Shimtools Optimisation

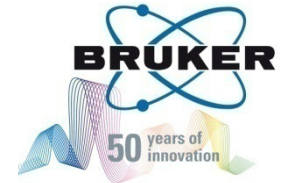Clemens Anklin, Detlef Moskau,
Rainer Kümmerle

pre-ENC workshop, April 2010

Shimming: which tools do exist?

- Operator / manual shim:

  - Maximize locklevel

  - GS-mode: observe FID (shape, length) or real-time FT

- Maximize locklevel automatically:

  - BSMS AUTOSHIM

  - „tune": different algorithms

- Gradient Shim:

  - „gradshim": first version of gradient shim

  - „topshim": improved gradient shim

Bruker BioSpin
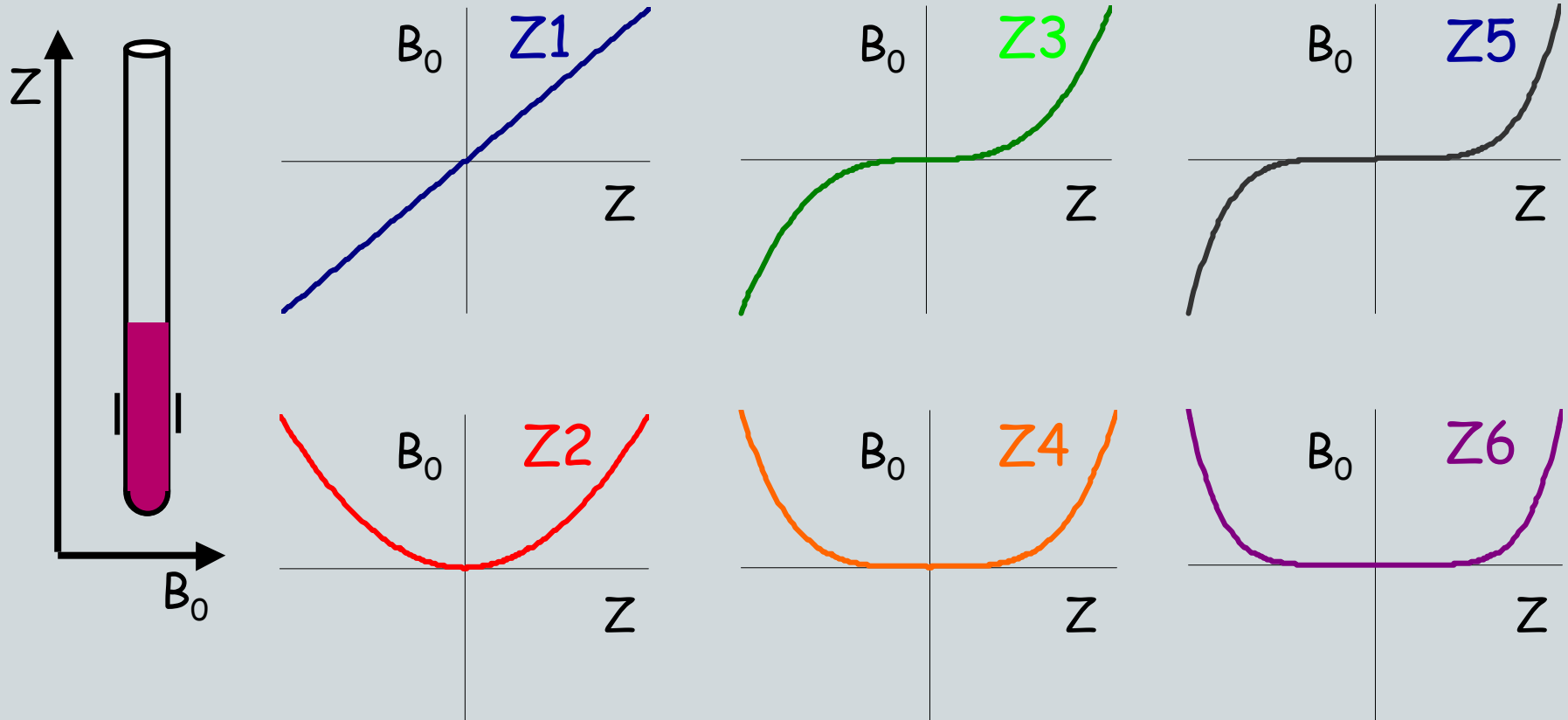
Shimming: some preparation...

- Manual Shim & automatic lock level optimization require:

  1. Correct lockphase

  2. Correct lock-power for solvent

  3. Idle time (waiting) after changing a shim

  4. Correct lock PID (feedback loop) parameter settings

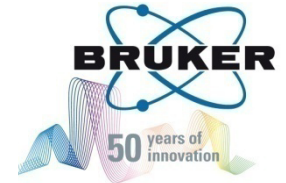- Gradient shim requires:

  1. (almost) no preparation

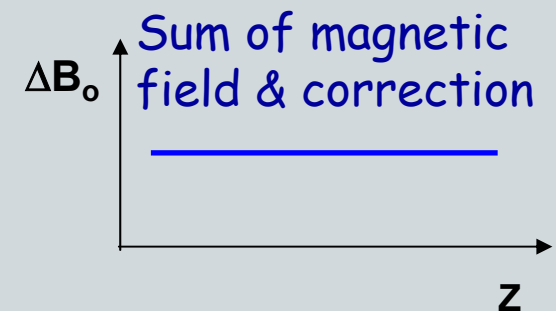**Bruker BioSpin**
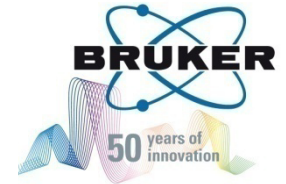
Manual Shim: Basics
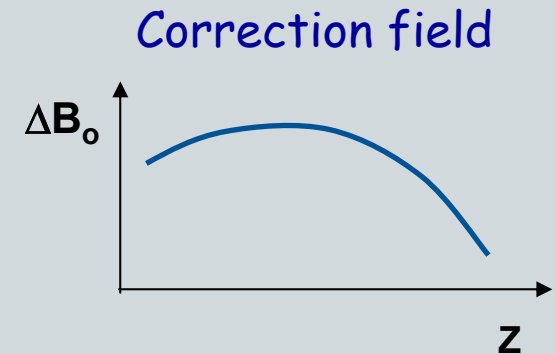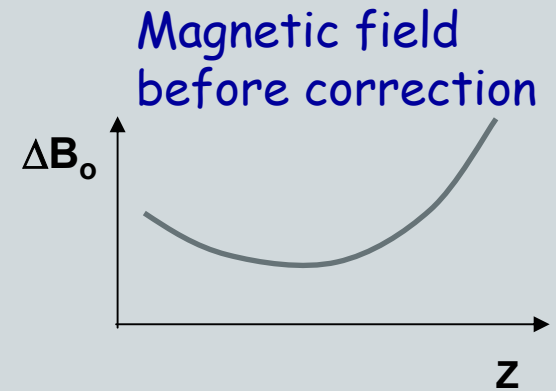
„On-axis" (Z or spinning) shims
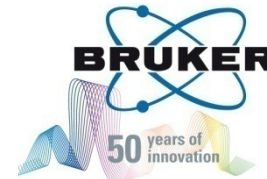
Manual Shim: Basics

Example of field inhomogeneity due to Z1 & Z2 mis-setting.

Correction achieved by:
applying correction field of same magnitude but opposite sign

Magnetic field before correction

ΔB_o

Z

Correction field

ΔB_o

Z

Sum of magnetic field & correction

ΔB_o

Z

Bruker BioSpin

Manual Shim: Basics

- Start with "reasonable" shim file (same probe(type), recently saved, same solvent, …)

- start spinning (20 Hz for 5mm, 14 Hz for 10mm)

- optimize Z1 - Z3 (maximize lock level) in iterations

- stop spinning, optimize Z1, Z2 (sample sits now on turbine)

- optimize off-axis shims (X, Y, X^2-Y^2, XY, XZ, YZ, …)

- go back to on-axis shims (Z1 - Z5)

- check lineshape:
  > sharp singlet in spectrum
  > water sample: residual water after presat (water line width without presat is entirely determined by radiation damping, NOT shim)
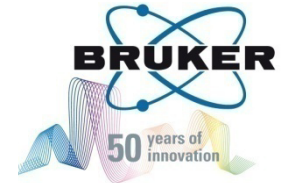
Bruker BioSpin

Manual Shim: Basics
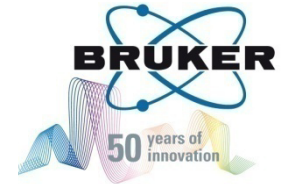
Lineshape with imperfect On-axis shims (Bruker Magnets)

