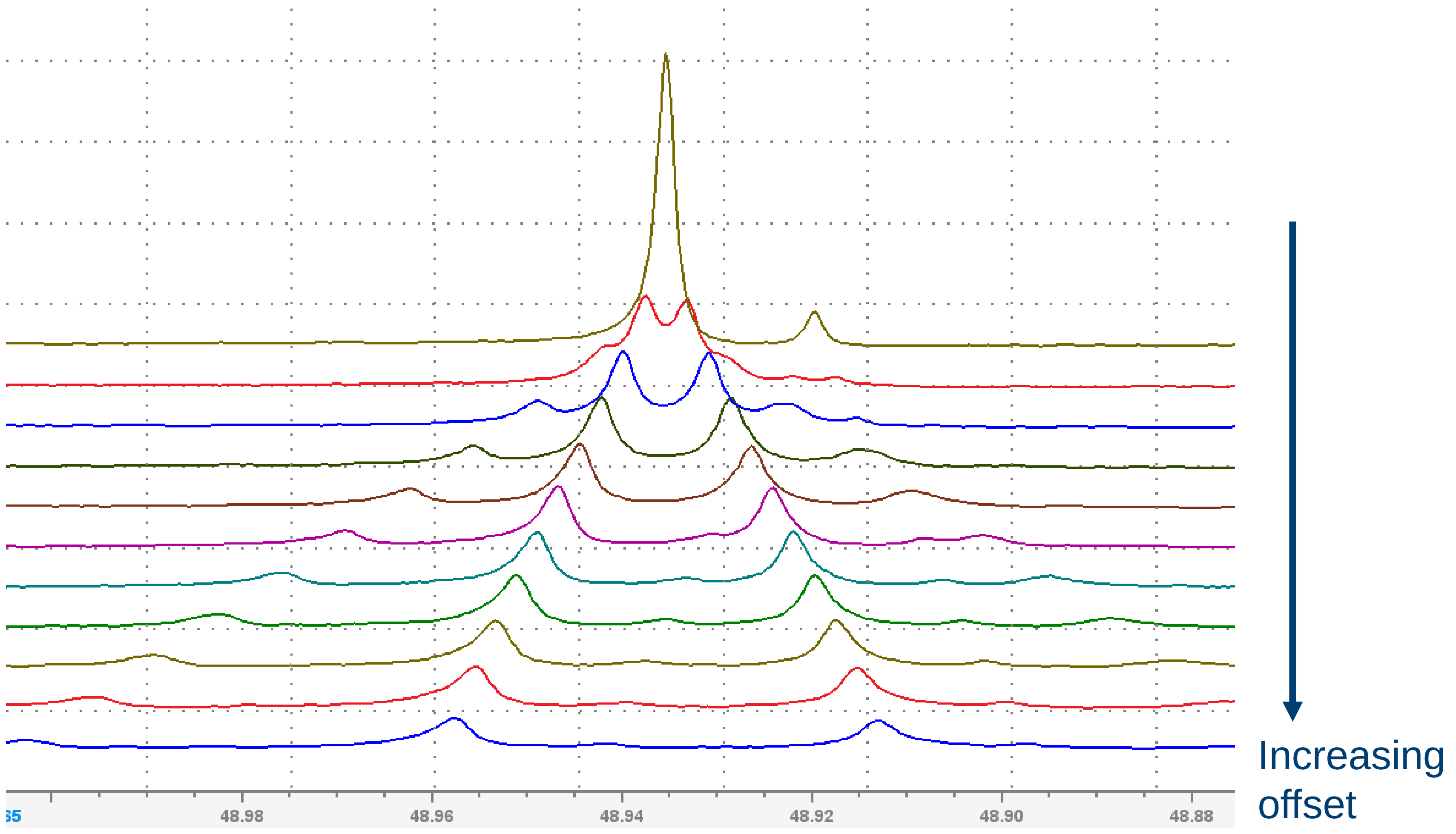
Experimental validation

- To really check the results we need to measure spectra
- I have used POPT here; we can save the data as pseudo-2D
- Need to have FT params set correctly
  - FT_MOD = FQC
  - PH_MOD= PK
  - WDW = whatever you want

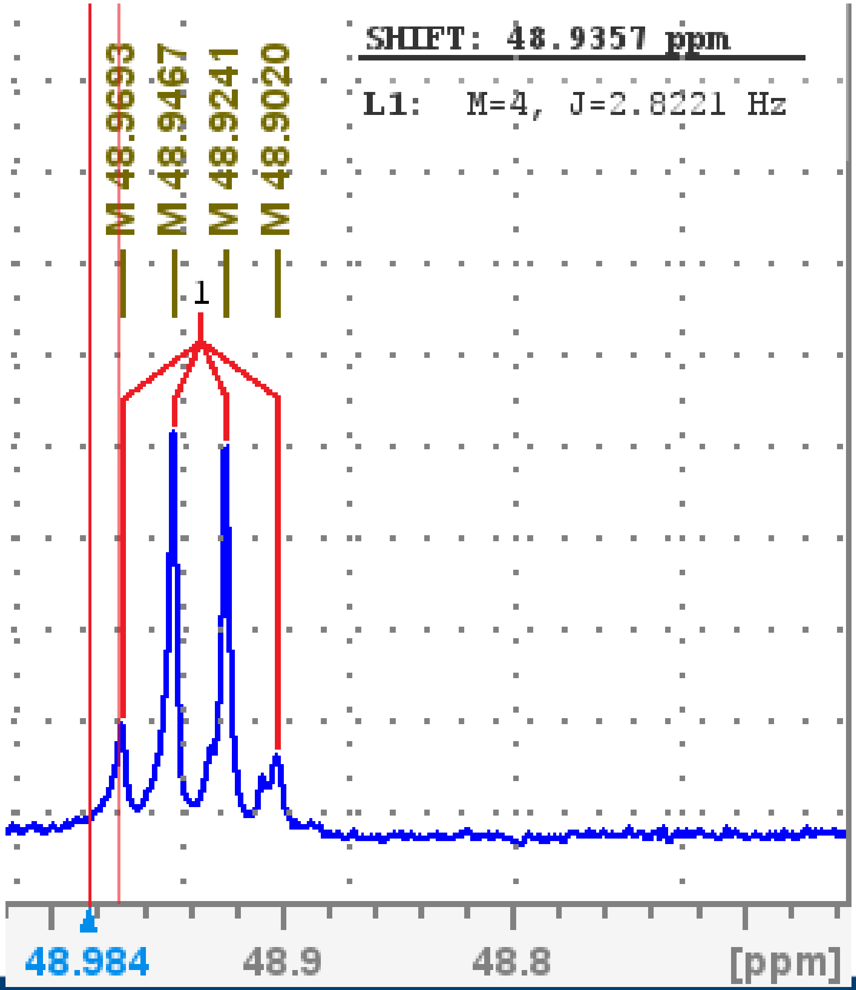
CW decoupling 2.2kHz RF field



CW decoupling



Scaling under CW decoupling



Offset = 50Hz
Nominal RF field 2200Hz

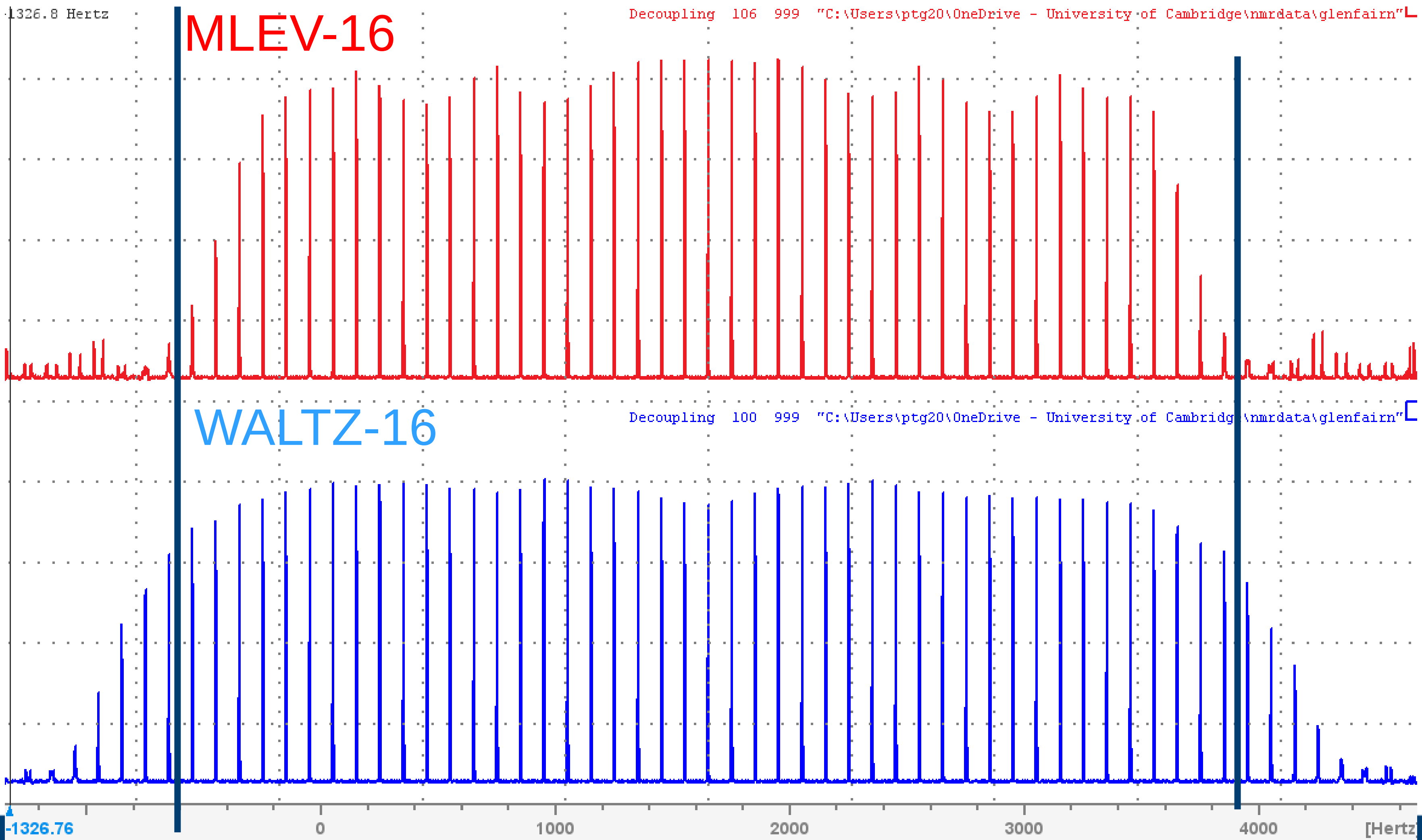
Actual coupling 140Hz

Scaling factor = offset/RF field

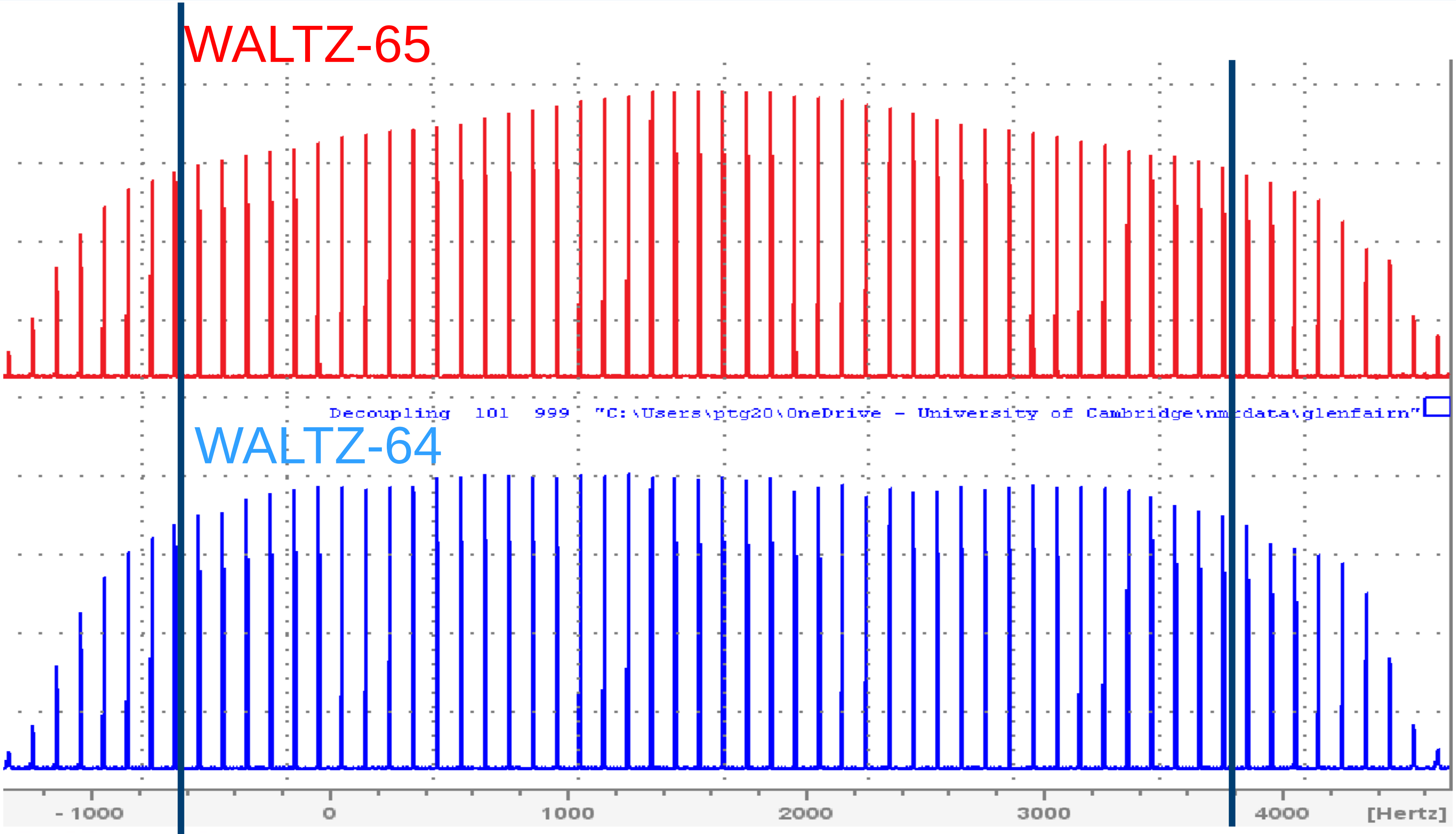
140*50/2200 = 3.18Hz

Working backwards:
RF field = 140*50/2.28 = 2482Hz

CPD bandwidth
+/- 1x RF field strength



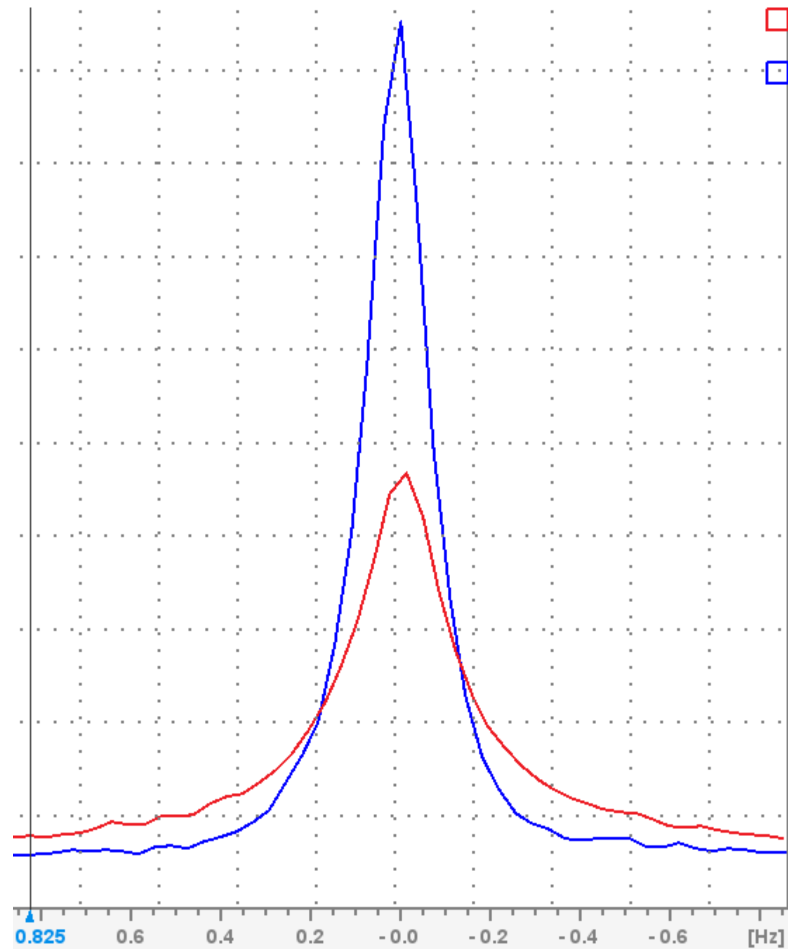
CPD bandwidth
+/- 1x RF field strength



Looking closely:

