FOCUS

Image Based Automatic Shimming Using B_0 Gradients

Installation and Users Guide
Version 0.9

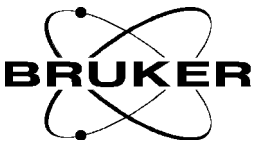

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TABLE OF CONTENTS

1. Introduction

FOCUS (Field Optimization by Computed Update of the Shims) is a fast shimming procedure that requires a Z-axis or XYZ-axis gradient probe for generating two profiles at two different echo times, TE1 and TE2 from which a phase or field map is generated. The first step involves mapping each of the shims for a given shim value setting. This procedure need not be repeated unless a different gradient coil is used or the orientation of the probe within the shimsystem is changed. The field map of a given sample is then generated and the new shim values are calculated. The procedures are completely automated so that after the initial setup, all operations such as acquisition, calculation, and loading of new shim values can be executed using a single button click.

2. FOCUS Installation

2.1. Preparations

Before FOCUS can perform automatic shimming, it has to generate the shim map: i.e. measure the effect of a known current in a specific shim. This calibration procedure is specific for a particular gradient probe and need to be carried out only once.

The initial setup is done by shimming on the water resonance of an aqueous sample and, in order to generate a reliable shim map, the initial magnet homogeneity needs to be good. Start by inserting a sample in water (90 % H_2O) and establishing reasonable homogeneity by reading in an appropriate shim file and/or manual shimming. It is essential for the procedure to have only a single chemical shift, in this case the water signal. All other signals are too small compared to the unsaturated water resonance.

The shim map procedure needs to know which probehead it is mapping and, also, it needs appropriate NMR parameters for the imaging experiment. Define the current probehead by executing the command **edhead**, clicking on the button **Define current** and highlighting the gradient probe currently in use.

Then, if this has not been done already, execute **expinstall** (you have to know the super user password for this) select your spectrometer system and select **Install Pulse Programs**, **Install Library Gradient Files** and **Convert Standard Parameter Sets**. This will a.o. install the pulse programs **imgegs1d** and **imgegs3d**, the gradient files **Imgegs1d** and **Imgegs3d** and the parameter sets **gradshim1d1h** and **gradshimdata**. See chapter 4 for information how to customize these parameter sets.

The FOCUS software is driven via a tcl/tk script that provides a simple graphical user interface to control all parameters and execute all functions. It can be started by typing **gradshim**.

2.2. Generating the Shim Map or Reference Field

The first time **gradshim** is called, it opens up two windows: the main window "Shim Sample" (see figure 1) and the info window "Gradient Shimming" (see figure 2). If this second window has been closed, it can be reopened via the menu „Window | Show Info“. This second window gives information about the autoshim setup and controls the generation of the shim map. If no shim map has been measured yet, then click on the

button **Shim Map Functions** to go to the shim map control window "Create ShimMap" (see figure 3).