OK	Z1 wrong	Z2 Too high	Z3 wrong	Z4 too high
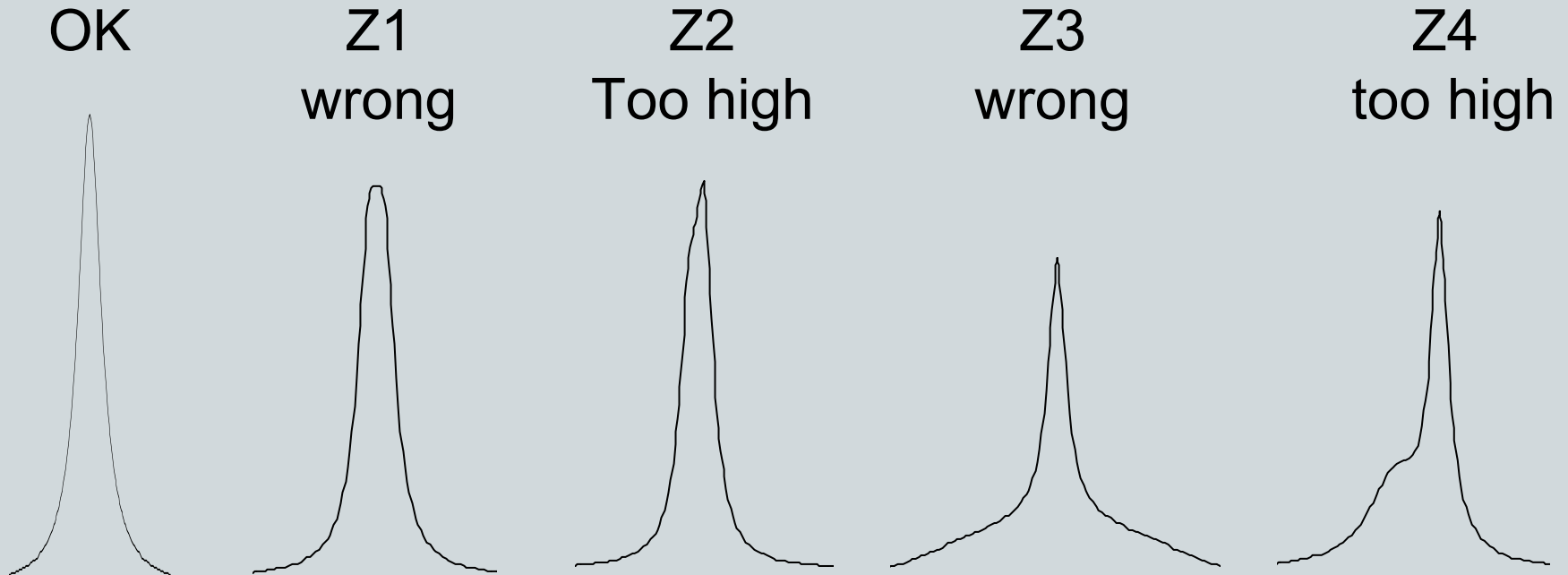
Z5 behaves like Z3, but lower in hump
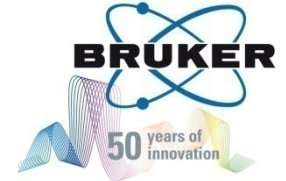Z6 behaves like Z4, but lower in hump

Bruker BioSpin

Maximize lock level automatically

- BSMS AUTOSHIM

- TUNE (different algorithms)

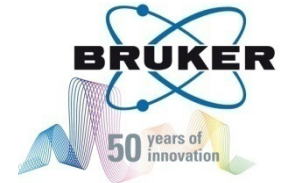- Difference between AUTOSHIM & TUNE ?

Bruker BioSpin

Maximize lock level automatically

AUTOSHIM:

- stepwise variation of selected shims (correct stepsize!)

- approaching good shim

- Long term: autoshim can maintain homogeneity
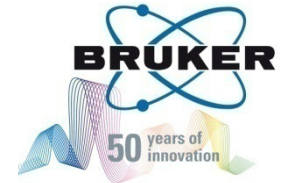
- Short term: random variation of shims & lineshape

Bruker BioSpin

Maximize lock level automatically

Use of AUTOSHIM:

- In case of shim drift

- Rather bad homogeneity

- Compensation of cryogen evaporation & sample evolution

- Not necessary / reasonable if shims are stable

- Not necessary / reasonable for short-term experiments

- Can increase t_1-noise in 2D-experiments

Bruker BioSpin
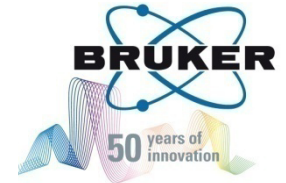
Maximize lock level automatically

tune:

- Optimization of a selected shim (locklevel)

- Optimization of subsequent shim (locklevel)

- Stops after a given number of iterations

- Used to optimize homogeneity before a NMR experiment

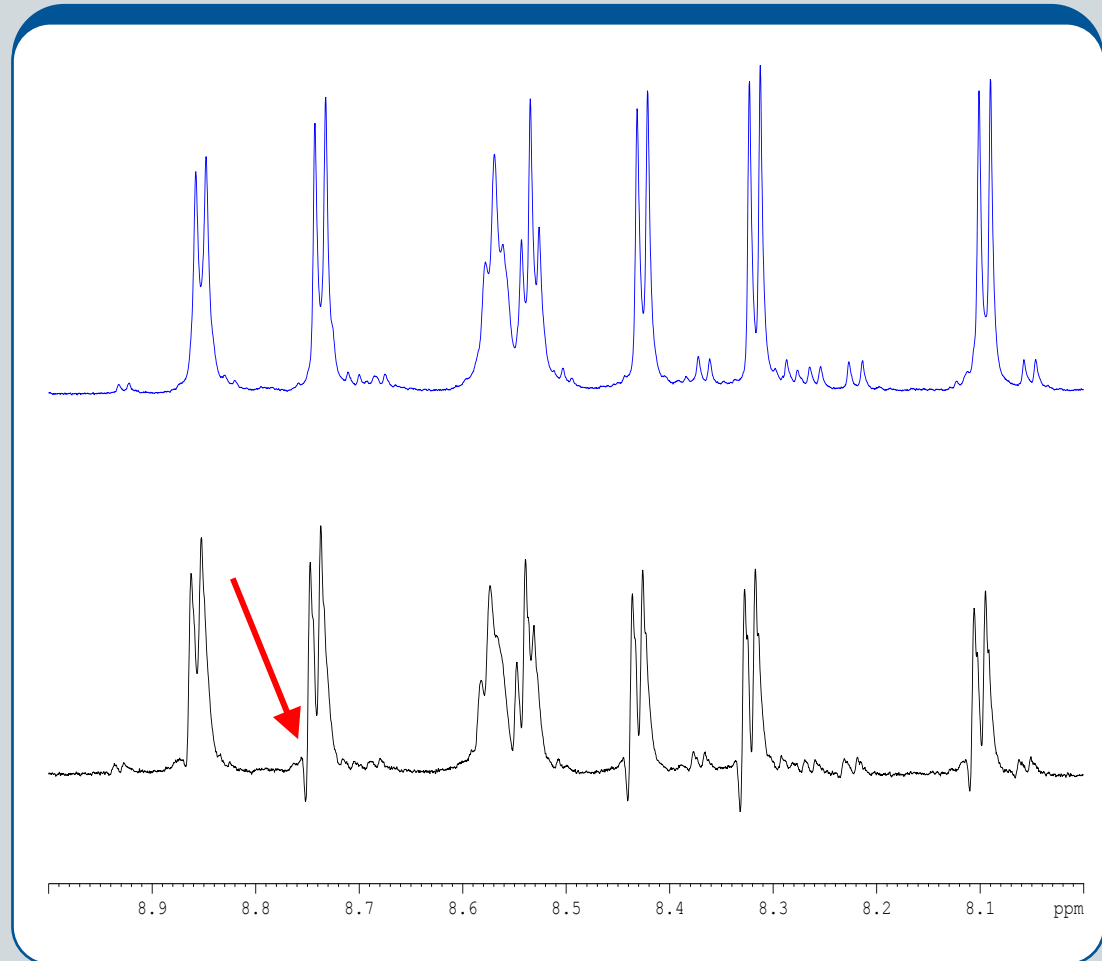- Can be combined with Topshim

Bruker BioSpin

TOCSY wihtout gradients: t_1-noise

- AUTOSHIM:

- Can increase t1-noise

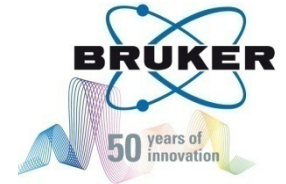- Especially critical for lossy aqueous solutions