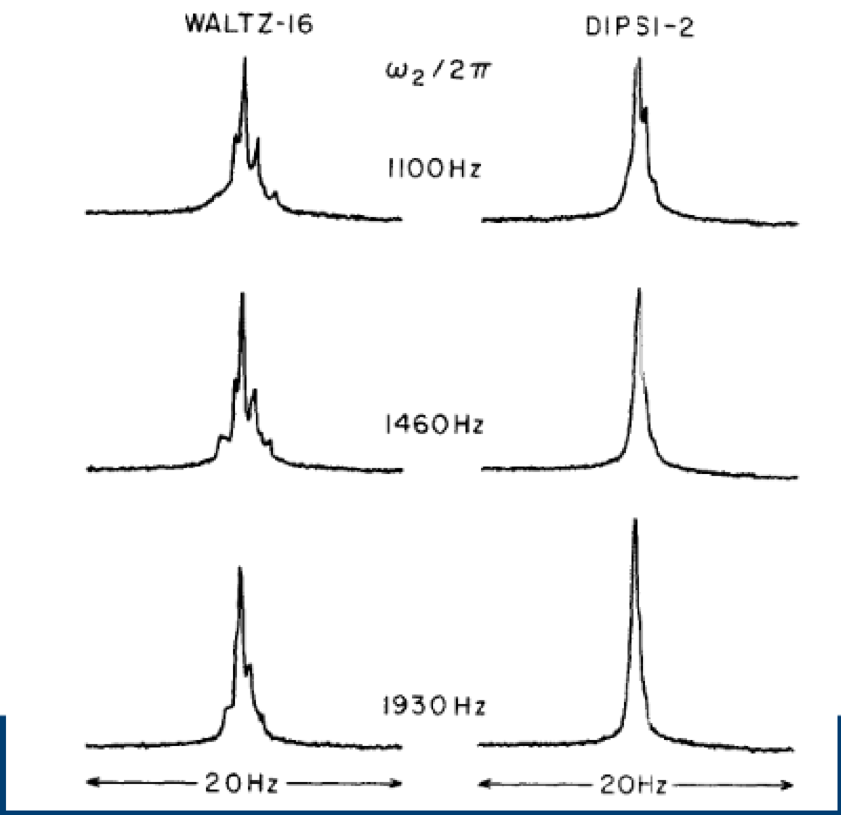
- WALTZ-16: on res linewidth ~ 0.16Hz
  - Not a real sample!
- Linewidth at +2300Hz = 0.26Hz
- Still ~insignificant broadening
- Better magnet, spinning:

Width[Hz/ppm]= 0.074/



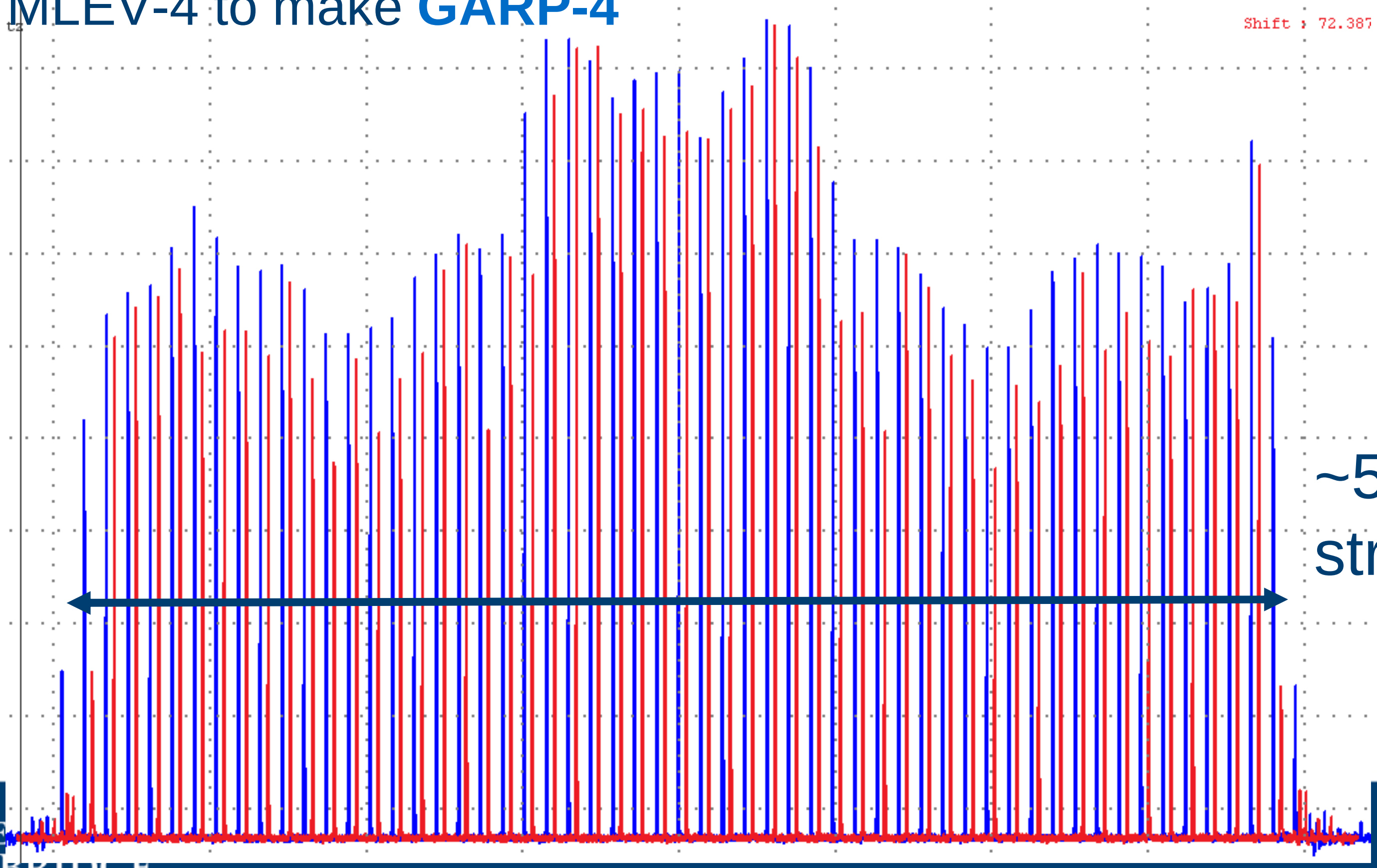
Interference of homonuclear coupling

- Most decoupling schemes evaluated for I-S pair
- What if coupling between the nuclei that are being decoupled?
- Example: ethyl iodide
- DIPSI-2 vs WALTZ-16:



More bandwidth?

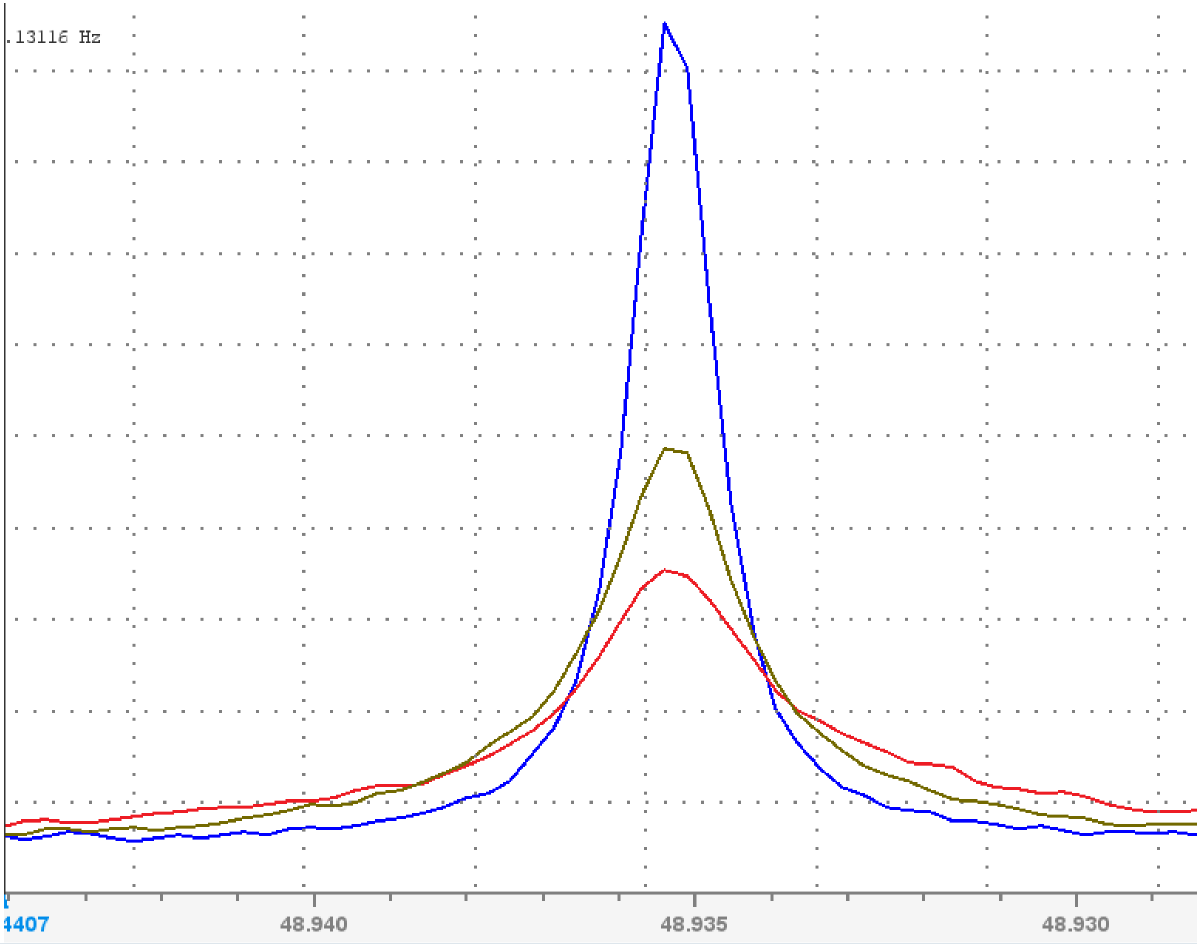
- WALTZ-16/64 is only enough for proton decoupling
- **GARP-1** (Globally optimised Alternating-phase Rectangular Pulses)
- Add MLEV-4 to make **GARP-4**



~5x RF field strength

GARP performance

- Best case: 0.17Hz ~WALTZ
- Worst (GARP) 0.38Hz
- Worst (GARP4) 0.29Hz



Even more bandwidth?

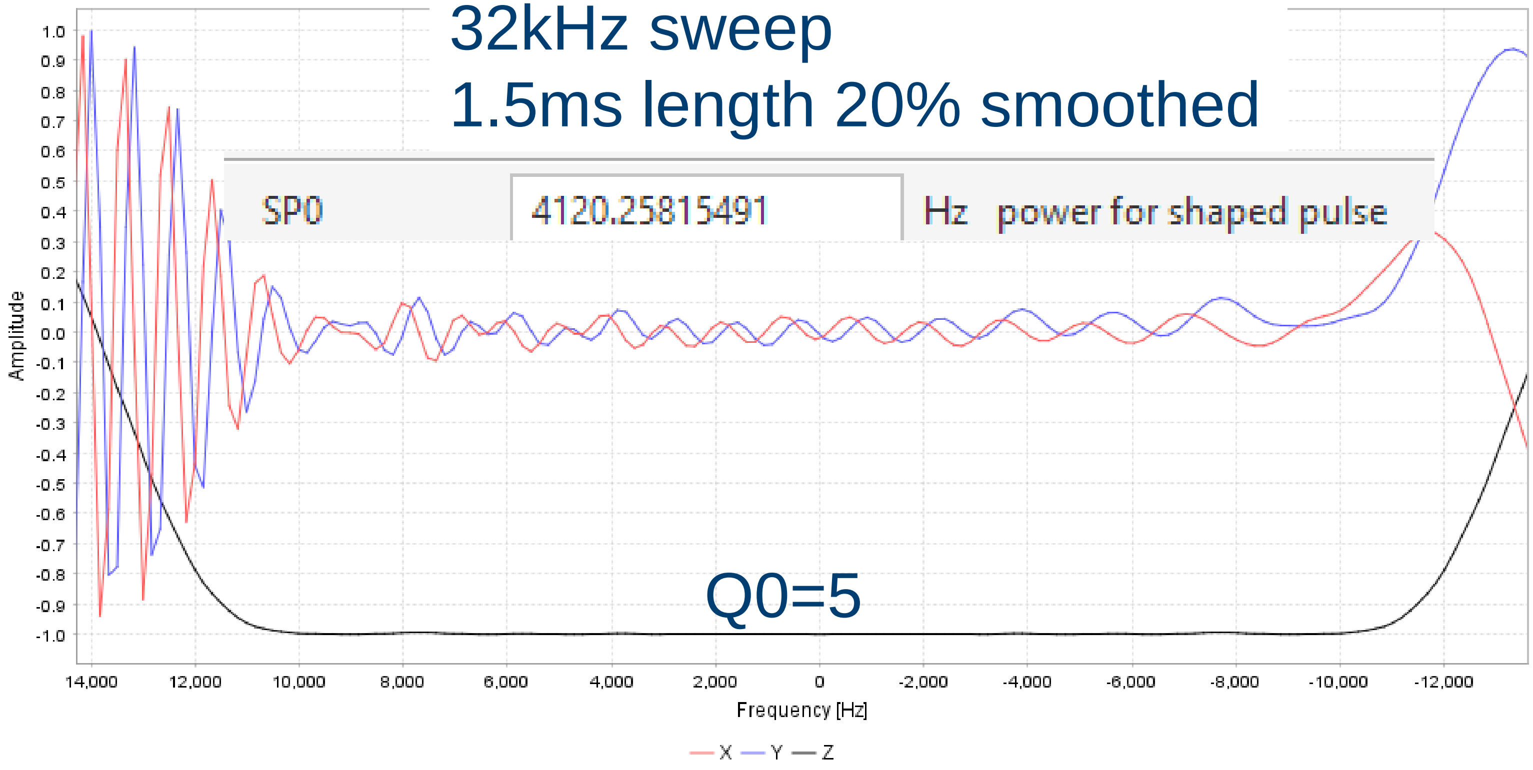
- Broadband inversion? **Adiabatic pulses**

$$Q_o = \frac{2\pi * RF^2}{SweepRate}$$

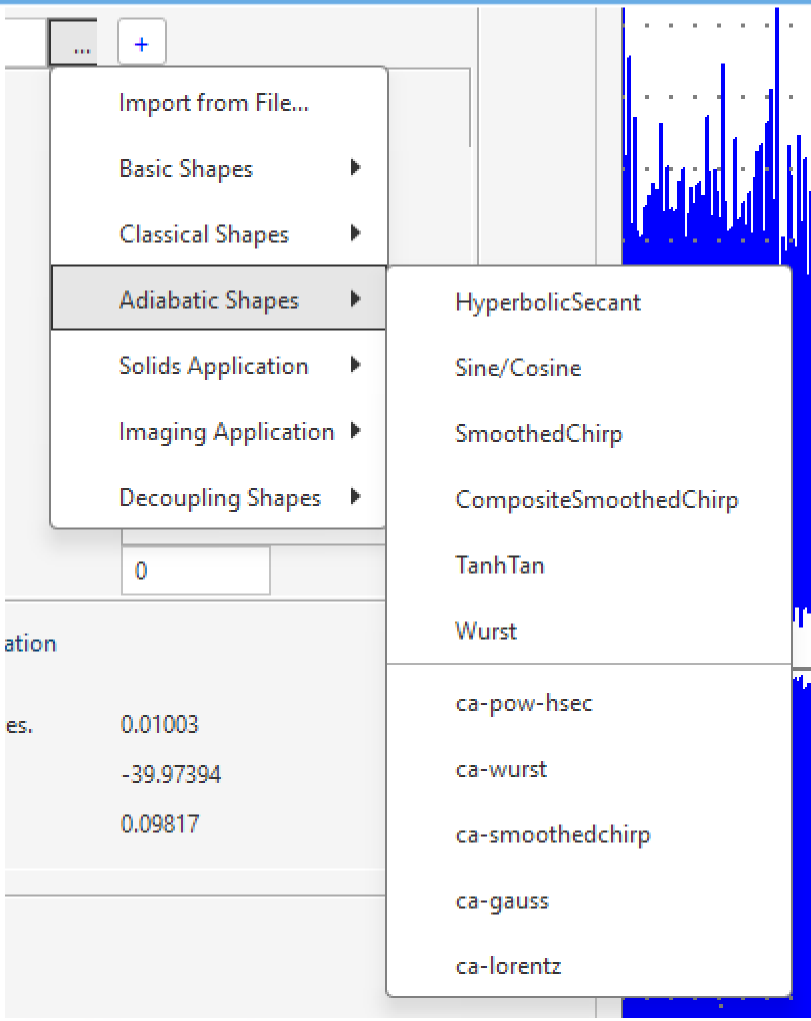
Crp32,1.5,20.2
32kHz sweep
1.5ms length 20% smoothed