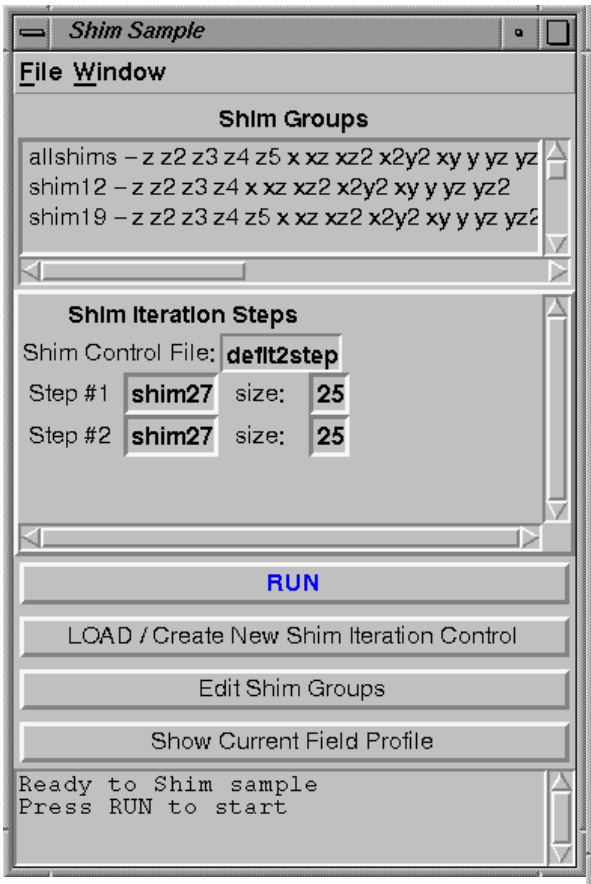

Figure 1: Main Shim Control Window

Figure 2: Shim Map Information Window

The "Create ShimMap" window comes up with the reference field parameters and the first thing to do is to select the Data Set Dimension. The default is 3D (for which a three axis gradient probe is required). If you want to do single axis shimming only then click on 1D and note the x- and y-size of the Matrix sizes are updated automatically.

Now click on **Edit shimdata params** to define the name for the temporary shim file and the directory path (Disk and User) for the autoshim data (see figure 4).

The data for the shim maps and for the actual shimming are written to an XWIN-NMR dataset and the dataset name parameters can be adjusted in this window under Acquisition File Name. The shimming procedures obtain the appropriate NMR parameters from a parameter set which has the same name as the dataset (see figure 4, file). The parameter sets delivered with the software are called **gradshimdata** for 3D shimming and **gradshim1d1h** for 1D. Therefore these names have to be specified if these parameter sets are to be used. Only specify another name if you have provided a parameter set with the same name you specify !!