increased t_1-noise
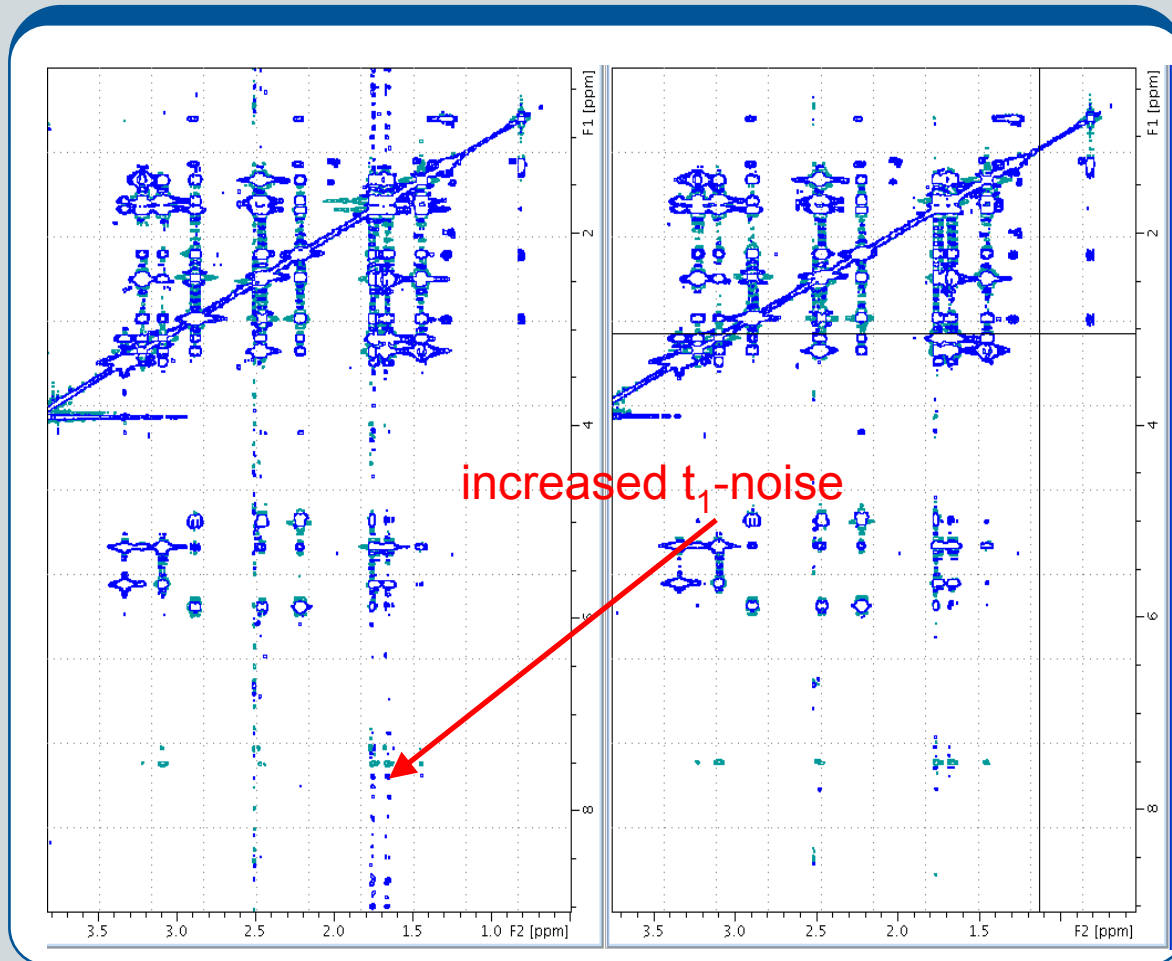
WATERGATE: gradient effects
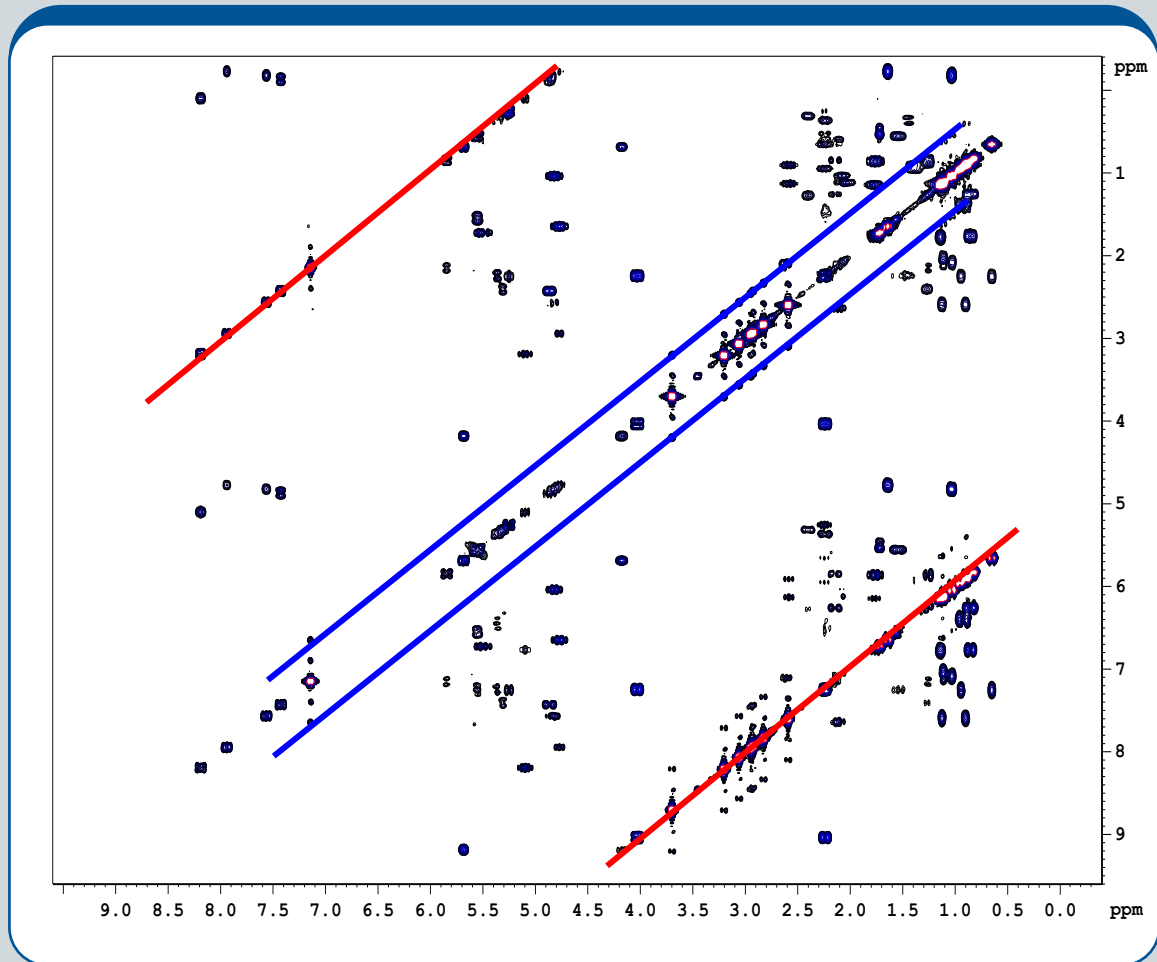
- WATERGATE:

- Lockphase wrong (30º)

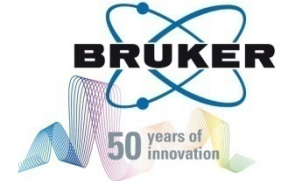- Depending on offset (positive / negative) artifact can be on right or left side of signal
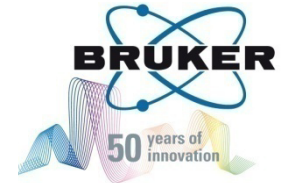
Gradient-COSY

- COSYGPQF:

- Lockphase wrong by ca. 40°

Gradient shim methods: preparation...

- Gradient shim methods require basically no preparation

- BUT:

  - Lock parameter must be correct, especially phase

  - Gradshim requires existing shim map

  - Topshim requires existing reference pulse widths

- AND...

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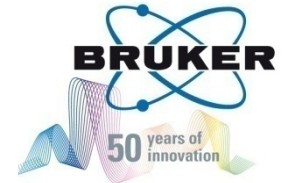
Gradient shim methods: preparation...

AND... What else should we know?

- Gradient shim is based on a 1D- or 3D-imaging experiment

- Homogeneity is measured via localized frequency (phase)

- Anything that influences the quality of the imaging experiment will have consequences for the result of the the gradient shim
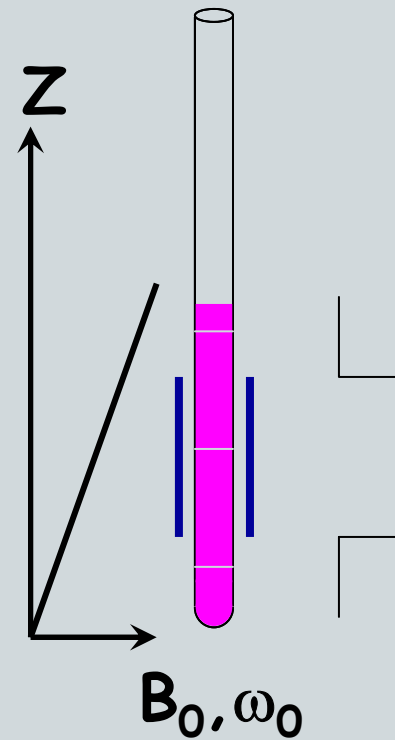
Bruker BioSpin

Gradient Shimming

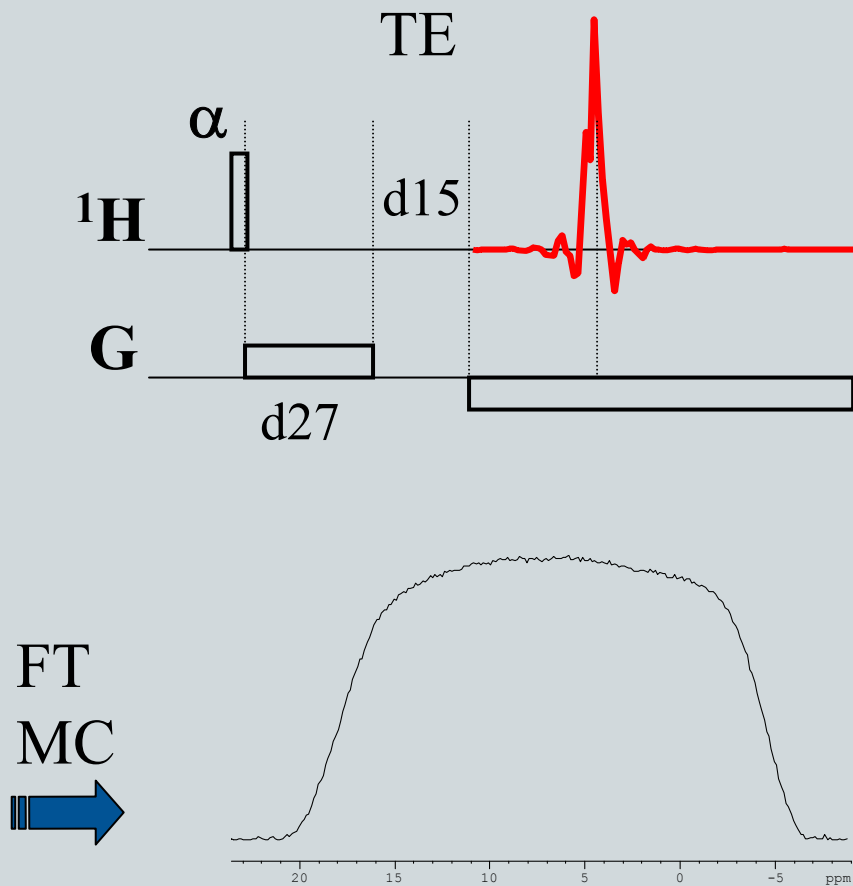- "Gradient Shimming" uses simple gradient echo sequence to localize the frequencies along the Z (X,Y) axis