SP0 | 4120.25815491 | Hz power for shaped pulse

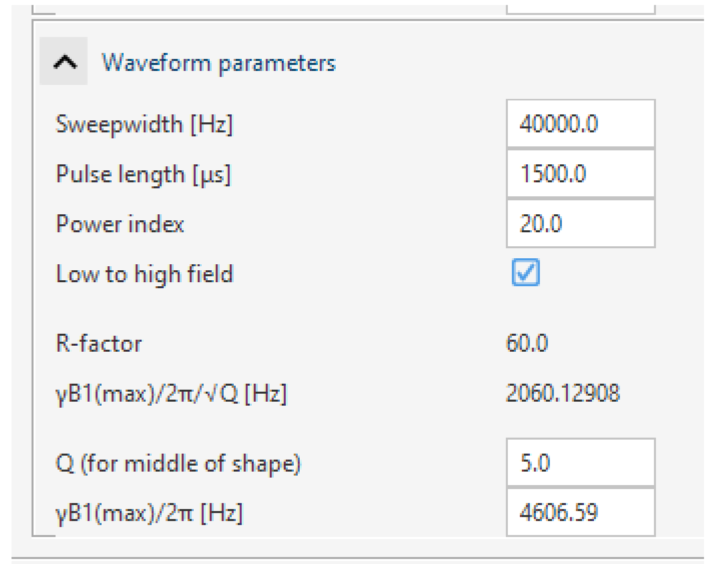
Q0=5



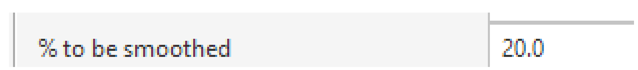
Creating adiabatic pulses



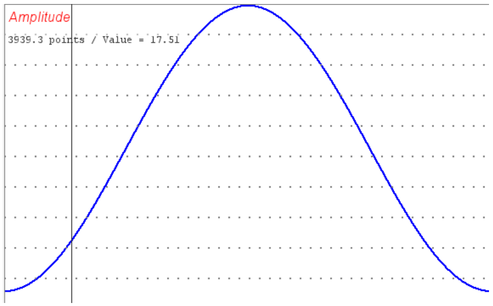
WURST

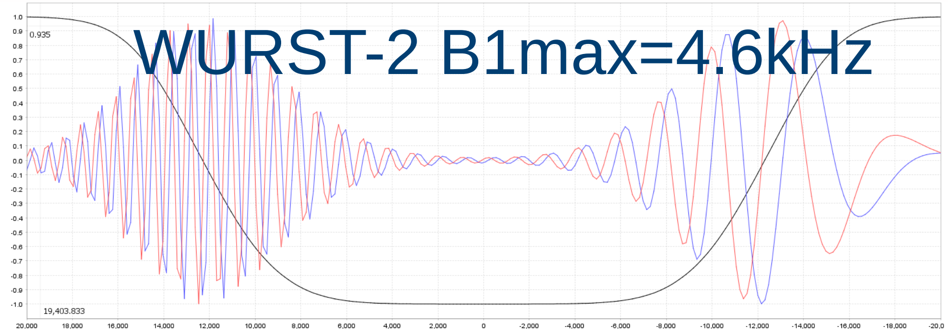


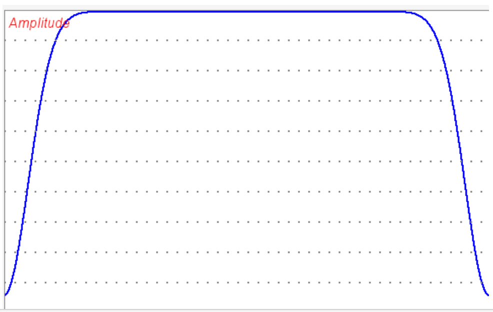
Smoothed Chirp

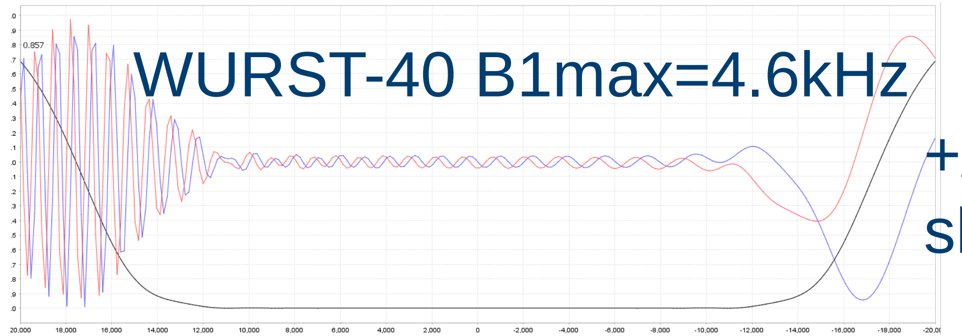


Amplitude and phase modulation
Fixed 1.5ms pulse length and 60kHz sweep

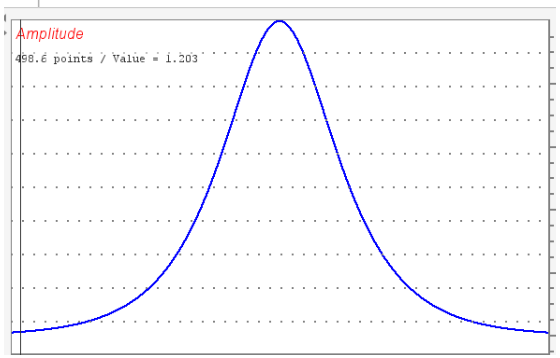


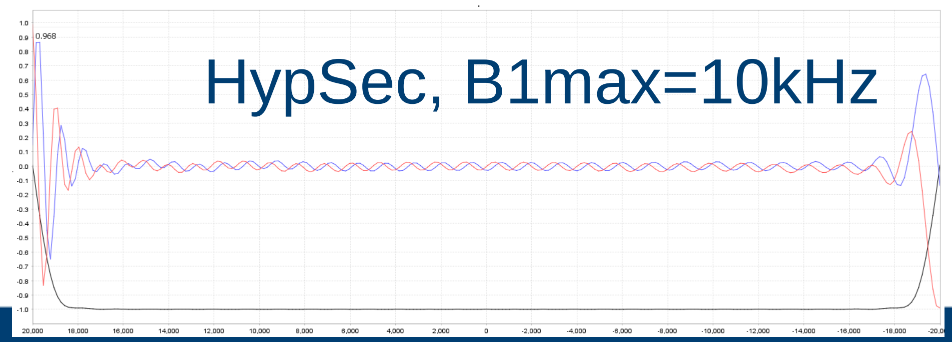






+/- 20 kHz shown





Power setting in adiabatic pulses

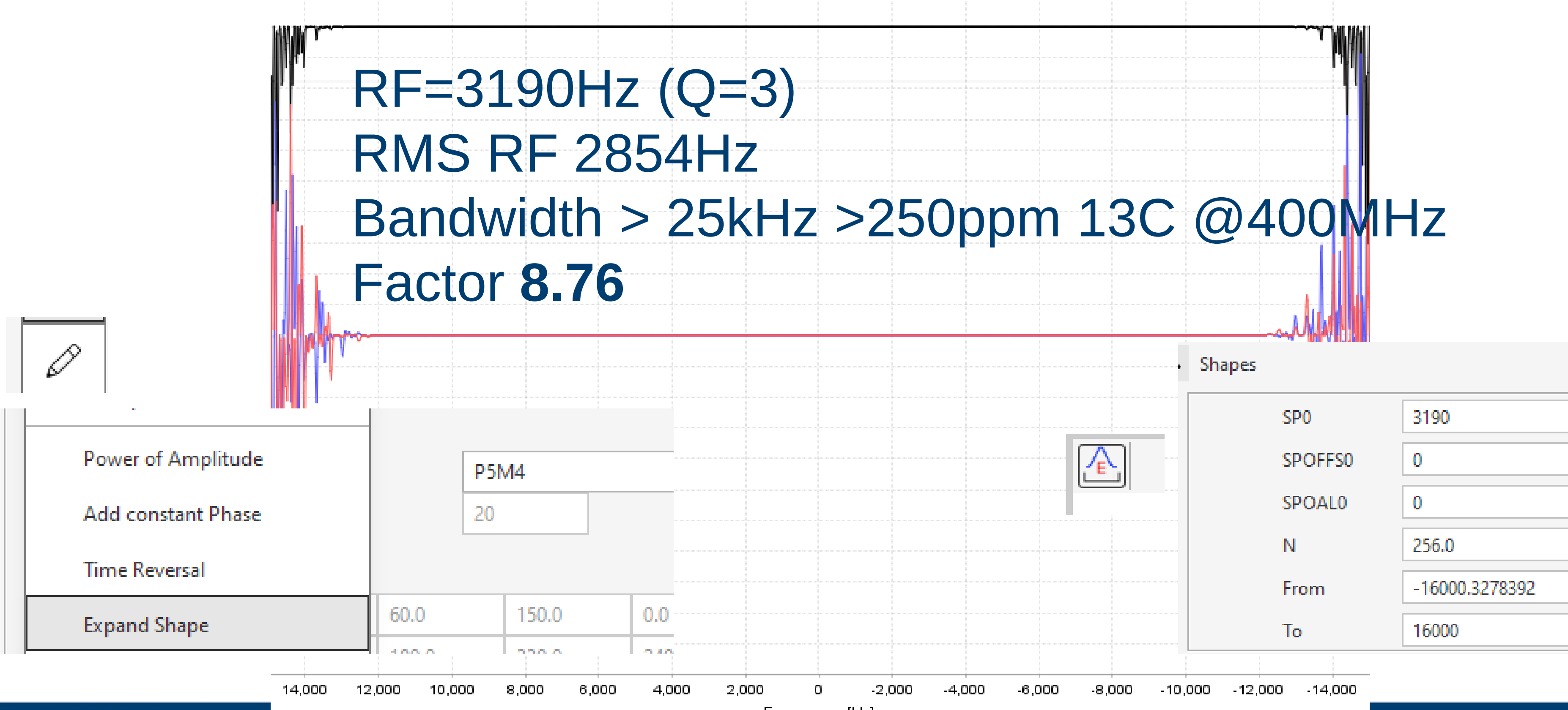
```
20  ##$SHAPE_INTEGFAC= 1.0444279E-01
```

- Q=5 is fine for normal inversion
- Unnecessarily high for decoupling with supercycle
- Change integral factor in shape file
- $= \frac{Length\ of\ hard\ pulse\ of\ same\ flip\ angle\ and\ RF field}{Length\ of\ shaped\ pulse}$
- $Q \propto RF^2$
- To change Q by a factor, change SHAPE_INTEGFAC by square root of that eg Q=5 -> Q=3 increase SHAPE_INTEGFAC by factor SQRT(5/3)

Add supercycle, reduce power

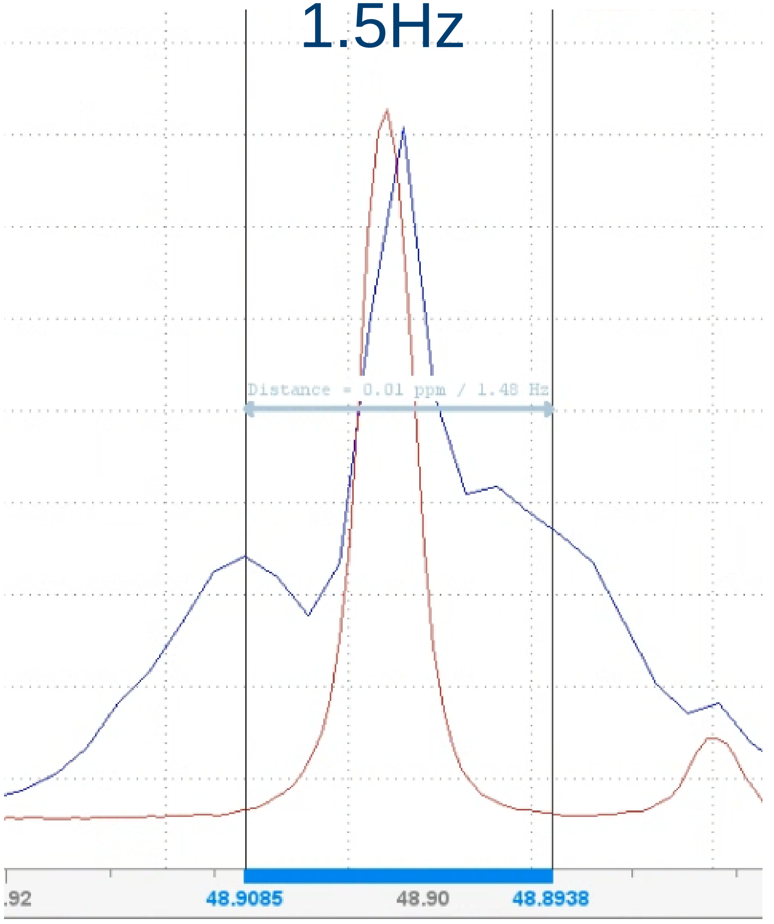
- "P5M4" $= RR\overline{RR}$ where $R = 180_0\ 180_{150}\ 180_{60}\ 180_{150}\ 180_0$

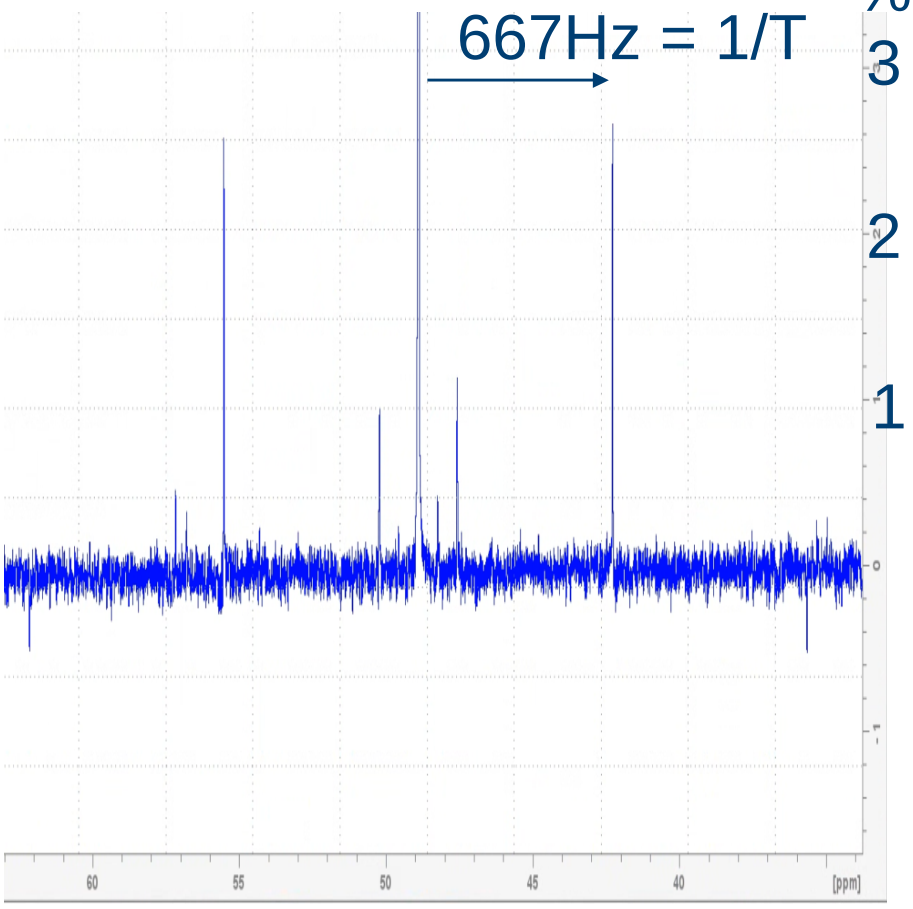
RF=3190Hz (Q=3)
RMS RF 2854Hz
Bandwidth > 25kHz >250ppm 13C @400MHz
Factor **8.76**



Results of adiabatic decoupling in13C{1H}:

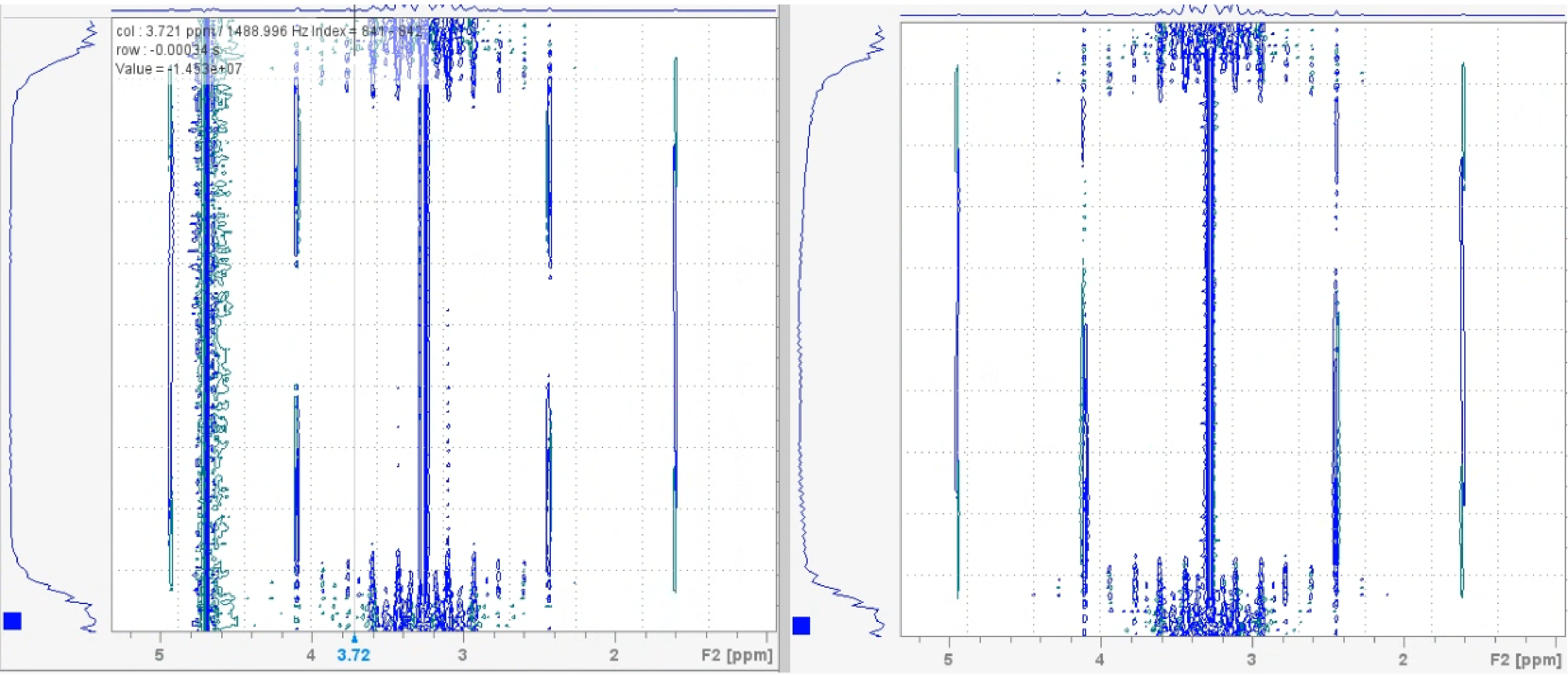
- Waltz, Adiabatic





Decoupling sidebands

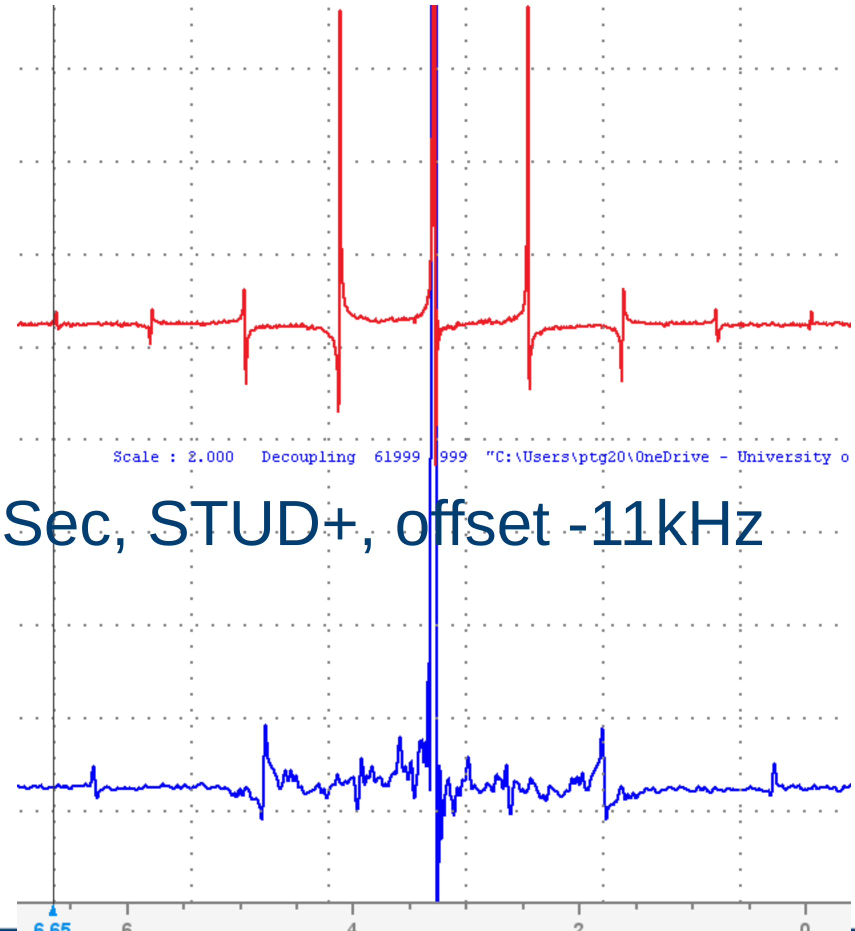
- Indirect dimension is decoupler offset
- 1D proton (13C labelled MeOH) vs HSQC, p5m4sp180.2