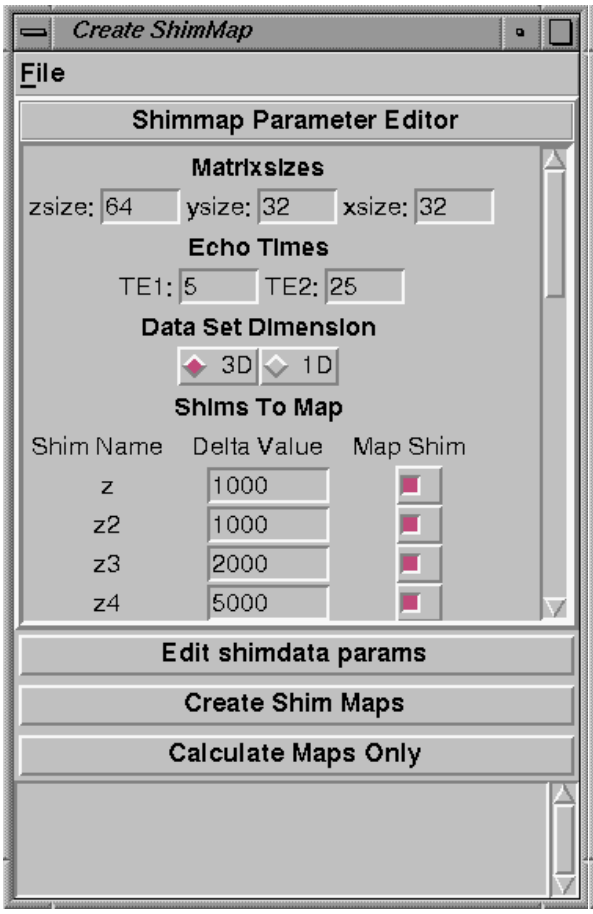

Figure 3: Shim Map Control Parameters

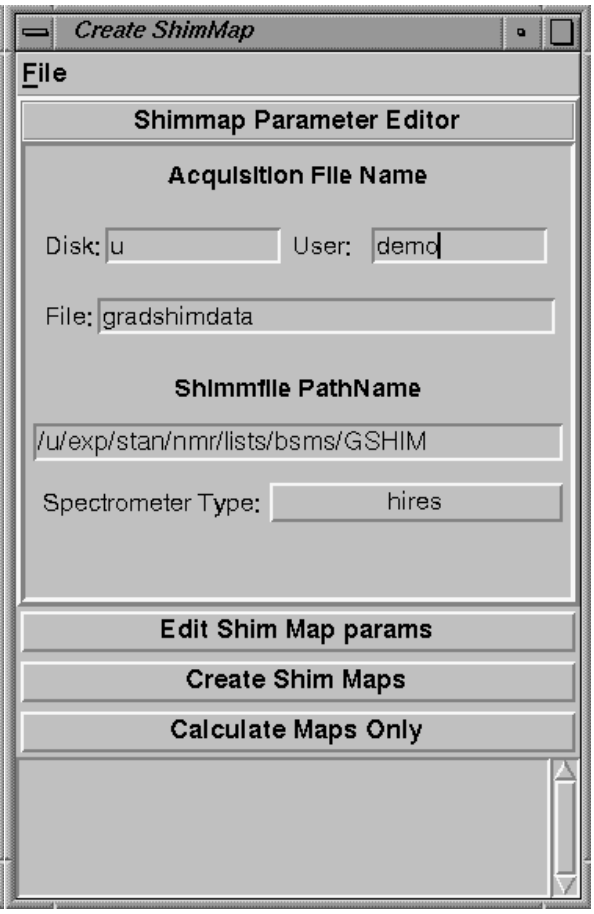

Figure 4: Shim Data Parameters

The shim map procedure will load offsets in individual shims and then reload the original values after the experiment has completed. Therefore it needs the name of a shim file with the starting values. This same file is used by the shimming procedure to calculate the new shim values. Its name (and full path) is specified in this window under Shimfile Pathname. After you have defined this name, make sure you store the current shim values in this file by typing **wsh GSHIM**. Note that during the gradient shimming this file will be overwritten so it should not be used to permanently record a specific set of shim values.

The actual contents of the shim files differs for different spectrometer types (e.g. high resolution spectrometers and biospec instruments). The correct spectrometer type should be indicated by activating the button **Spectrometer Type**. The default value for all Avance systems is **hires**.

Now click on **Create Shim Maps** to start the shim map procedure. For 1D shimming this will take approximately 5 minutes, for 3D 1 to 2 hours (depending on which shims are mapped). At the end of the experiment the program will display the measured maps for the Z-shims in a separate window (see figure 5). This window can be regenerated at any time after the shim map data have been acquired by clicking on **Calculate Maps Only** in the "Create ShimMap" window, if the corresponding datasets are still on the disk.

When the shim maps are available, the window "Gradient Shimming" contains the information about how the shim maps were acquired and, consequently, how the shimming will be done (see figure 6).

This window can be called up again at any time in the future by clicking on the menu bar "Window | Show Info" in the "Shim Sample" window, as already mentioned.

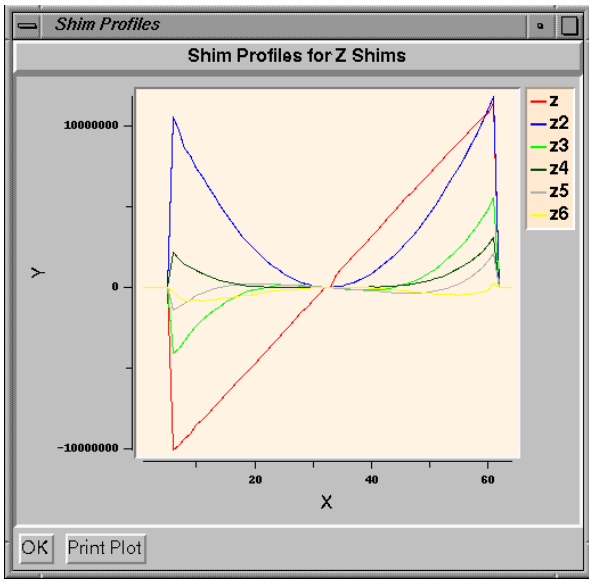

Figure 5: Shim Maps for Z-shims

2.3. The shimming parameters

Now the shim map has been generated, all windows can be closed except the main window "Shim Sample". This window shows the shim control parameters and allows to modify, save and recall these. The parameters are divided into two groups: the Shim Groups and the Shim Iteration Steps. First click on **Edit Shim Groups** to setup groups of shims that will be shimmed together (see figure 7).

2.3.1. The Shim Groups

The shim group editor allows you to edit existing shim groups, define new groups and remove unwanted ones. Some example shim groups for 3D shimming (i.e. shim12, shim19, etc.) and for 1D-shimming (i.e. lowz, midz, highz) are already predefined.