- Those frequencies are a measure of the homogeneity

- For better precision, frequencies are expressed as phase

TE

α

^1H

d15

G
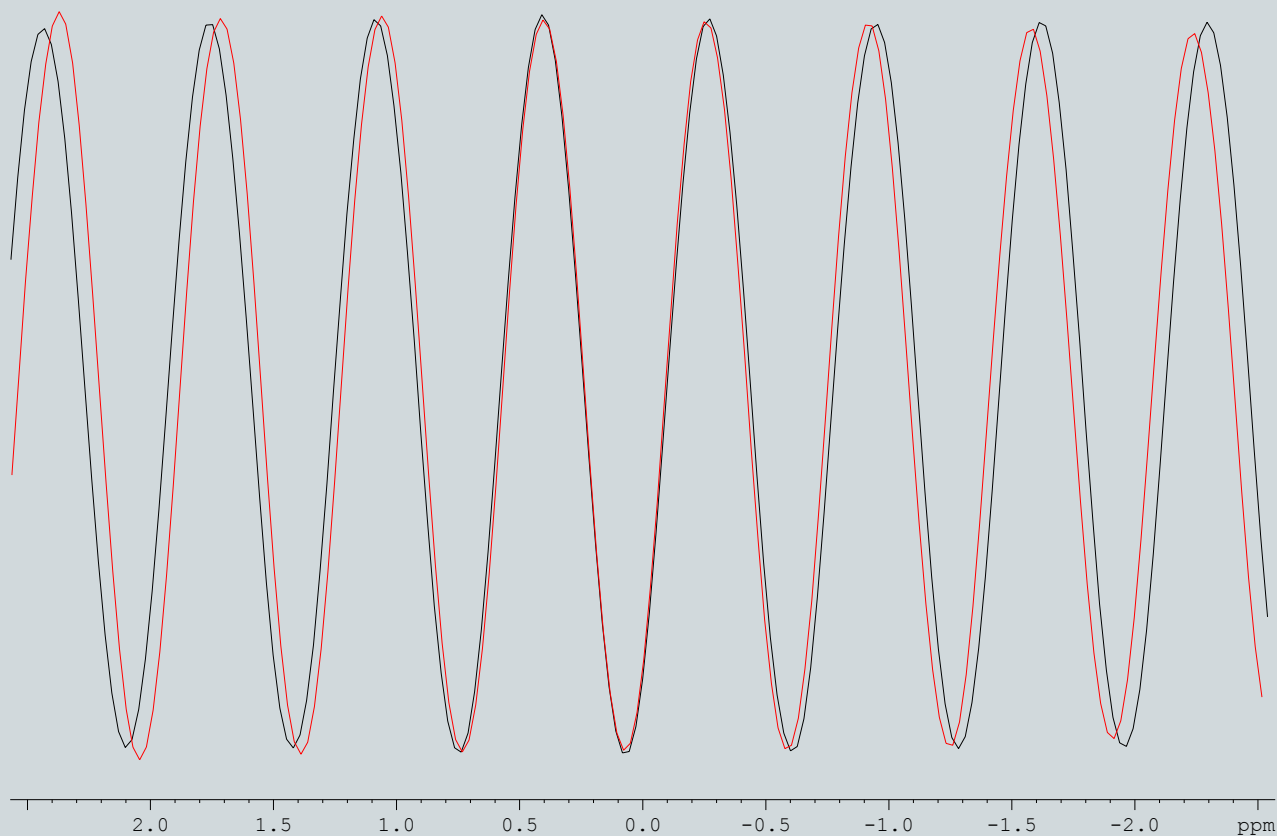
d27

FT
MC

Z

B_0, ω_0
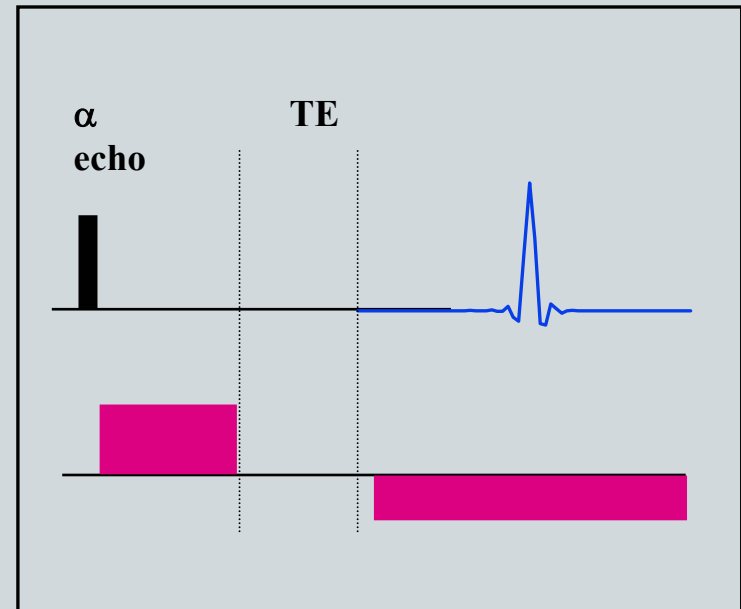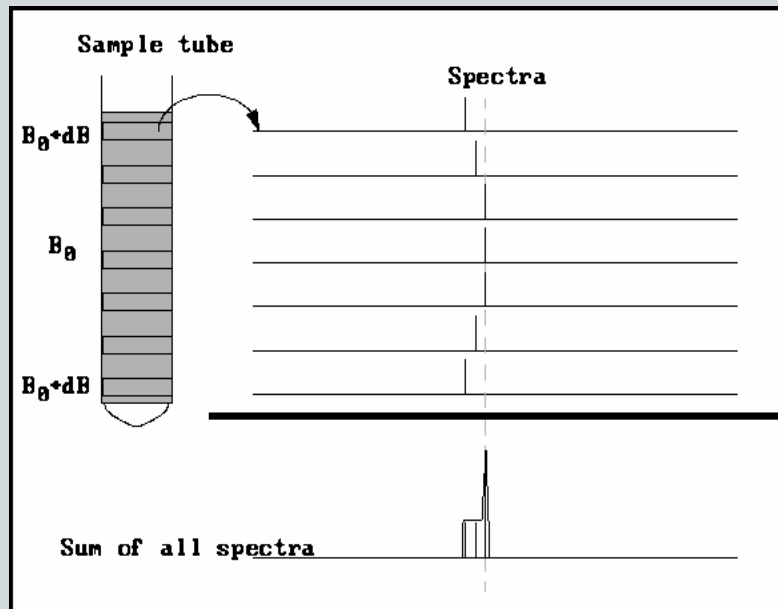
Gradient Shimming: the mapping information