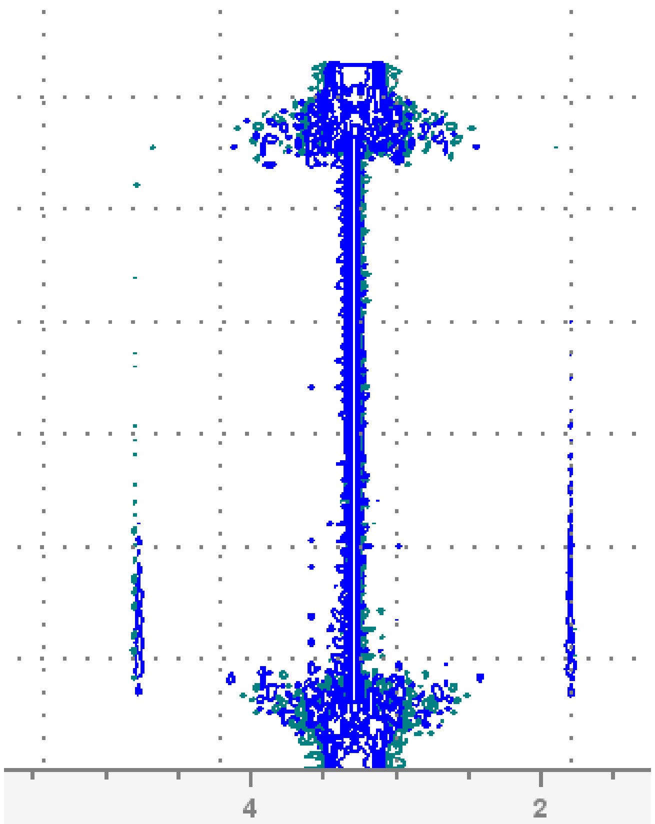


Reducing sidebands: eg STUD+

Crp32, P5M4, offset -11kHz

HypSec, STUD+, offset -11kHz



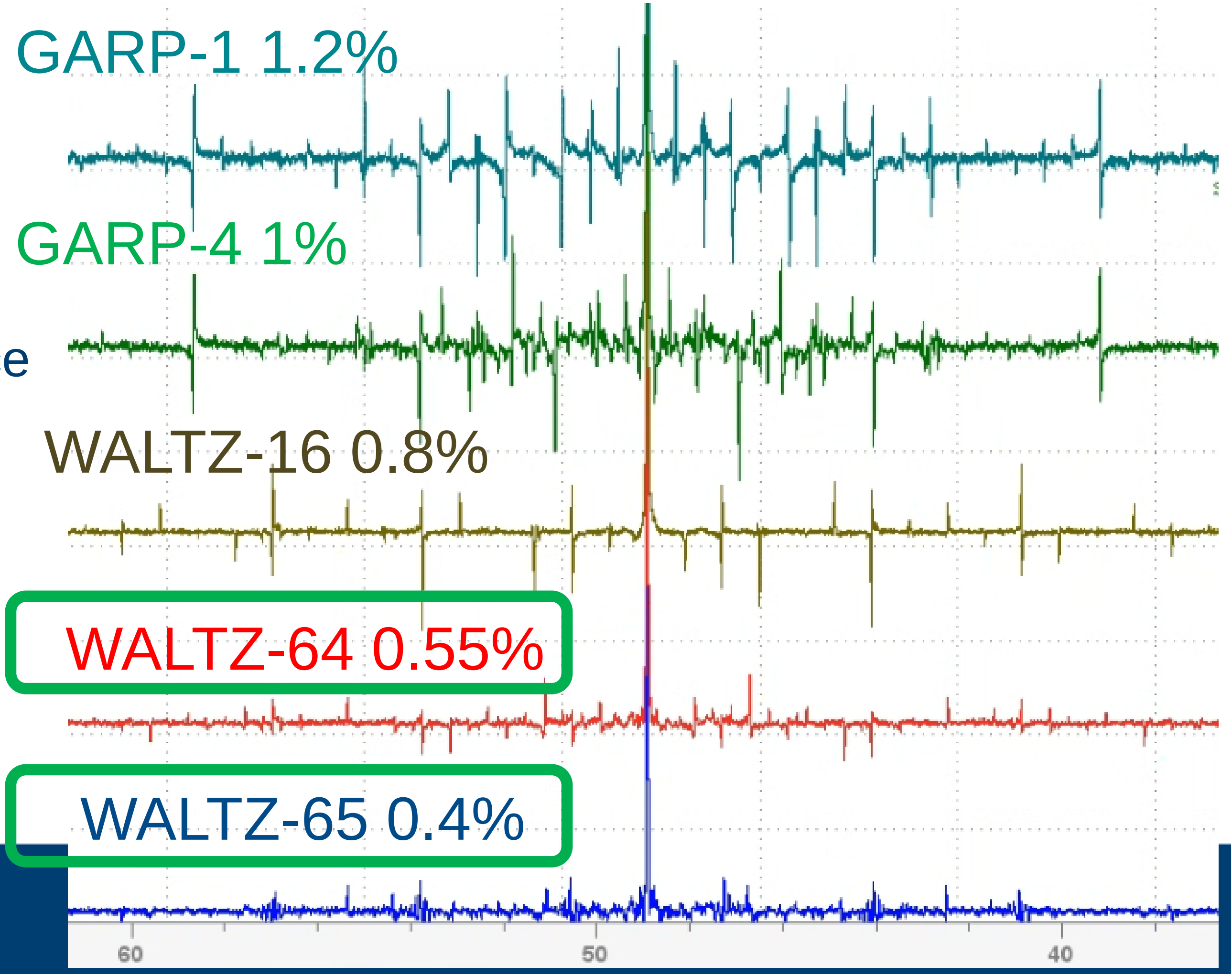


What about sidebands in normal CPD?

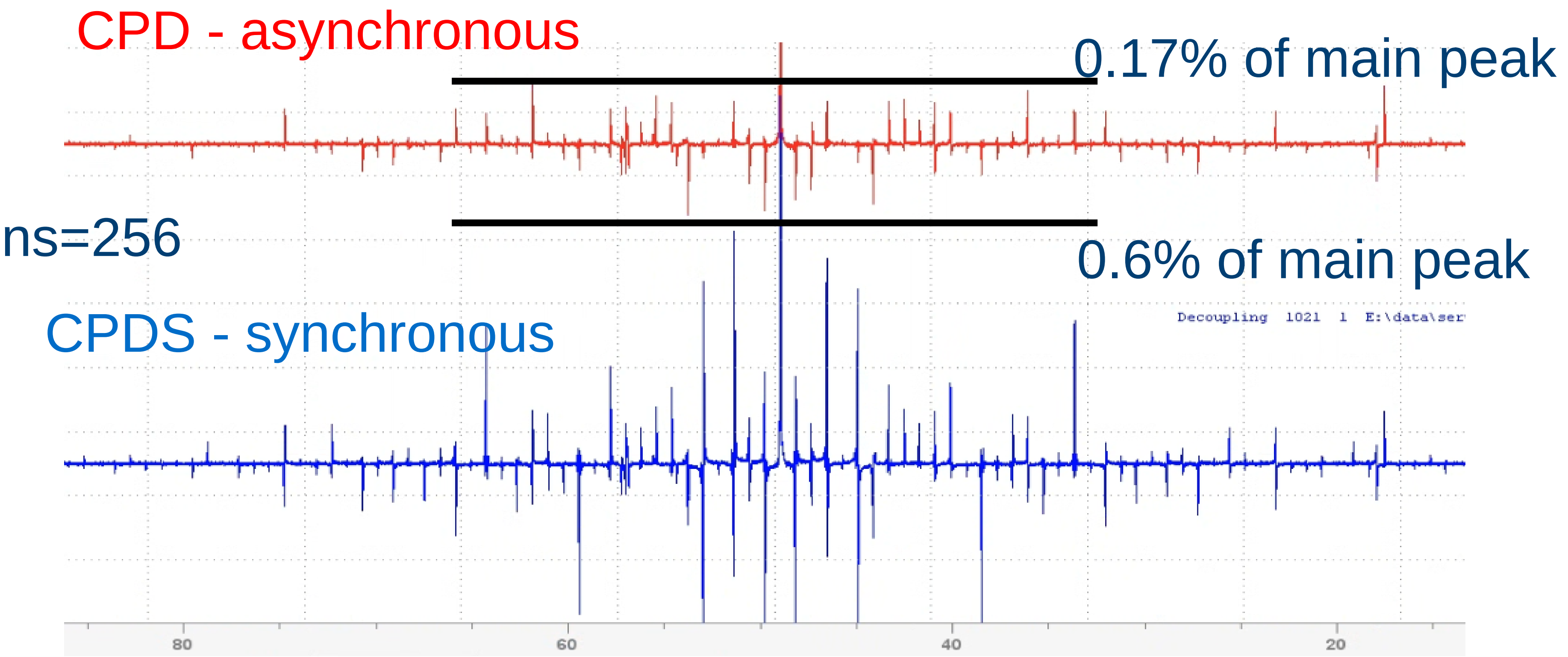
- Sidebands are still there, just usually less obvious
- 1 scan
- pcpd2=128us

(==90us @ J=200Hz)

Decoupler on resonance

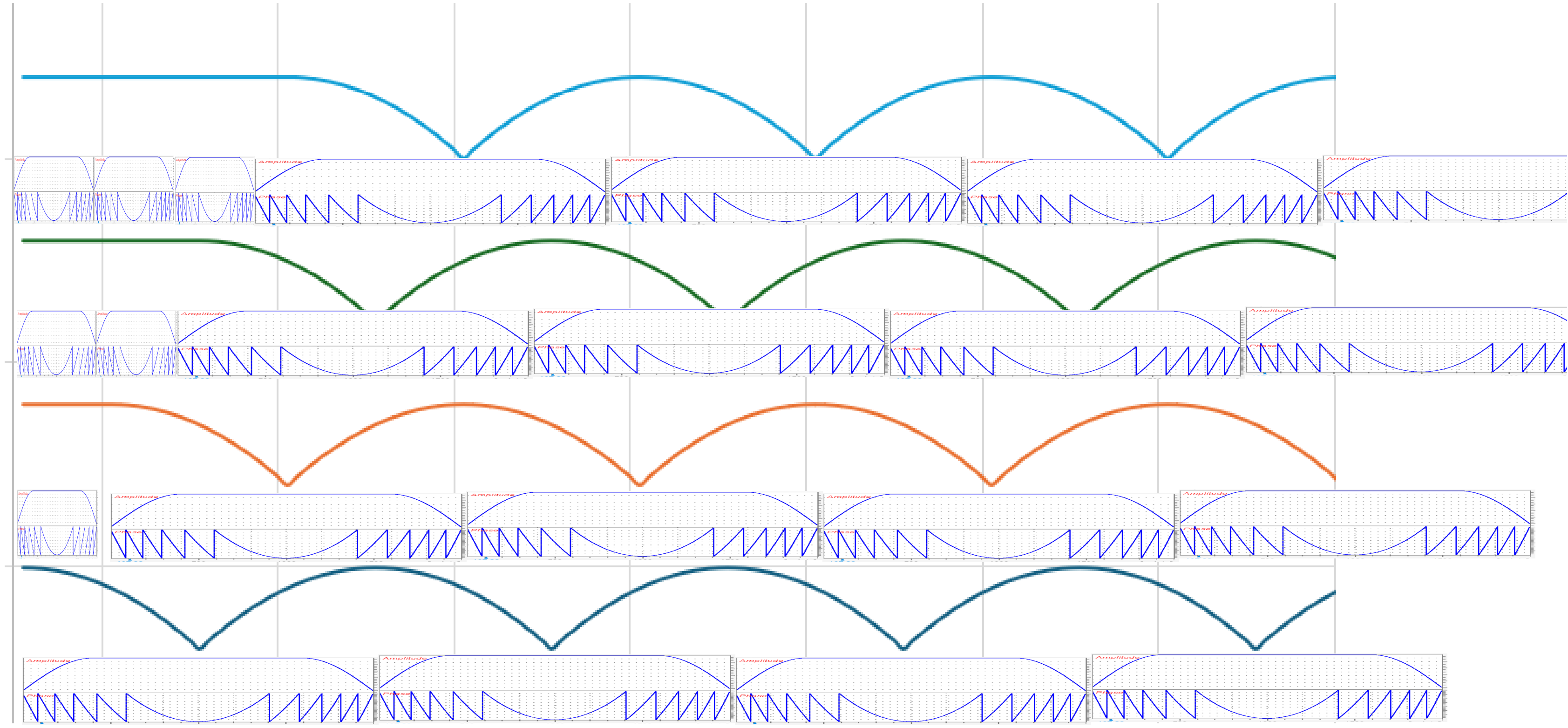


“synchronous” vs “asynchronous” CPD



Bilevel decoupling

- Controlled cancellation of decoupling sidebands?



Bilevel cpd programs: bi_p5m4sp_4sp.2

```
#setphase
bilev "l31=(nsdone+ds)%4+1"
1 p63*0.5:sp14:0 pl=sp14
  lo to 1 times l31
  p63:sp31:0 pl=sp31
2 p63:sp31:150
  p63:sp31:60
```

Bilev statement forces synchronous CPD

Number of loops to do set by nsdone

SP31 for main part

SP14 for bilevel part

P63 for length of main pulse

SPNAM 14	Crp32,0.75,20.2		File name for SP14
SPOAL14	0.500		Phase alignment of freq. offset in SP14
SPOFFS14 [Hz]	0		Offset frequency for SP14
SPW14 [W, -dBW]	1.2921	-1.11	Shaped pulse power SPW14
SPNAM 31	Crp32,1.5,20.2		File name for SP31
SPOAL31	0.500		Phase alignment of freq. offset in SP31
SPOFFS31 [Hz]	0		Offset frequency for SP31
SPW31 [W, -dBW]	0.64603	1.90	Shaped pulse power SPW31