To edit an existing group, click on its name and click on edit. Clicking on one of the Available Shims will add that shim to the group, clicking on a Member Shim will remove it. Click on Apply when the edit operation is complete. If you do not have a BOSSII shim system, then you may well want to edit the supplied shim group **allshims**.

To define a new group, click on New and type a new group name e.g. **shim5**. Now add shims from the Available Shims by clicking on them e.g. **z z1 z2 z3 z4 z5** and consolidate by clicking on **Apply**. It is essential that no shim group should be used containing shims for which no shim map was generated. Therefore, if operating in 1D mode, shim groups should be defined with Z-shims only.

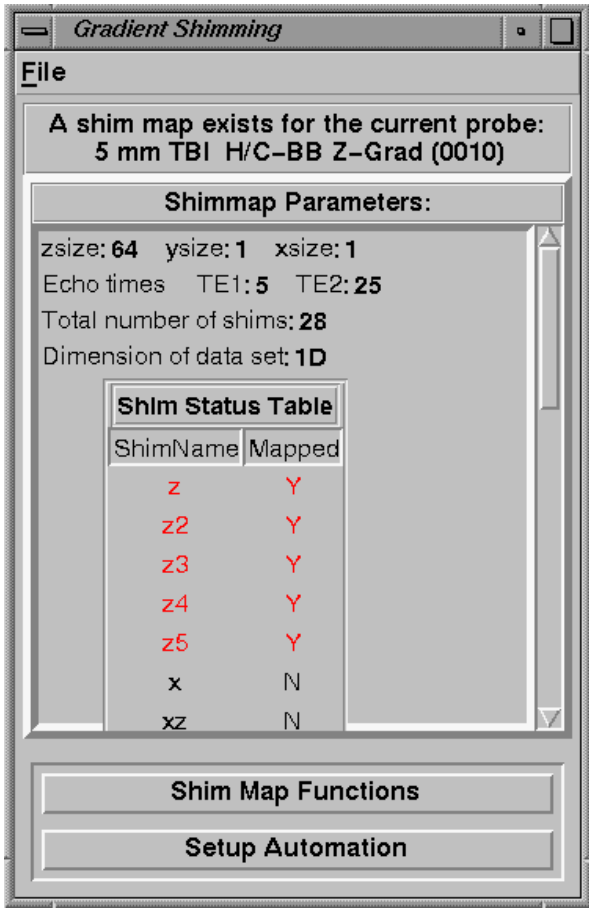

Figure 6: The Info Window with Shim Map parameters.

If it is not intended to work with 3D shimming, then the default shim groups for 3D shimming should be deleted. To delete a group, click on its name and then click on **Delete**.

All shim group editing operations are user specific, so each user can setup his own shim groups. The shim groups are stored in a file in the users autoshim directory called: **$HOME/.xwinnmr/autoshim/shimgroups**. Initially, the default shimgroups are copied to this file from **/u/conf/instr/autoshim/shimgroups**.