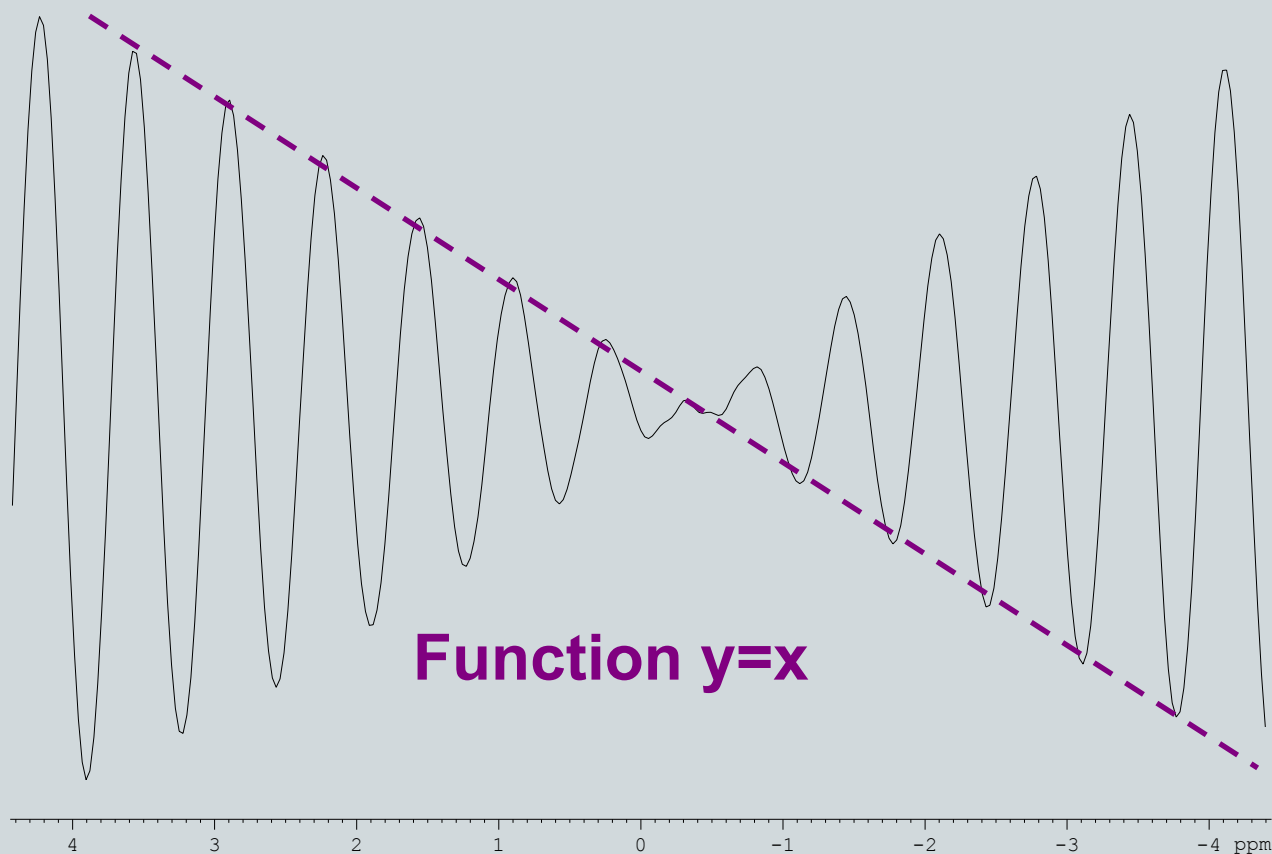red: profile with Z-shim detuned

black: all shims perfect

Bruker BioSpin

Gradient Shimming: the mapping information

Difference of profiles with perfect shims & Z-shim detuned

Function y=x

Bruker BioSpin

Difference of profiles with perfect shims & Z2-shim detuned

Function $x=y^2$

7   6   5   4   3   2   1   0   -1   -2   -3   -4   -5   -6   -7   ppm

Bruker BioSpin
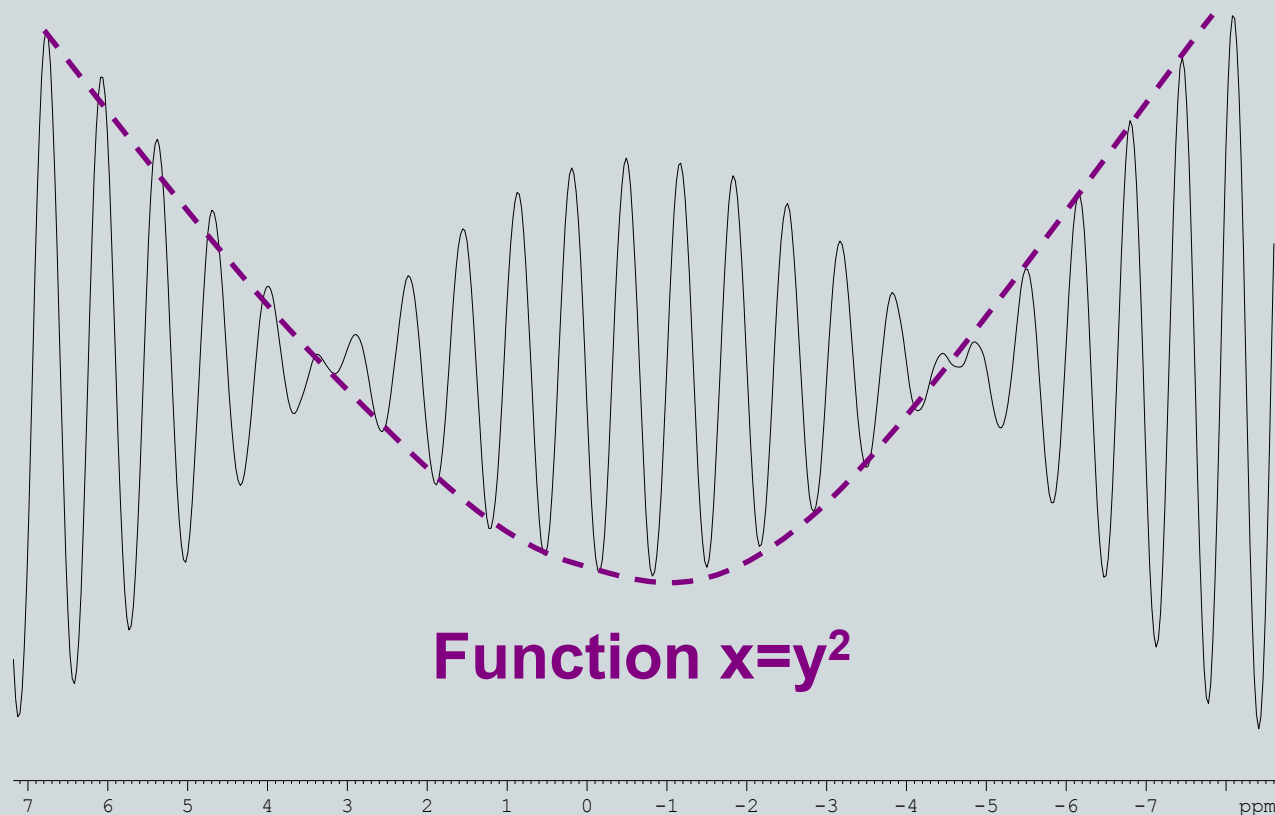
Gradient shim: typical problems
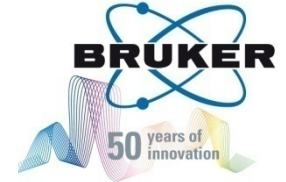
1. Partial or complete loss of magnetization during echo time TE:

   - Starting shim is very bad
   - Very short T_2
   - Sample presents severe inhomogeneity (air bubble, ...)
   - Diffusion
   - Convection

2. Solvent molecules are not stationary during experiment

   - Diffusion
   - Convection

Bruker BioSpin

Gradient Shimming & Convection

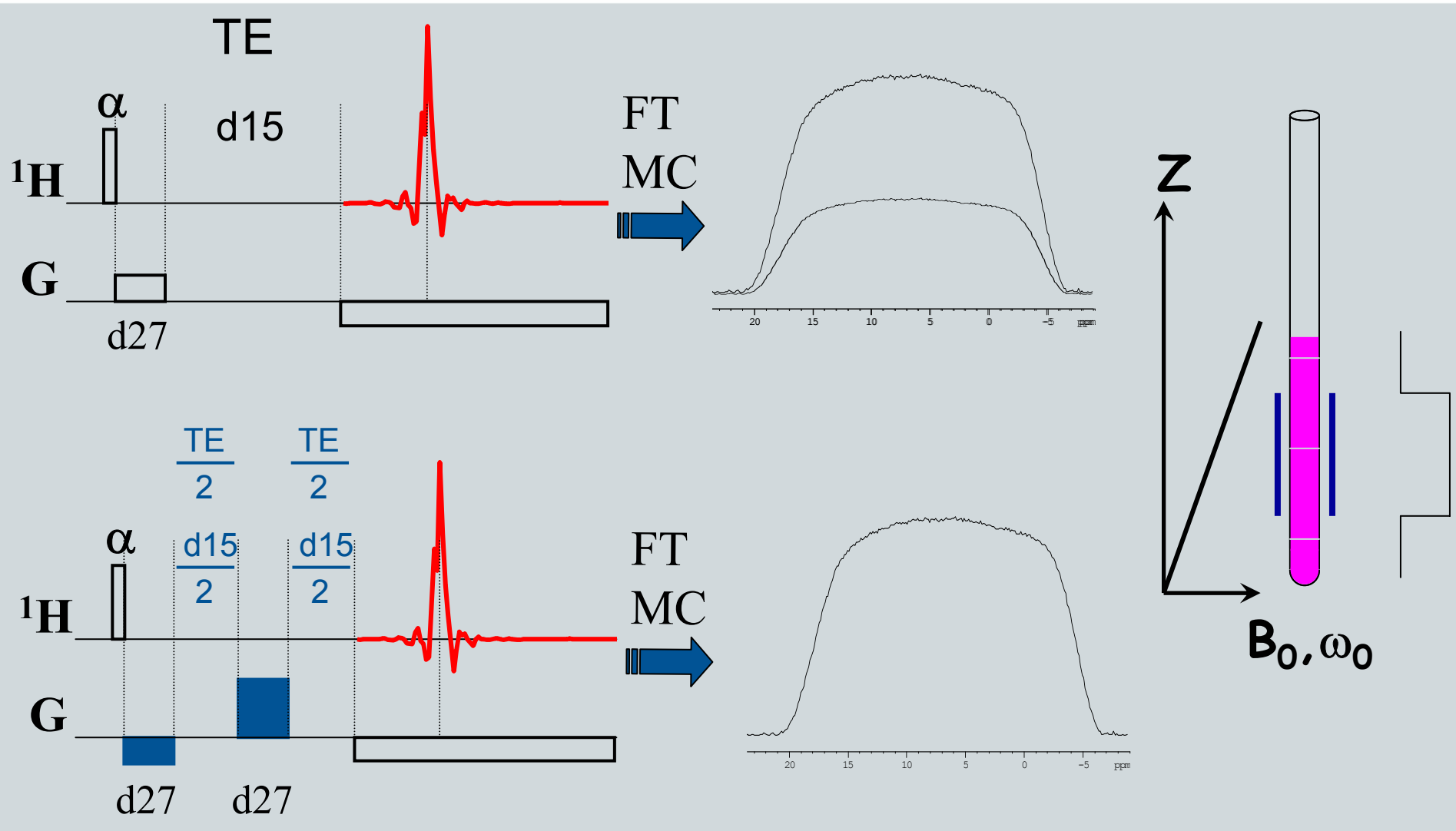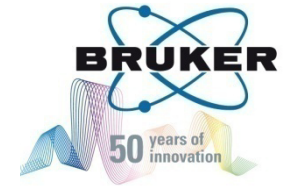# Gradient shim: Convection

- First priority: eliminate / reduce convection

    - Sample filling height =< 40 mm.