Shapes for bilevel adiabatic decoupling

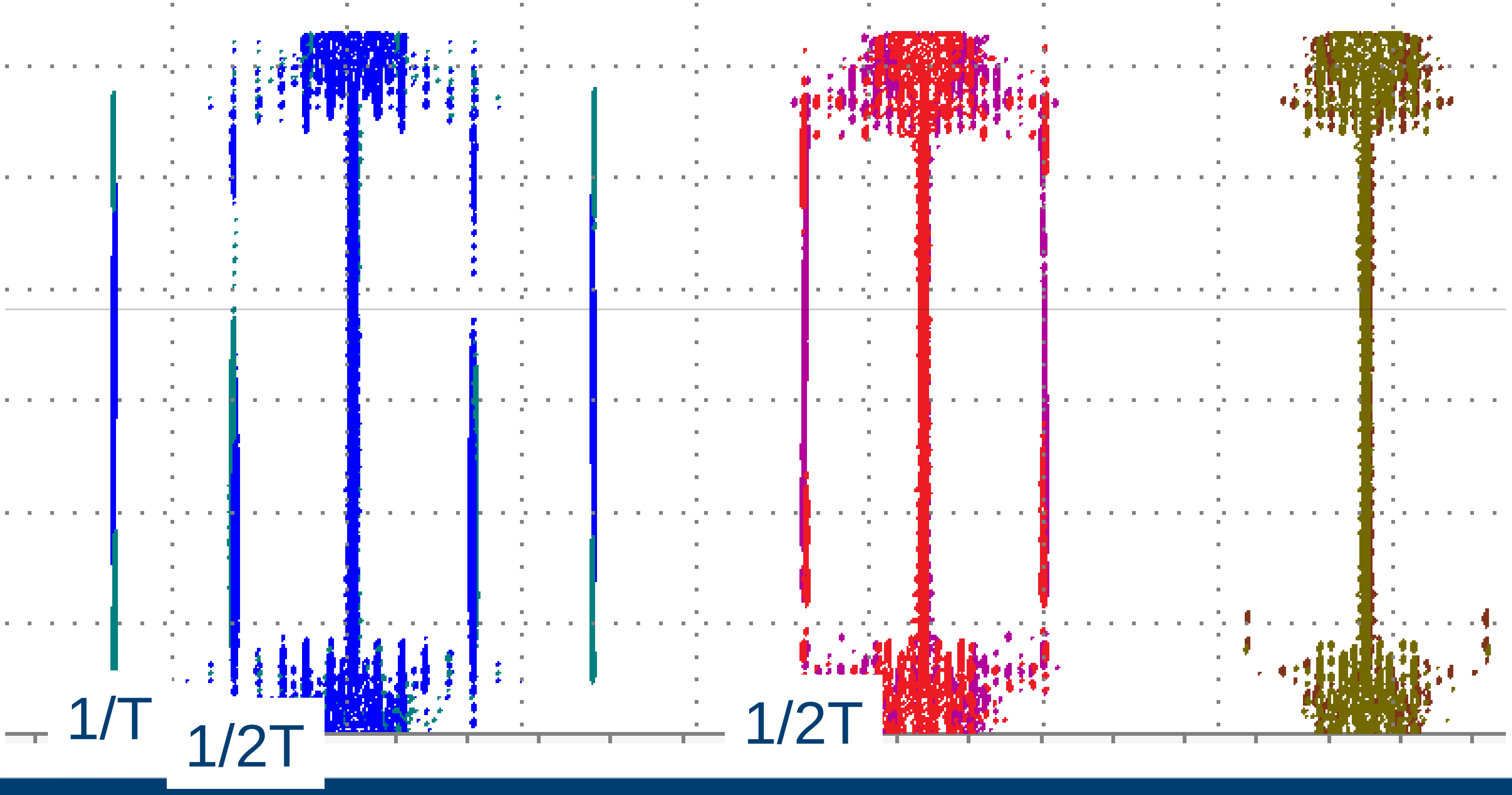
- Historically we just used the same shape for both parts
- But running the same shape in half time doubles the sweep =. 4x power
- Make new shape => only twice power

12	adiabatic decoupling	Crp32,1.5,20.2	...	3191.54	1500.00	0.64603
13	adiab. decoupling (bilev part)	Crp32,0.75,20.2	...	4513.52	750.00	1.2921

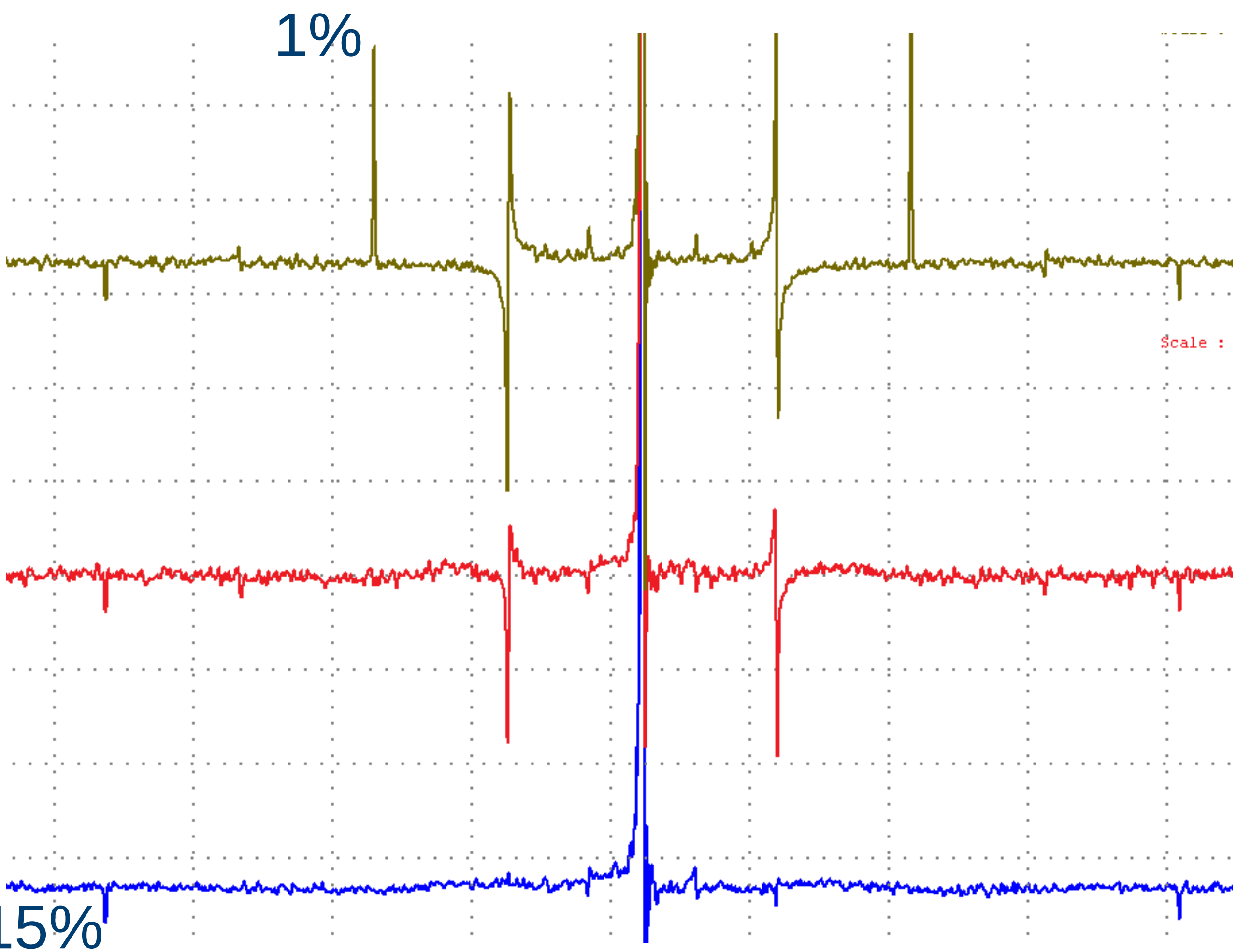
- Shapes adjusted for low Q – need to do this if making your own

Adiabatic bilevel decoupling results

- 1 scan, 2 scans, 4 scans
- Lowest contour 0.5% of highest point

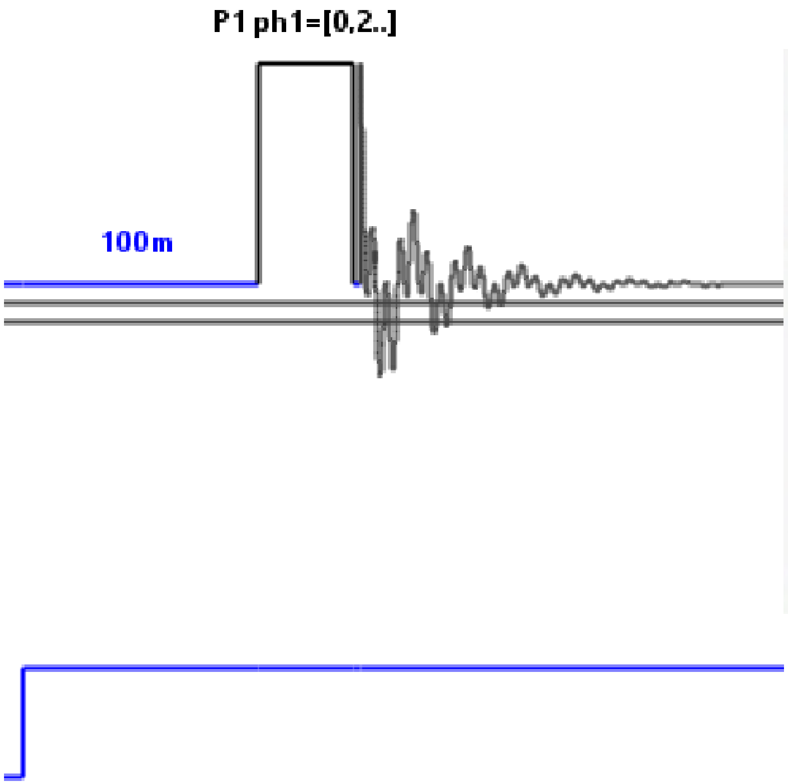


On resonance slices



Bilevel decoupling in zgpg: bi_waltz65_128 / 256

- Start decoupling before excitation pulse




```
bilev "l31=(nsdone+ds)%128+1"
1 pcpd*3.68133:0
  lo to 1 times l31
2 pcpd*3:0          ; R
  pcpd*4:180
  pcpd*2:0
  pcpd*3:180
```

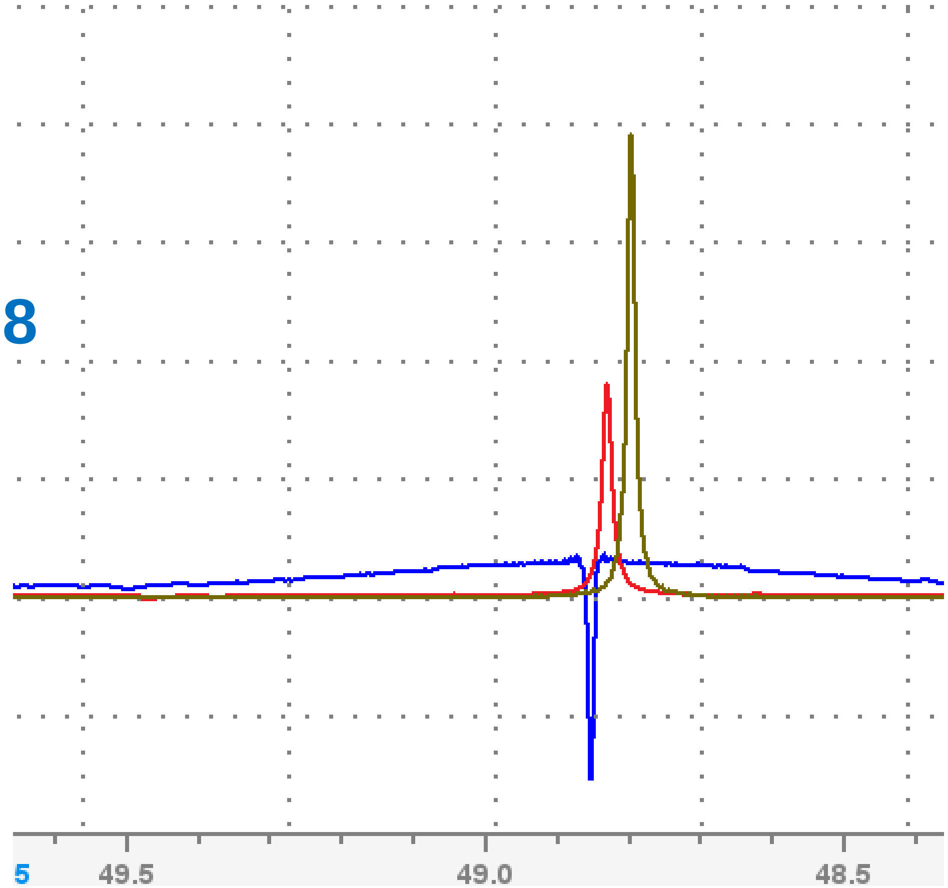
- CW decoupling period in this 100ms
- Start point of CPD sequence varies in controlled manner

DEPT experiments (also relevant for zgig)

ns=8, waltz65

ns= 8, bi_waltz65_128

ns= 32, bi_waltz65_128



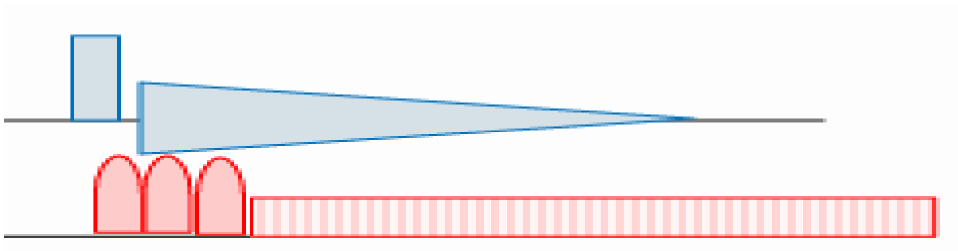
Bilevel decoupling in zgig / DEPT

- Can't use this trick as is – v bad decoupling in CW part
- PL switching: cpdprg2=bi_waltz16_32pl

```
bilev "l3l=(nsdone+ds)%32+l"
l pcpd*1.500:0 pl=pl3l
  lo to l times l3l
  pcpd*3:180 pl=pl30
2 pcpd*4:0
```

0	cpd	2777.78	90.00	0.14578
6	bilev cpd (cw part)	5555.56	45.00	0.58311

Shaped pulse bilevel decoupling
Clemens Anklin, Bruker US, unpublished?



Use shaped pulses for bilev part – eg BIP720,0.5,20.1

Supercycle the shapes eg P5M4

```
bilev "l31=(nsdone+ds)%128+1"
1 p63:sp15 ph21^ pl=sp15
lo to 1 times l31
2 pcpd*3:0 pl=pl12          ; R
  pcpd*4:180
```

```
  pcpd  :0
jump to 2
ph21=(360) 0 150 60 150 0 0 150 60 150 0 180 330 240 330 180 180 330 240 330 180
```

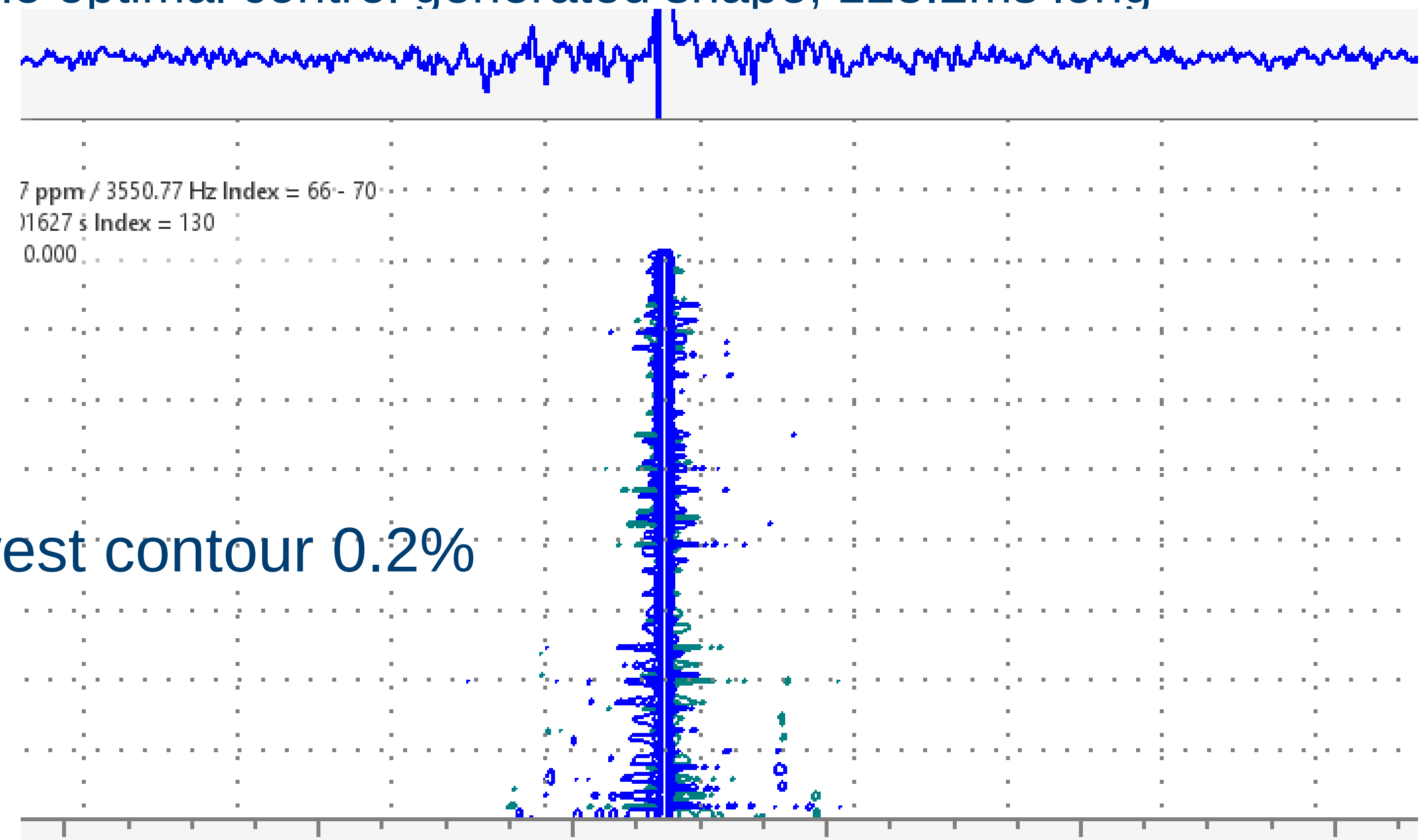
Pulse has to have a certain length, related to CPD supercycle length

BUSS decoupling

Next-Generation Heteronuclear Decoupling for High-Field Biomolecular NMR Spectroscopy†

Dr. Franz Schilling, Dr. Lisa R. Warner, Dr. Naum I. Gershenzon, Prof. Dr. Thomas E. Skinner, Prof. Dr. Michael Sattler, Prof. Dr. Steffen J. Glaser