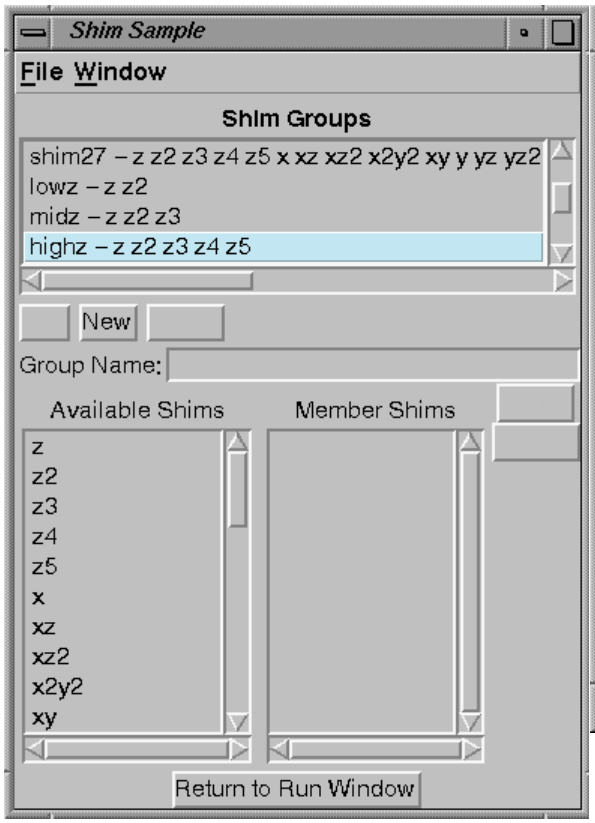

Figure 7: Shim Group Editor

Figure 8: Shim Iteration Control Editor

2.3.2. The Shim Iteration Control

When all required shim groups have been setup, then click on **Return to Run Window** and move on to the Shim Iteration Control Editor (see figure 8) by clicking on **LOAD/Create New Shim Iteration Control**.

Each time an autoshim procedure is executed a number of iterations can be performed. The shim iteration control editor allows specification of the number of iterations and, for each iteration, which shim group and which "shim range" or size is being used. This size specifies the number of points on either side from the centre of the profile (64 points) that contribute to the fitting of the current field map to the reference field when calculating the new shim currents.

The Shim Iteration Control Editor shows which shim groups have been defined and which is the current iteration control file. An existing control file may be opened by clicking on **Open** and selecting a file. Alternatively, a new control file may be generated by clicking on **New** and typing a new file name.

The number of iterations in the current control file can be modified by clicking on either of the buttons **New Step** or **Delete Step**. For each Step # the name of the shim group can be

entered plus the size of the shim range. The value for size depends on the sample height and the RF-coil height. Click on **Save** to consolidate any changes.

As for shim groups, each user can setup his own control files. They are stored in files called: **$HOME/.xwinnmr/autoshim/shimcntls/<fname>**. Initially, the default shimgroups are copied to the shimcntls directory from **/u/conf/instr/autoshim/**.

2.4 Running gradient shimming

Once suitable shim iteration controls have been setup, select the one to be used and return to the run window. Click on **RUN** to start the auto shimming procedure. Note that each iteration stores shim values in the temporary shim file (e.g. **GSHIM**) before the new ones are loaded.

At the end of the experiment, for each iteration the measured field maps (before shimming!) along the Z-axis are displayed together with a scroll window showing the new shim values and some statistical information on the measured field (see figure 9). The X-axis in these figures represents the B_0 field (in arbitrary units) and the Y-axis the spatial dimension, where the unit is data points in the measured profiles. The shim ranges for each iteration are indicated by differently coloured dots on the measured field map curves. Dark blue dots indicate the points which are **not** used for the fitting calculation.