    - Increase VT gas flow (if possible)

    - Spin sample (if possible)

    - Lower sample temperature (if possible)

    - Use solvent with higher viscosity (if possible)

    - Use shigemi or smaller sample diameter

Bruker BioSpin

Gradient shim: Convection

- Pulse sequences with convection compensation for Gradshim (imgegp**cv**1d; imgegp**cv**sp1d2h):

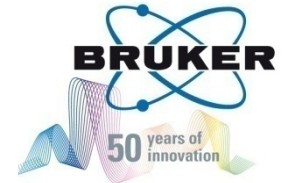   - Topspin 2.1 patchlevel 5 / Topspin 3.0

- Topshim with convection compensation option („convcomp"):

    - Topspin 2.1 patchlevel 5 / Topspin 3.0

- Older software versions: pulse sequences available on request (topshim for Topspin 2.1, gradshim any Topspin or Xwinnmr 3.5 version)

Bruker BioSpin

TOPSHIM

TOPSHIM: Basic Idea

- Make shimming as easy as possible

  - Push-button tool

  - Easy to use

  - Fully automated

  - Reliable

  - Fast

  - Good, guarantied results

- Replaces *GradShim*

TopShim™

Bruker BioSpin

Gradient Shimming

Map field inhomogeneity

B0(z)
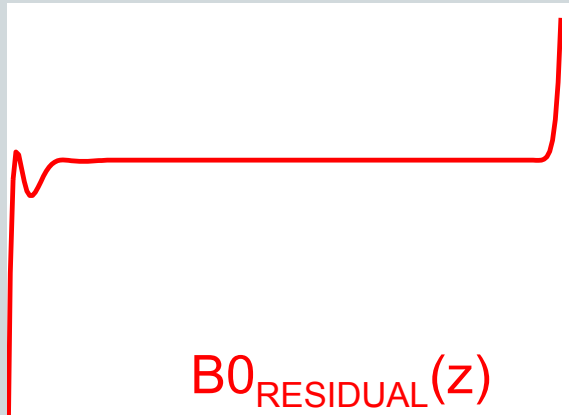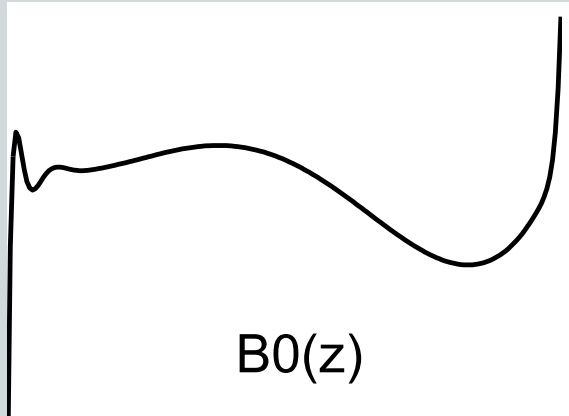
$B0_{RESIDUAL}(z)$

Shim system

$Z_i(z)$
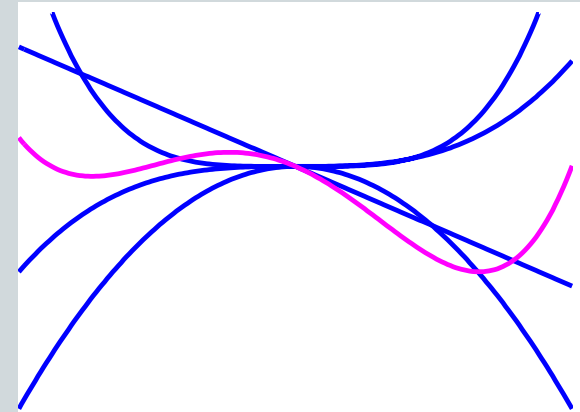
$\Sigma a_1 Z_1 + a_2 Z_2 + ...$

Compensate inhomogeneity

But: what is the best compromise for the residual field?

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Spectrum Optimisation
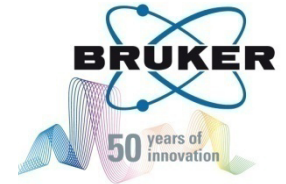
Assume shim setting

$B_{0\ RESIDUAL}(z)$

$B_1(z)$
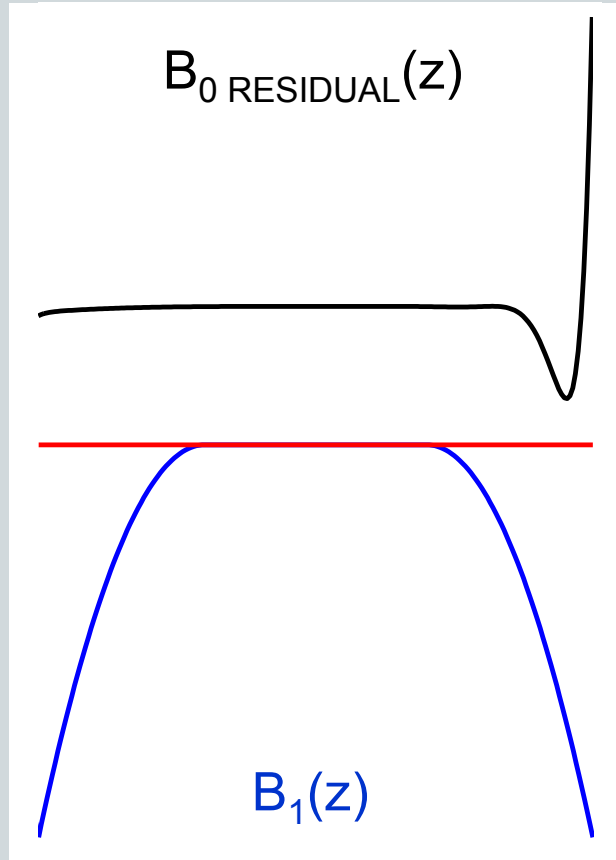
Incorporate B_1 of RF coil

Consider natural line

λ

Check quality of simulated lineshape

Optimisation: find best spectral lineshape possible for a probe.

Topshim & convection

1. Situation:
   - bad result   without Sample-Rotation
   - good result   with Sample-Rotation

2. Most likely cause:
   - convection

Bruker BioSpin

Topshim: troubleshooting

Warning message: „echo time must be reduced"

```
S TopShim                          ◻ ◹ ⊠
 Shim │ Report │ Service

 1D SHIMMING

 Parameters:
 maximum order = 5
 probehead = Z75003_0006
 solvent = Acetone
 shim nucleus = 2H
 nucleus optimised for = 1H
 o1p (from lock) = 2.04 ppm
 optimisation parameters = ls
 linewidth 1H = 0.10 Hz
 envelope shape / strictness = 2.00 / 200

 Results:
 echo time must be reduced
 echo time must be reduced
 initial B0 stdDev = 7.16 Hz
 sample size = 2.54 cm, position = −0.04 cm
 final B0 stdDev = 3.76 Hz > improvement = 1.9
 envelope width = 13.44 Hz
 shim changes:
 Z          +4
 Z2         +25
 Z3         +882
 Z4         +26
 Z5         −1346
 duration = 1 min 50 sec
 completed successfully
 finished Mon Jun  8 10:01:09 2009
```
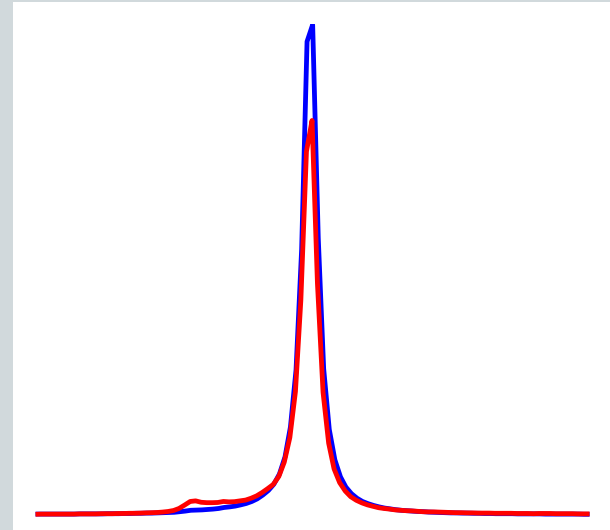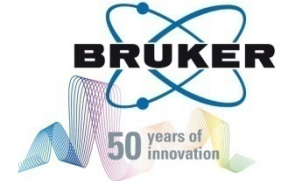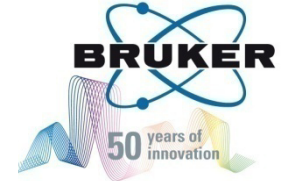
Results:
echo time must be reduced
echo time must be reduced
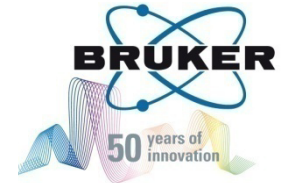initial B0 stdDev = 7.16 Hz