- Single optimal control generated shape, 123.2ms long



Lowest contour 0.2%

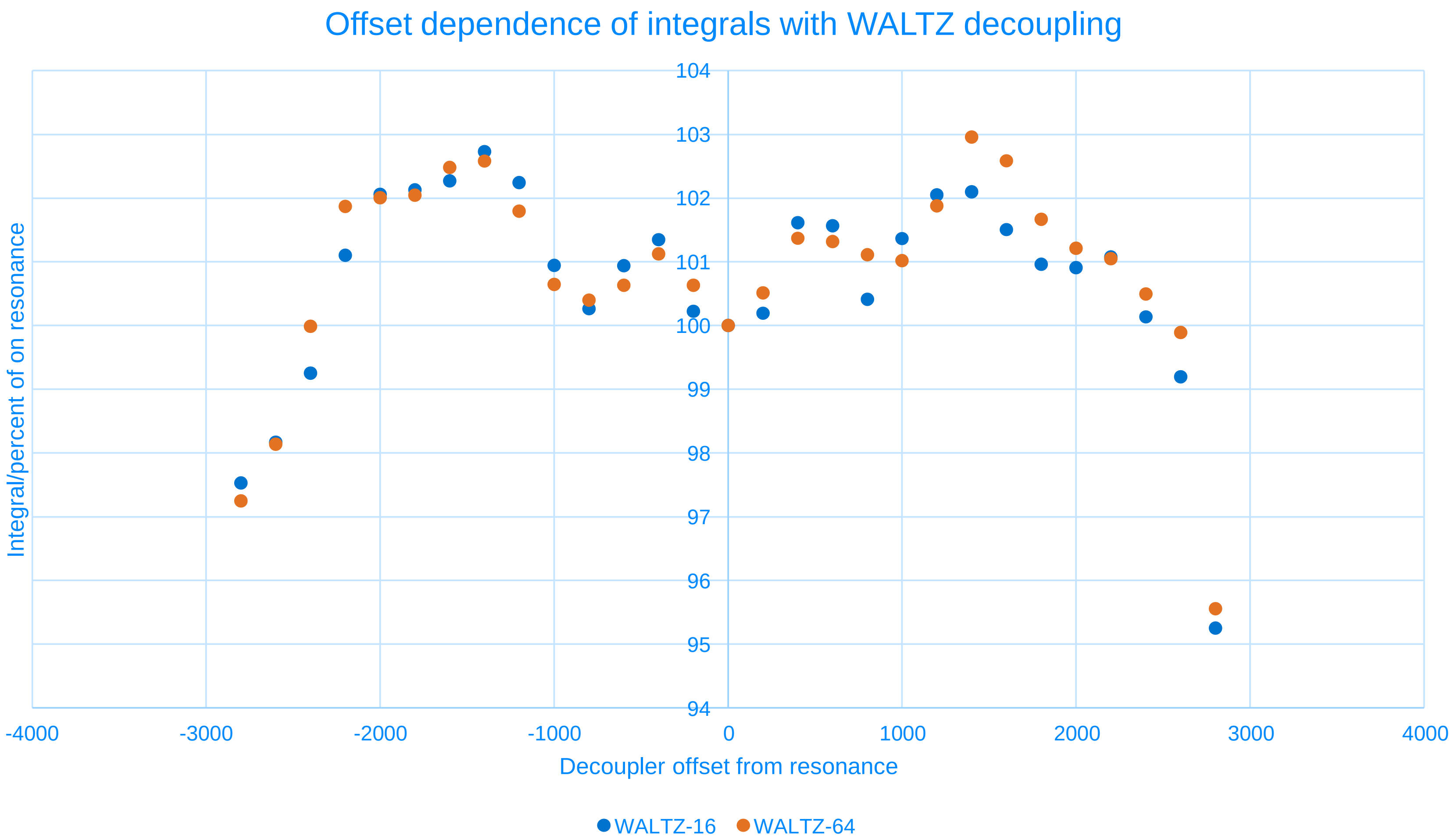
BUSS decoupling

8 ##$SHAPE_PARAMETERS= Type: 123.2ms RFmax=14.043kHz RFrms=4.4kHz BW=47kHz miscal=0

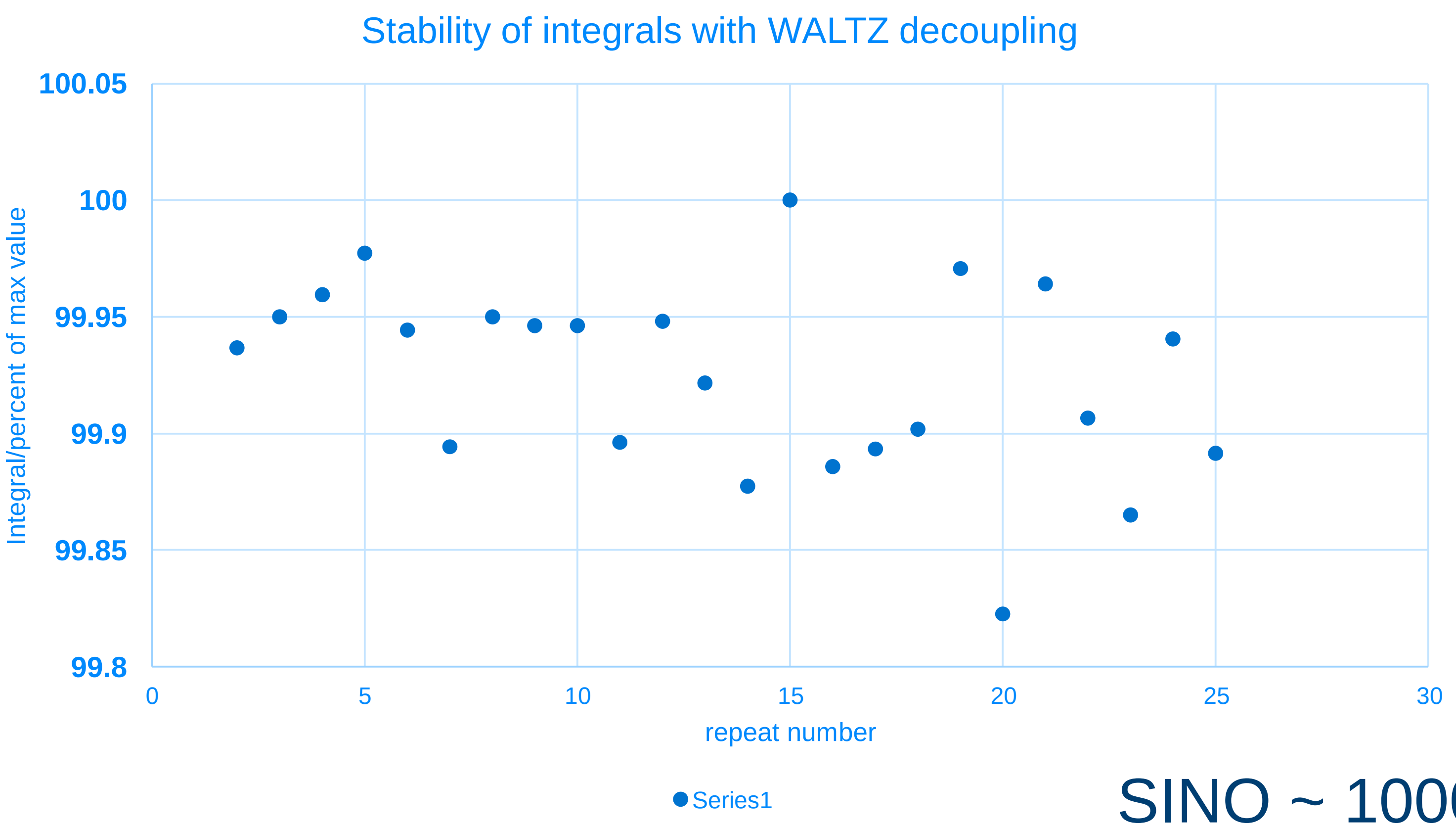
CPDPRG 2	bi_sp180pl.p63	...	E	File name for cpd2
SPNAM 63	Buss_dec	...	E	File name for SP63
SPW63 [W, -dBW]	11.641	-10.66		Shaped pulse power SPW63

- Power corresponding to 14.043kHz == 17.8us 90
- Shape is amplitude modulated – rms power 4.4kHz

Quantification



Quantification

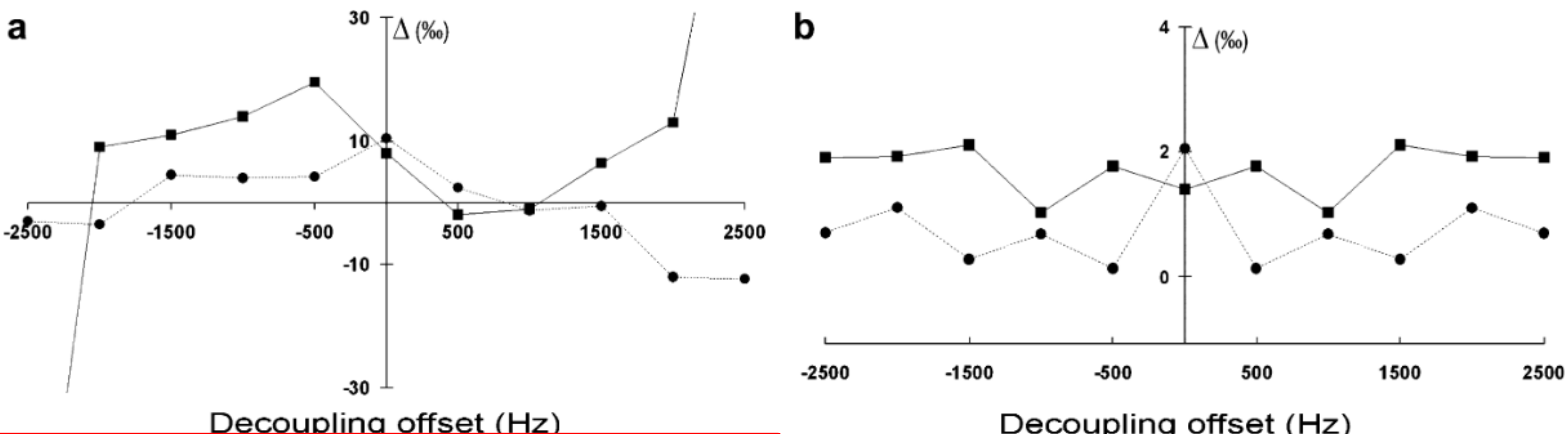


SINO ~ 10000:1

STDEV=0.04%

Quantification: adiabatic pulses for better uniformity

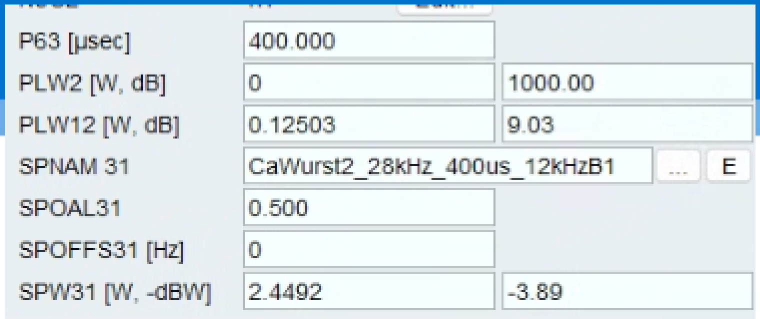
- Adiabatic 1H decoupling scheme for very accurate intensity measurements in 13C NMR, Eve Tenailleau, Serge Akoka
- https://doi.org/10.1016/j.jmr.2006.11.007



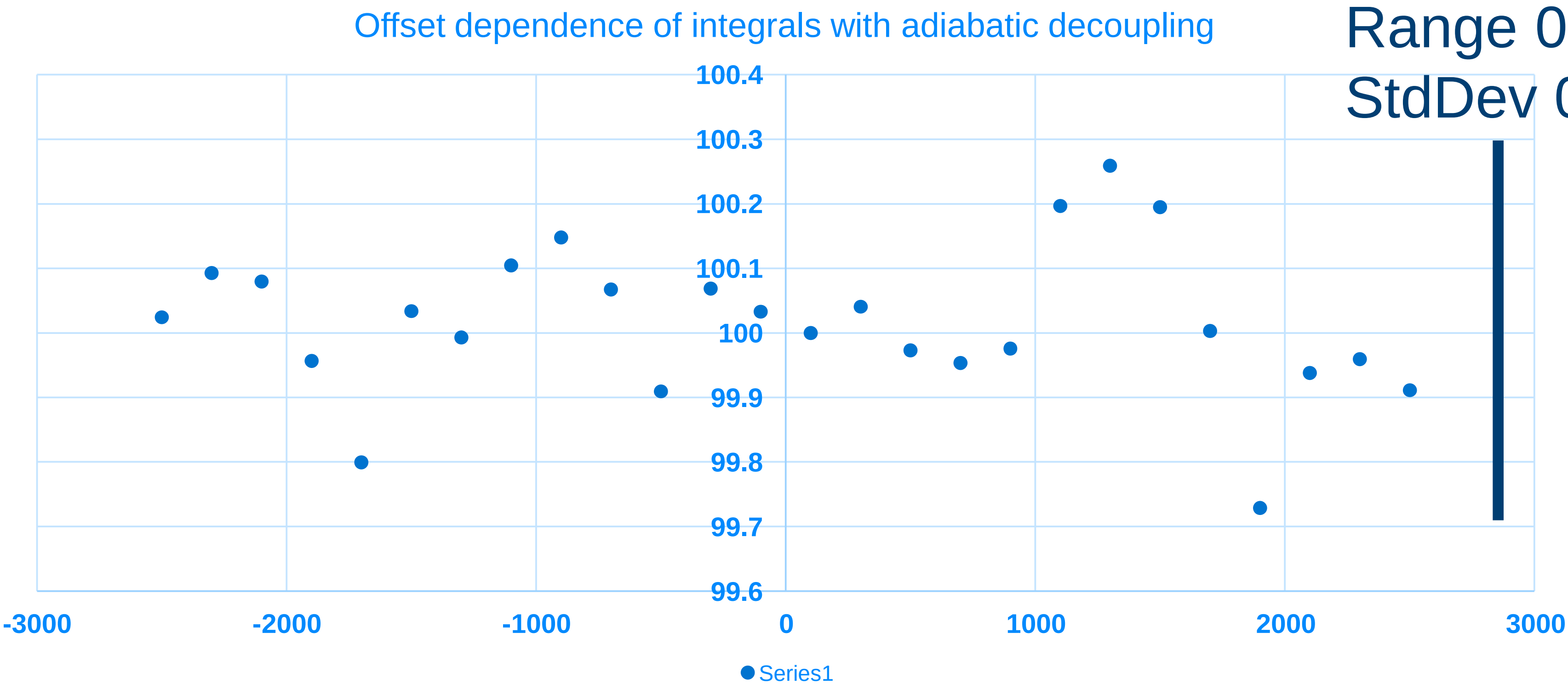
WALTZ-16 with $\omega_2^{max} = 53.1$ kHz.

cos/OIA pulses with $\omega_2^{max} = 75.2$ kHz, $T_p = 200\ \mu s$, $\Delta F = 14$ kHz

Quantification: adiabatic pulses for better uniformity

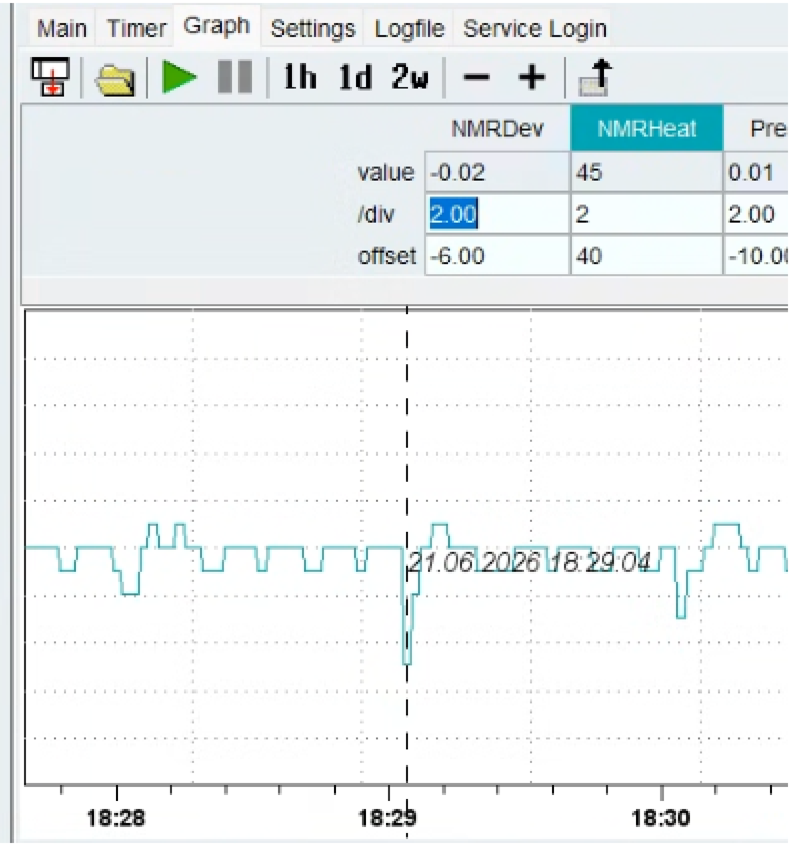


Range 0.5%
StdDev 0.12%



Cryoprobe monitoring

- Cryopanel
- Can set the plot scale for individual parameters
- Here coil heat drops from 50% to 45 percent with the pulse used on previous page
- This is absolutely fine
- If coil heater reaches zero, coil temp will increase and then warmup probe…



Setup tools: prosol

HR Square Pulses

0	cpd	2777.78	90.00	0.14578

HR Shape Pulses

Decouple

Nucleus 13C

12	adiabatic decoupling	Crp32,1.5,20.2	3191.54	1500.00	0.64603
13	adiab. decoupling (bilev part)	Crp32,0.75,20.2	4513.52	750.00	1.2921
34	low power adiabatic decoupling	Crp25,2.5,25.4	1784.12	2500.00	0.20188
35	low power adiab. decoupling (bi	Crp25,1.25,25.4	2523.13	1250.00	0.40377

Decouple

Nucleus 19F

12	adiabatic decoupling	Crp120,1.5,30.4	6180.39	1500.00	1.0451
13	adiab. decoupling (bilev part)	Crp120,0.75,30.4	8740.39	750.00	2.0902

Prosol defaults

- These are set from the files in <topspin>\exp\stan\nmr\lists\prosol
- Obs and dec files for H/C/N/F/P for different fields
- Care: default CPD pulse for carbon is too long at >=500MHz
  - <165ppm bandwidth with GARP4
  - But you should probably use adiabatic decoupling at this point!