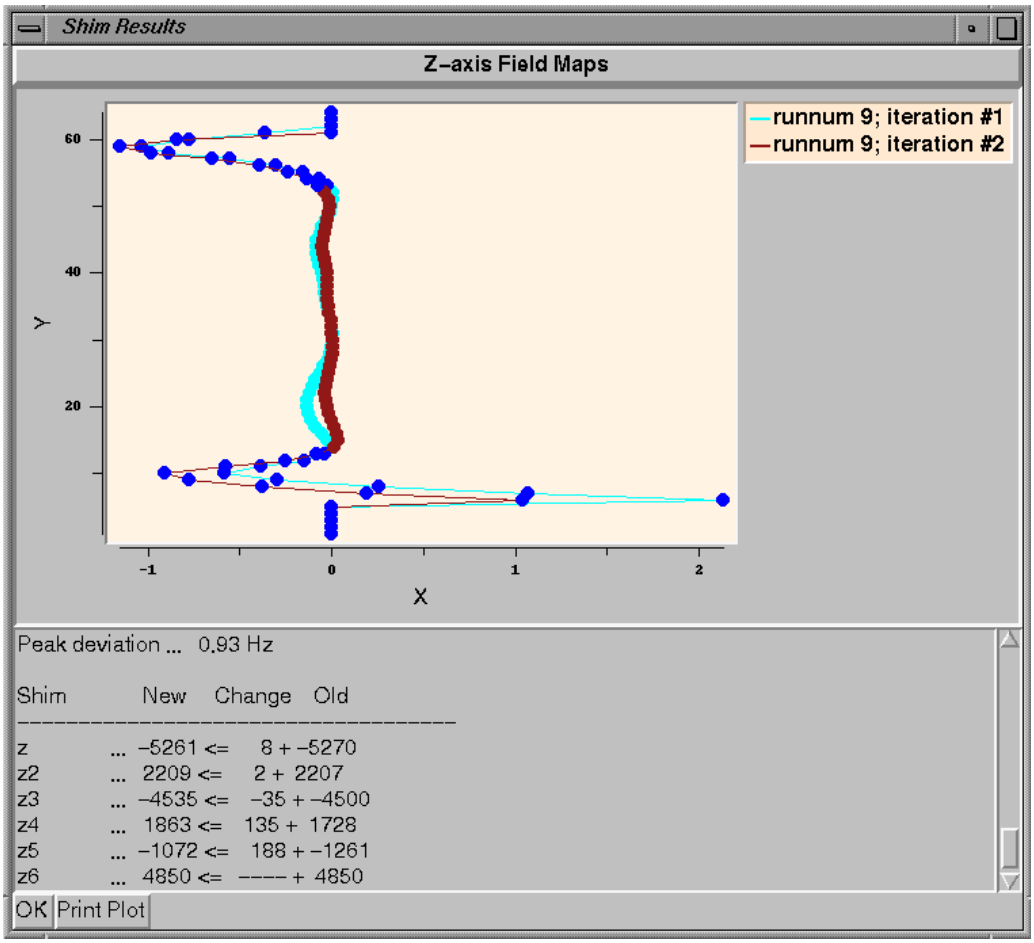

Figure 9: Z-axis Field Maps for a 2 iteration shim run.

3. Gradient Shimming in Automation

3.1. Automation Setup

not yet available

4. Advanced Techniques

The default parameters as used in the chapter 2 should normally provide good results. In this chapter it is described how to optimize these parameters and how to modify them to extend auto shimming to non-aqueous samples.

4.1. More about Shim Maps

The shim maps are always evaluated using 64 points in Z and 1 or 32 points in X and Y, depending which date set dimension is selected.

The Echo Times control the amount of time the magnetisation precesses in the (inhomogeneous) B_0 field for the two profiles that are measured. If the echo times are too long, then the signal to noise ratio in the resulting phase map will be poor. If, on the other hand, the difference between the two echo times is too small, then the difference between the two profiles will be small, again leading to a low signal to noise ratio in the phase map. The default values are adequate for most systems.

The table of Shims To Map shows the Shim Name of all available shims and indicates which Shim to Map. The Delta Value is the shim offset which will be loaded into each shim to calibrate its effect on the field homogeneity. The default values were chosen so that they produce a phase change of about +/- 180 degrees across the sample. If the Delta Value is set too low, the signal to noise on the phase map may be degraded. On the other hand, high values will cause distortions in the profile or loss of signal caused by de-phasing of the gradient echo signal. The optimum value is related to the sensitivity of the corresponding shim.

4.2. Parameter customization

To optimize the default parameters for 1D profile shimming on aqueous samples proceed as follows:

1. Place the standard sucrose, water suppression sample (2mM Sucrose in 90% H_2O and 10% D_2O) into the magnet.

   NOTE: DO NOT SPIN THE SAMPLE

2. Lock the sample.
   > lock d2o

3. Using standard proton parameters, run the one-pulse sequence, zg, and verify the transmitter is on resonance to the water.

4. Create a new data set.
   > edc

The data set name should be the same as the one you are going to use in the setup for the shimdata parameters, for example, gradshim1d1h.

5. Read in the default parameters for 1D profiling.
   > **rpar gradshim1d1h all**
   Check and set the following spectrometer related parameters using the eda command: spectrometer frequency and/or offset frequency: must be set on resonance (**o1p≅4.7**).

   Check also the hardware parameters that are system dependent, such as type of digitizer, etc.

6. Collect a gradient echo.
   > **zg**
   The echo must appear approximately in the middle of the acquisition window if digital filters are being used. If the analog mode is used it will appear at about 0.25*AT, where AT is the acquisition time.

   Fourier transformation and magnitude calculation should produce a z-axis profile.
   > **fmc**
   The Z profile should at least be about 70-80% of the spectral window. If the profile is too small or causes a fold over effect the gradient strengths in the gradient file Imgegs1d.r must be changed accordingly. This file resides in /u/exp/stan/nmr/lists/gp/. It can be edited from XWIN-NMR by:
   > **edcgp**
   For example, if the profile is too wide (or even folds over), then the gradients will have to be reduced. Change all values in the gradient file by the same factor.