Problem

second echo time too long, not enough magnetization (signal) left

Source of problem:
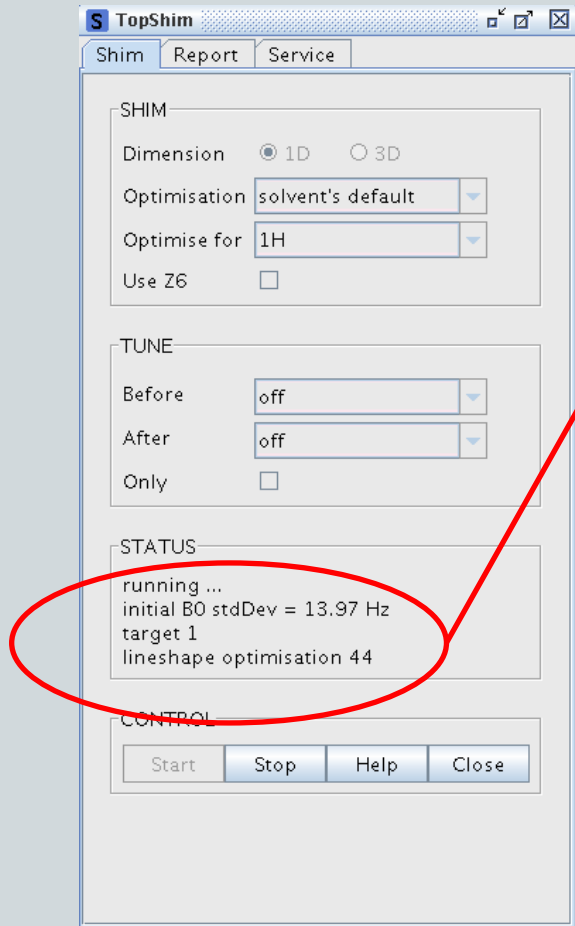
1. Start-Shim too bad

2. Too short T_2

3. Convection

Bruker BioSpin

Topshim: troubleshooting

Topshim requires a long time to converge
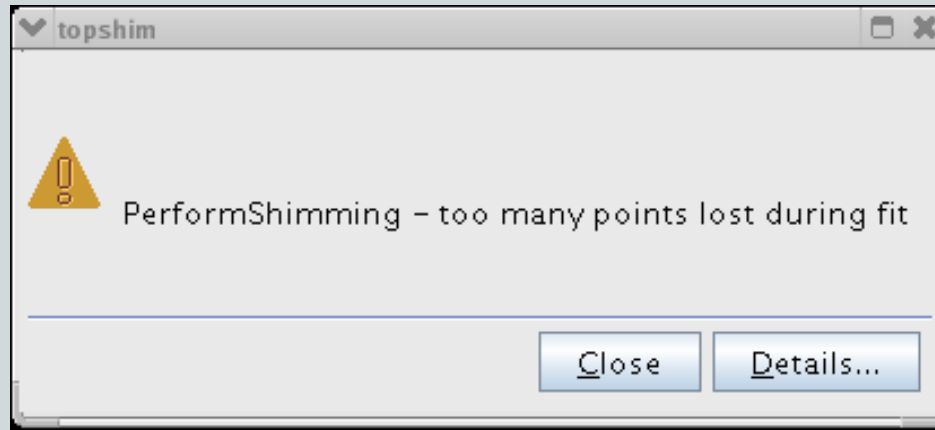

source of problem
1. Start-Shim is too bad
2. Convection

Bruker BioSpin

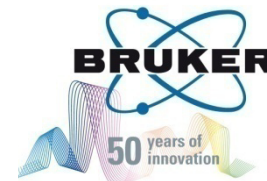# Topshim: troubleshooting

Error message: Too many points lost during fit
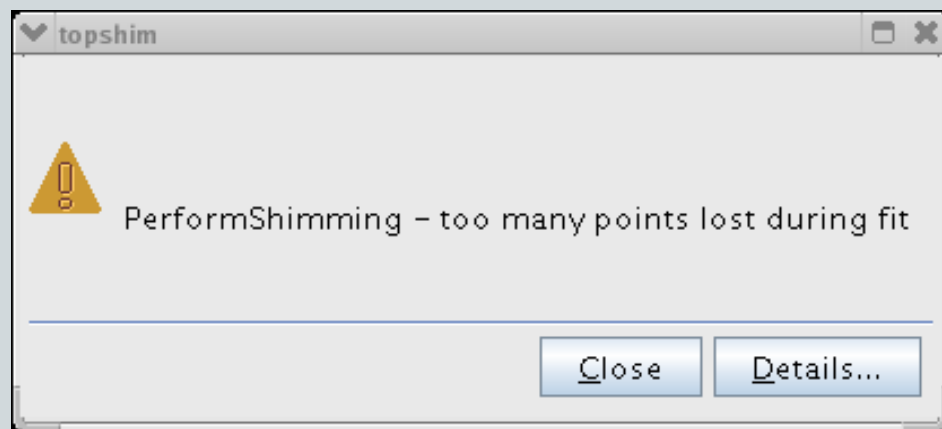

Source of problem

    1. Start-Shim is too bad

    2. Convection

Bruker BioSpin

Topshim: troubleshooting

Error message: Too many points lost during fit

Successive errors

1D SHIMMING

Parameters:
maximum order = 5
probehead = Z75003_0006
solvent = Acetone
shim nucleus = 2H
nucleus optimised for = in
o1p (from lock) = 2.04 ppm
optimisation parameters = ls
linewidth 1H = 0.10 Hz
envelope shape / strictness = 2.00 / 200

Results:
echo time must be reduced
echo time must be reduced
initial B0 stdDev = 13.97 Hz
shim changes: none
duration = 3 min 57 sec
completed with failure
finished Mon Jun 8 10:08:35 2009
PerformShimming – too many points lost during

PerformShimming – too many points lost during fit

Close   Details...

Bruker BioSpin
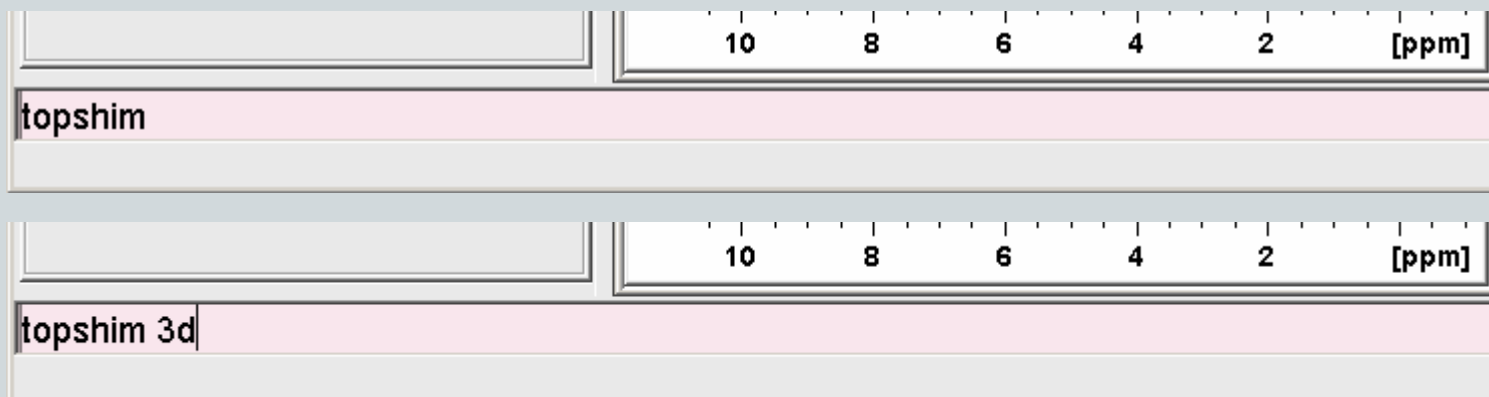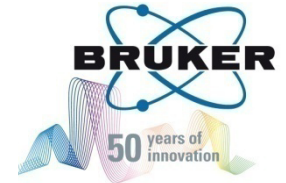
Working with Topshim

1. Open NMR experiment to be run (dataset)

2. Lock on correct solvent (*lock*)

3. Start Topshim

Working with Topshim

- topshim gui

- topshim 1d ordmax=6

- topshim lockoff nuc=1h o1p=4.7

- topshim nuc=1h o1p=3.49 selwid=0.3

- topshim plot

- topshim 1d shigemi

- topshim 1d zrange=1.1   [range in cm]

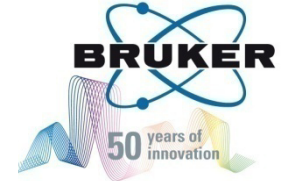- topshim 1d zrange=-0.9,1.1   [lower limit, upper limit]

Topshim error messages

- FileOpen - failed to open file C:/Bruker/TOPSPIN/conf/instr/topshim/gradients/grad13_1D.zfdf - No such file or directory