BUSS decoupling in prosol

HR Shape Pulses

Decouple

Nucleus 13C

Decouple

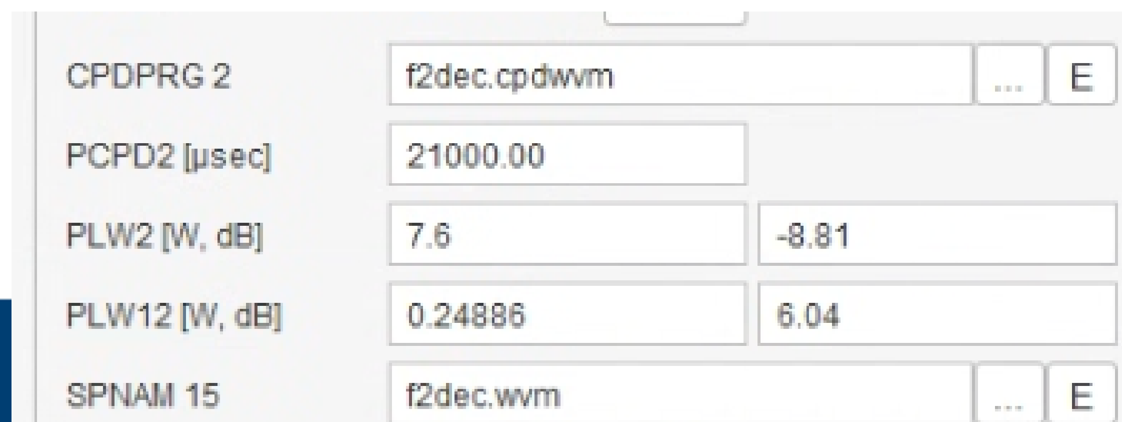
12	adiabatic decoupling	Buss_dec	...	14043.00	123200.00	12.508	

- Make a cpdprg:

```
#setphase
bilev "l3l=1"
1 p63:sp31:0 pl=sp31
  jump to 1
```

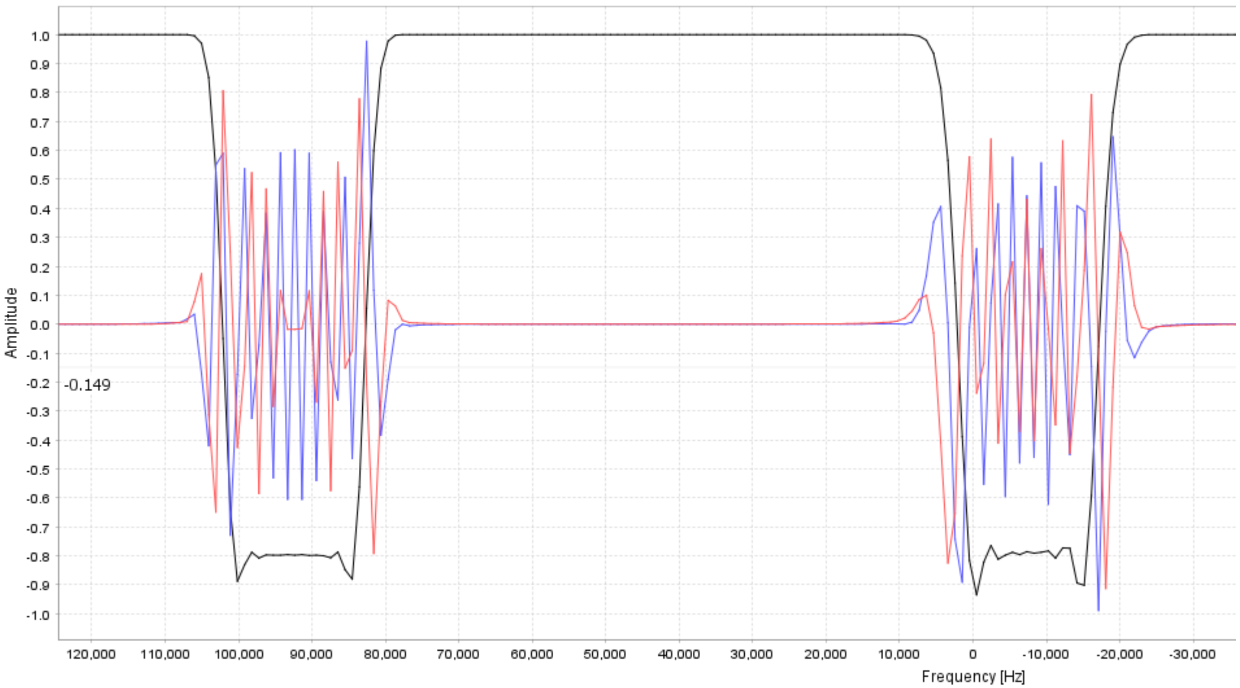
Setup tools: Wavemaker

- Wavemaker: automated shaped pulse setup
- Eg: adiabatic decoupling for f2 channel:
  - USERA2 = cpd2:wvm:f2dec: cawurst_d(cnst50 ppm, cnst54 us; Q=cnst55, sucyc=[p7]m4)
  - Or:
  - **WAVEMAKER2 = create_shape(cpd2, cawurst_d, name=f2dec, bandwidth=$cnst50 ppm, length=$cnst54 us, Q=$cnst55, supercycle=[p7]m4)**



Multi-band decoupling with wavemaker

- USERA2: cpds2:wvm: cawurst_d-8(20000Hz, 1 ms, 0ppm; Q=1.3, sucyc=[p7]m4) cawurst_d-2(20000Hz, 1 ms, 100000Hz; L2H, Q=1.3, sucyc=[p7]m4)



Local lists in TS4

- NB in TS4, the generated shapes created thus by wavemaker are (only) stored locally in the dataset (in the lists/wave subdirectory of the expno directory), not in the global exp/stan/nmr/listswave/user. Likewise the cpd prog in lists/cpd.

lists	15/06/2026 12:07
pdata	15/06/2026 11:03
acqu	15/06/2026 12:38
acqus	15/06/2026 12:38
audita.txt	15/06/2026 12:07
format.ased	15/06/2026 12:38
wvm.log	15/06/2026 12:12
wvm.par	15/06/2026 12:12
wvmPPInfo.xml	15/06/2026 12:12

Performance summary

- WALTZ-64/65 : Bandwidth **2.2x RF field strength**
  - Mostly only 1H decoupling
- GARP-4 : Bandwidth **>5x RF field strength**
  - For large couplings and small bandwidths
  - Or where shaped pulses are a problem
- Adiabatic decoupling: Bandwidth prop.to **(RF field strength)^2**
  - Can be adapted to almost any case
  - **13C QNMR**
- BUSS decoupling: Fixed bandwidth of **47kHz**
  - **Should we use this more regularly?**

Overview of CPD sequences in topspin

- Waltz16 / waltz64/ waltz65 / Garp / garp4 / dipsi2
- Bi_waltz65_128/256 – bilevel waltz for zgpg
- Cwp – continuous wave (implemented as a repeated identical pulse)
- Bi_p5m4sp_4sp.2 – bilevel shaped pulse dec with p5m4 and different shapes
- bi_sp180pl.p63 – single shape repeated p63/sh63, no supercycle
- P5m4sp180* - versions of p5m4 supercycle of a shaped pulse
- Mlevsp180* - versions of mlev16 supercycle of a shaped pulse

Example cases: 1H{13C} 2D

- Cpdprg2= bi_p5m4sp_4sp.2
- Set shapes in prosol to give eg >200ppm inversion
- Crp32 is a bit tight @500MHz => Crp42 (~same power as 70us CPD)

- Or BUSS

Example cases: 1H{13C} 1D

- Eg QNMR

PULPROG	zgigld
CPDPRG 2	bi_p5m4sp_4sp_lp

```
#setphase
bilev "l31=(nsdone+ds)%4+1"
1 p60*0.5:sp59:0 pl=sp59
  lo to 1 times l31
  p60:sp60:0 pl=sp60
2 p60:sp60:150
  p60:sp60:60
```

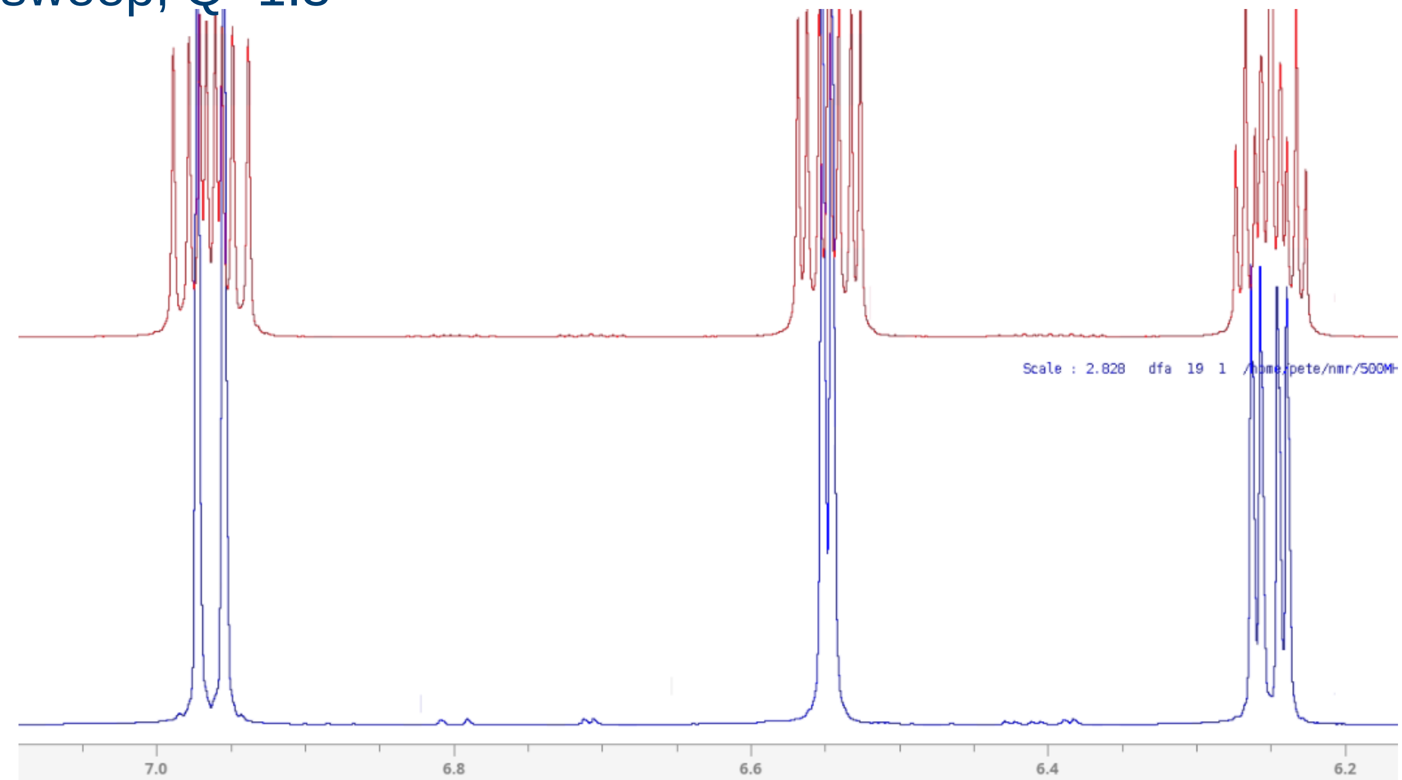
TS4:

34	low power adiabatic decoupling	Crp38,2.5,25.4	...	180.00	2199.62	2500.00	0.16257	
35	low power adiab. decoupling (bil	Crp38,1.25,25.4	...	180.00	3110.73	1250.00	0.32514	

P[60]	=	SHPW[34]	*	1.0	2	# 180 deg adiabatic low power dec., F2, 13C
SH[60]	=	SH[34]	*	1.0	2	# adiab. low power dec., F2, 13C
SH[59]	=	SH[35]	*	1.0	2	# adiab. bilev low power dec., F2, 13C

Example cases: 1H{19F}
NB filters!!

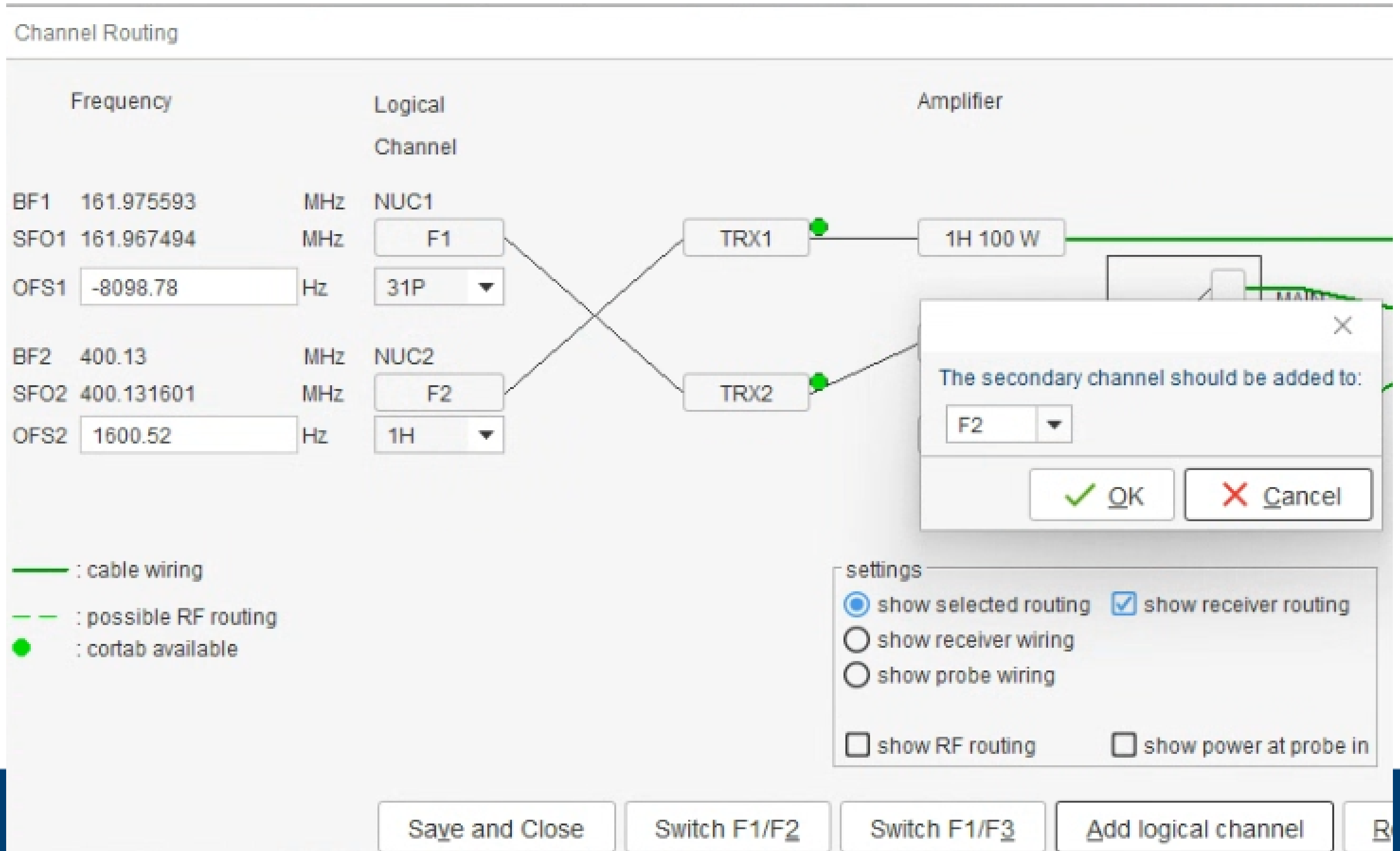
- Large BW but small J => Long adiabatic pulse OK
- 4.5ms, 180kHz sweep, Q=1.3



		Filename	∡ [°]	RFF[Hz]	PuW[µs]	Pw[W]
12	adiabatic decoupling	Crp180,4.5,20.1_q	180.00	2857.58	4500.00	1.0041
13	adiab. decoupling (bilev par	Crp180,2.25,20.1_	180.00	4050.05	2250.00	2.0171

Example cases: 31P{1H}

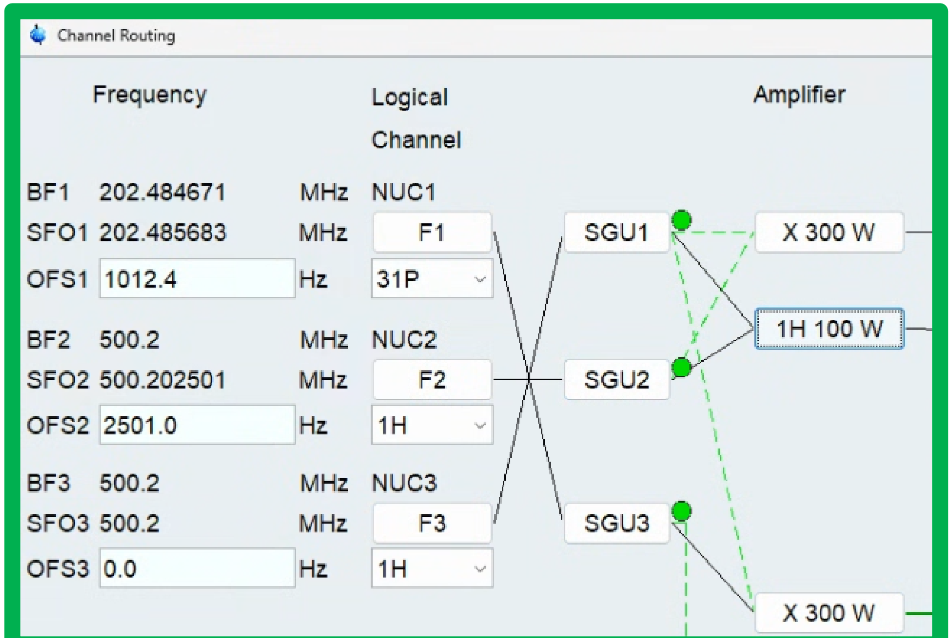
- Bi_waltz65_128 / 256
- CPD + CW:



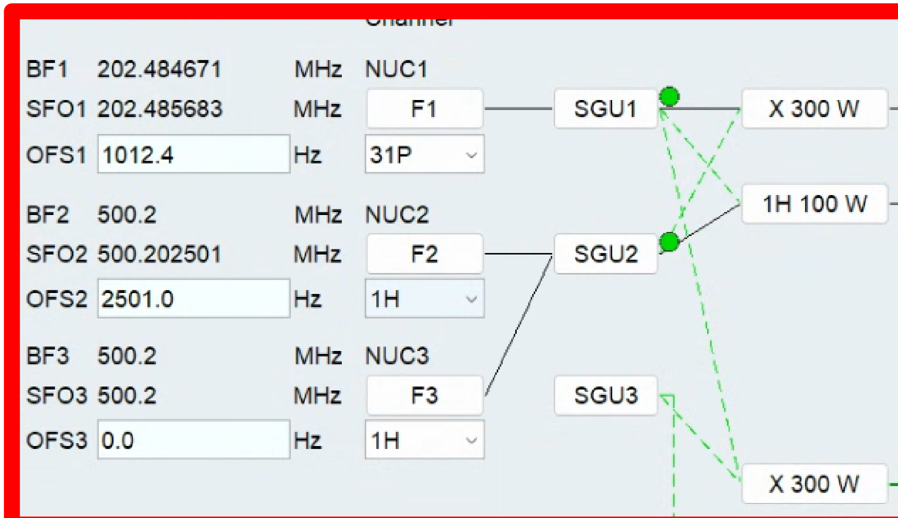
Example cases: 31P{1H}

- CPD + CW on AVIII:

OK

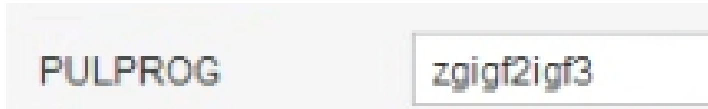


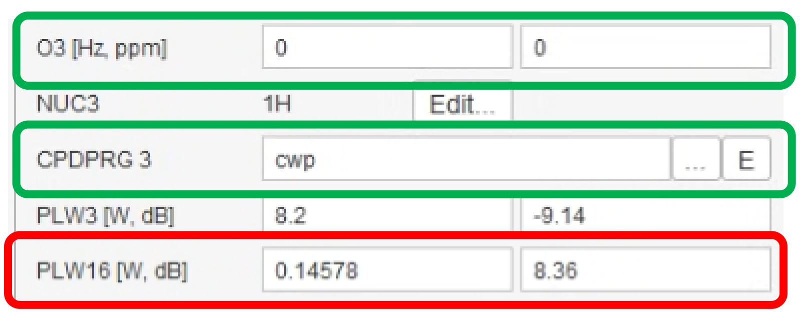
NOT OK!!



Example cases: 31P{1H}

- CPD + CW:





Set exactly on res

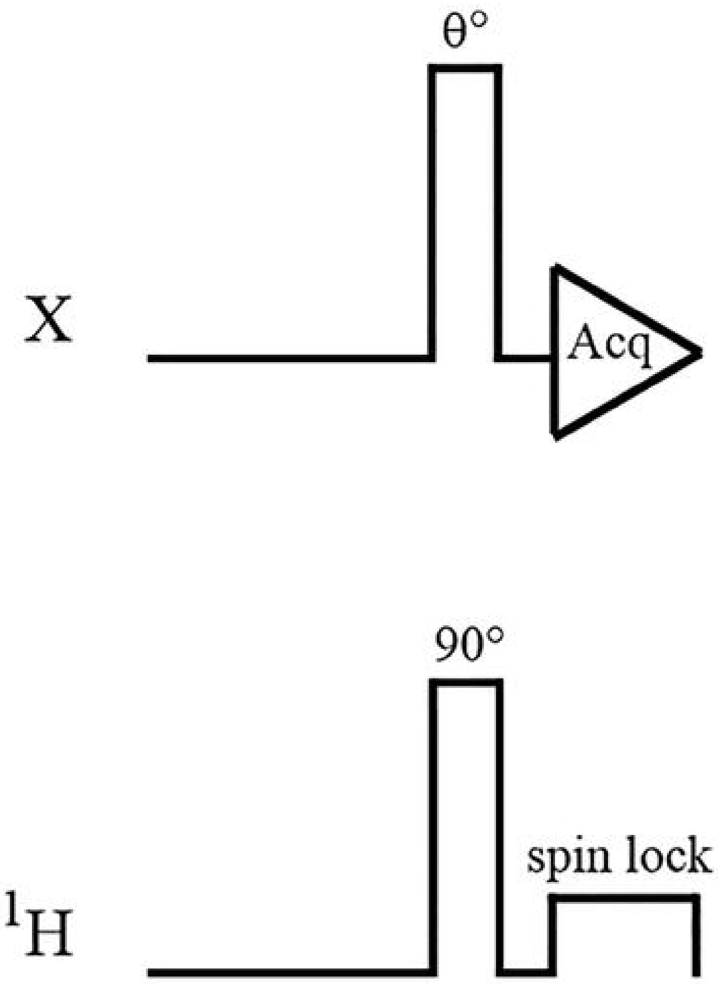
Could use (much) less power

Alternative possible approach

- Adiabatic spin locking

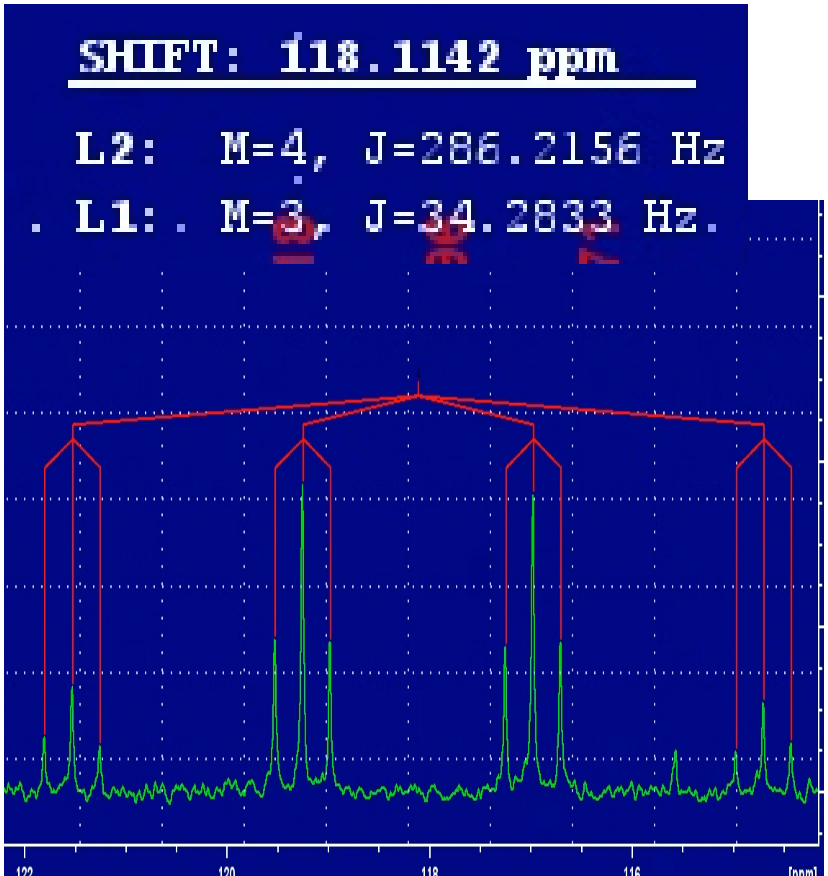
- **Complete elimination of decoupling sidebands in the case of very large heteronuclear scalar coupling by spin locking using adiabatic pulses**

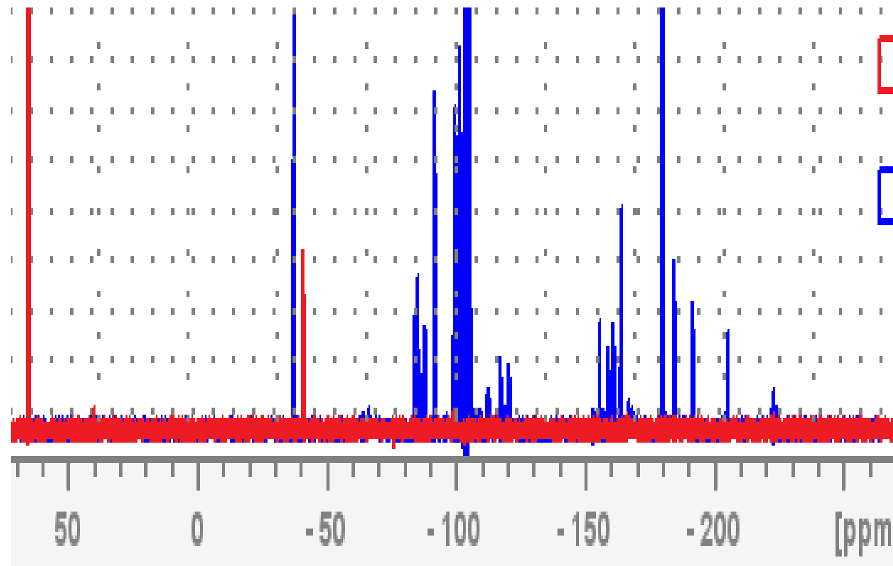
Kilka, Spectroscopy Letters 2026



Example cases: 13C{19F}{1H}

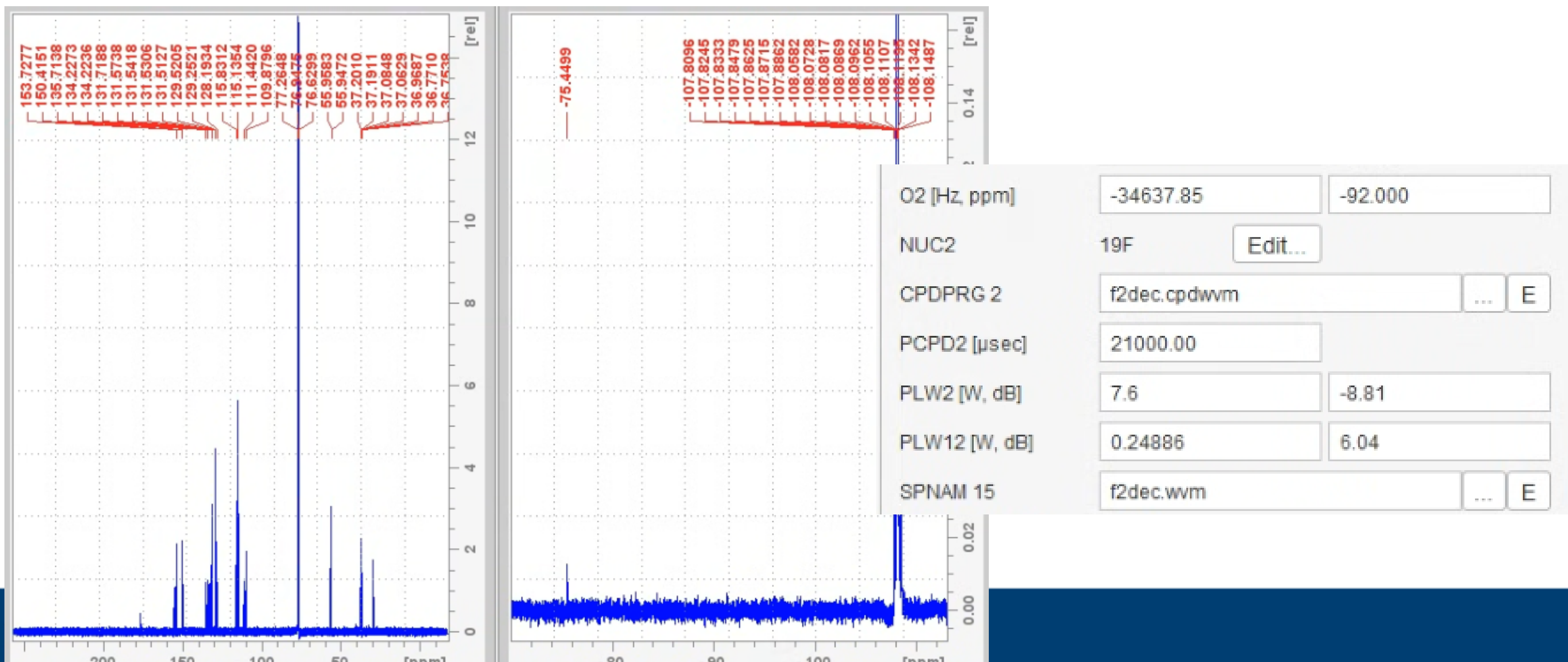
- Very challenging due to large bandwidth (>300ppm) and J (~300Hz)



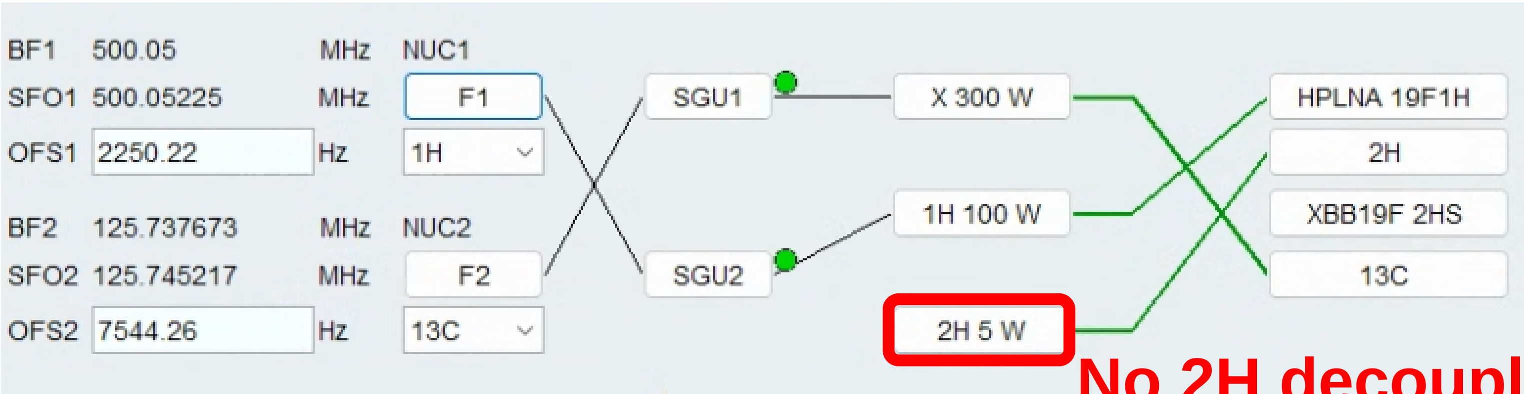


Setup tools: AU programs

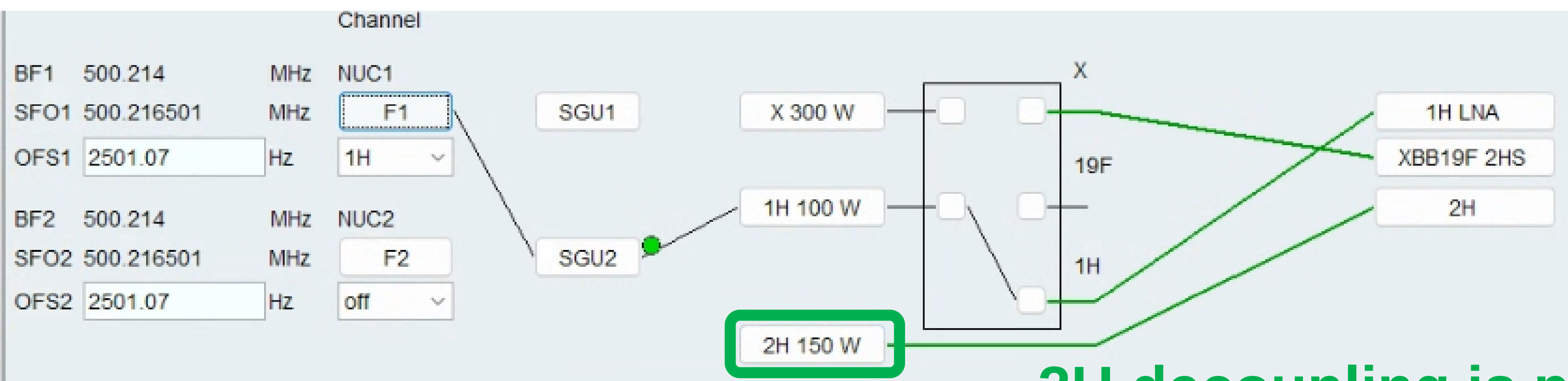
- “au_getlim3” – WIP, ask Bruker…
- Eg for 13C{19F}: expno 9 = 13C, expno 10 = 19F, expno 11 = 13C{19F}
- **au_getlim3 ref=9,10 drange=2000 wvm=1**



Considerations for 2H decoupling



No 2H decoupling possible



2H decoupling is possible!

Considerations for 2H decoupling

- In order to switch between the lock pulsing / decoupling: pp **zgig2h**
- Lock can be on during D1
- Enforce short AQ: UDEFT?

SFO2 [MHz]	107.4853392		Frequency of ch. 2
O2 [Hz, ppm]	376.20	3.500	Frequency of ch. 2
NUC2	2H	Edit...	Nucleus for channel 2
CPDPRG 2	waltz16	... E	File name for cpd2
PCPD2 [µsec]	500.00		F2 channel - 90 degree pulse for decoupling sequence
PLW2 [W, dB]	0	1000.00	Power PLW2
PLW12 [W, dB]	2.492	-3.97	F2 channel - power level for CPD/BB decoupling

Example 13C{2H}{1H}