  - Probe requires more recent gradient definition file (Topspin version too old)

- No error message: "topshim finished" message immediately (but no shim optimisation)

  - Update from Topspin 2.0 to 2.1 has been done, but no "edhead" execution has been done: connectivity information missing
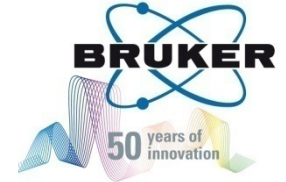
Bruker BioSpin
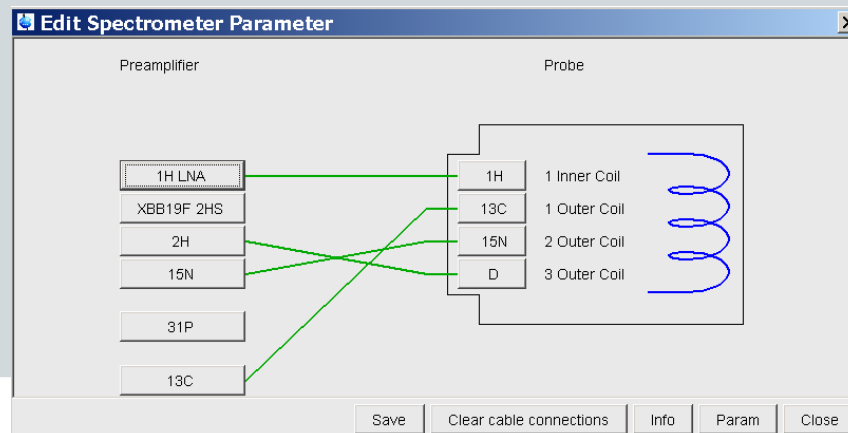
Topshim error messages

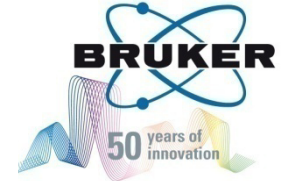- PrepareLock – lift is on: please switch off for shimming
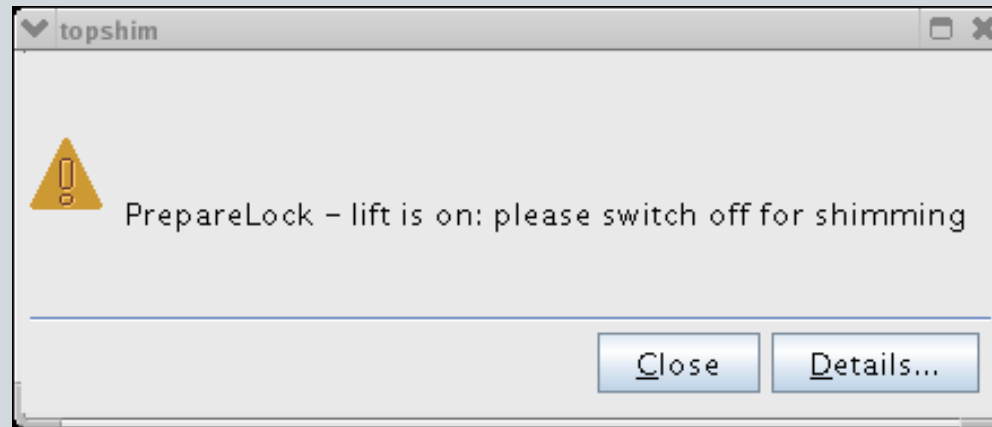
Bruker BioSpin

Topshim: define new solvent

- edsolv: define new solvent name

- edlock: set up locking paramters for new solvent

- Topshim works... BUT

  - Is everything working perfectly?

  - Which parameters can / must be defined?

Topshim: define new solvent
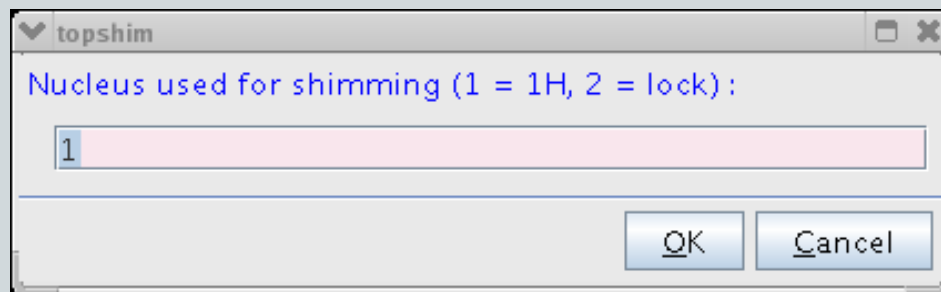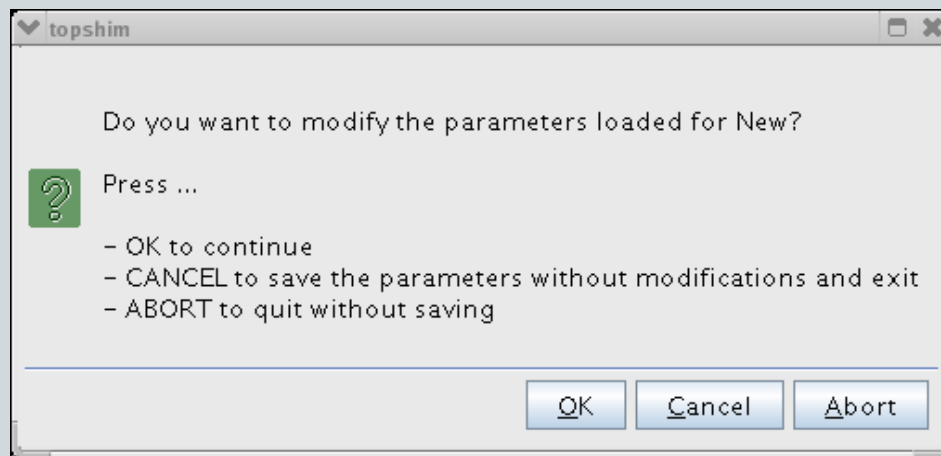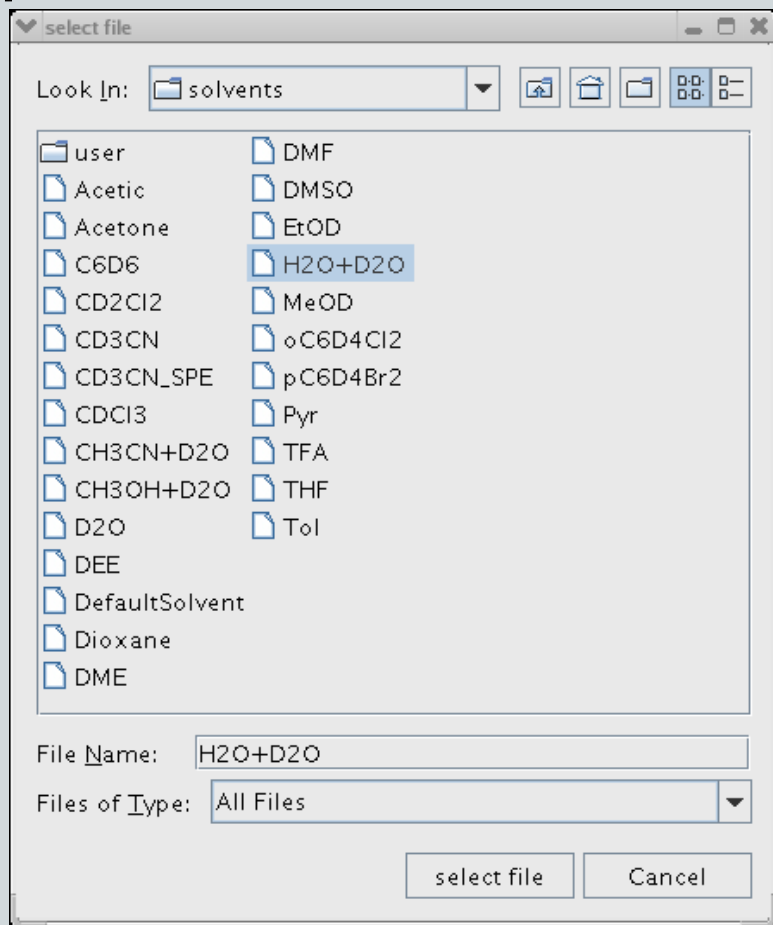
- edsolv: define new solvent name

- edlock: set up locking paramters for new solvent

- topshim solvcal solvent=<new solvent name>

Bruker BioSpin

Topshim: define new solvent

topshim solvcal solvent=New

Bruker **BioSpin**

Topshim: define new solvent

topshim solvcal solvent=New

topshim

Mode for setting excitation frequency o1p (1 = lock shift, 2 = manual):

```
1
```

OK   Cancel

topshim

Selective excitation (1 = off, 2 = on):

```
2
```

OK   Cancel

topshim

Excitation bandwidth [ppm]: 0.01 – 10.00

```
0.02
```

OK   Cancel

Bruker BioSpin

Topshim: define new solvent

topshim solvcal solvent=New

topshim

Approximate T1 relaxation time [s] : 0.01 – 1000.00

3.00

OK   Cancel

topshim

Specific optimisation parameter file :

ss

OK   Cancel

topshim

For 1H shimming no further information is required.
The current solvent parameters will be stored now.

Press OK to continue or CANCEL to abort.

OK   Cancel

Bruker BioSpin