7. Optimize the pulse power.

   Set the pulse length p0 and power pl1 to give about 30º flip angle (Optimize to give a 90º pulse, then reduce pl1 by 10 dB).

8. Optimize the gain.

   Set the **rg** value so that the echo is not clipped (overflows the digitizer).

9. Optimize the relaxation delay d1 in order to avoid saturation effects.

   This optimization is only needed if time averaging is required for the profile experiment, i.e. NS > 1. In that case it is important that the flip angle be chosen so that saturation effects are avoided. A simple way to check for saturation effects would be to compare the intensity of the profile of a single scan versus that taken with two scans. It must be twice as high, otherwise it indicates saturation.
   > **ns 1**
   wait for spins to relax.
   > **zg**
   > **fmc**
   note the signal intensity
   > **ns 2**
   wait for relaxation
   > **zg**
   > **fmc**
   compare the signal intensity with previous profile

10. After optimizing **d1**, you may have to optimize the receiver gain, **rg**, again.

11. Save the 1D profiling parameters for use in the automatic shimming procedures:

> **wpar gradshim1d1h**

4.3. Shimming non-aqueous samples

When non-aqueous samples are used, then water is no longer the overwhelming resonance (to the extent that, without water suppression, it may be considered the only resonance). The automatic shimming procedure, however, is designed to map the field, using a single resonance. Making use of selective excitation the resonance used for shimming can simply be selected by setting the parameter O1P to the chemical shift of the biggest signal, preferably a singlett, but other multiplicities work as well. If sufficient TMS is present (>= 2 %), set O1P to 0.

This neccessary pulse sequence can be generated from the standard profile pulse program by replacing the hard pulse by a soft pulse:

> **edpul imgegs1d**
replace the line **p0:f1 ph1** by **p0:sp1:f1 ph1**
save the program as **imgegs1dsel**

> **edc**	Create a new data set e.g. **gradshim1dsel**
> **rpar gradshim1d1h all**	Read FOCUS parameters
> **pulprog imgegs1dsel**	**C**hange the pulse program name
> **o1p 0**	Set on resonance for TMS

Now set the shaped pulse parameters spoffs1 to 0, and spnam1, sp1 and p0 to give a sinc shaped pulse with 1 cycle and 5 ms duration and at about 60 dB. You may optimimize the amplitude of the shaped pulse to give about 60^{o} flip angle and the duration p0 to result in profile which is similar to the profile of acqueous samples (compare chapter 4.2). Because of the long relaxation time of TMS (or many other resonances other than water), time averaging is rarely a useful option.

> **wpar gradshim1dsel all**	Store modified parameters using the same name as the data set name.

Now selective auto shimming on TMS can be performed by setting the shim data parameters to **gradshim1dsel.** Even though you are using a different acquisition scheme for shimming non-aqueous samples, the reference map generated with the sucrose sample (see section 2.2) can be used for this.

5. Appendices

Appendix 1: Pulse program for 1D profile acquisition

```
;imgegs1d
;avance-version
;1D Gradient Echo for gradshim-procedure

#include<Avance.incl>
#include<Grad.incl>

;;"d11=30m"

1 ze
  d11 UNBLKGRAD
2 d1
  p0:f1 ph1
  2u:ngrad
  d27
  2u:ngrad
  d15
  2u:ngrad
  d21 ph30 syrec
  2u adc ph31
  aq
  2u:ngrad
  rcyc=2
  400m wr #0
  d11 BLKGRAD
exit

ph1=0
ph30=0
ph31=0

;pl1 : f1 channel - power level for pulse (default)
;p0 : f1 channel -  small flip angle              [2 usec]
;d1 : relaxation delay
;d11: delay for disk I/O                          [30 msec]
;d15: echo time
;d21: gradient stabilisation delay
;d27: length of dephasing gradient (phase encode time)
;NS: 1
;DS: 0
;use gradient program (GRDPROG) :  Imgegs1d
;this program can be used for dmx as well
```

Appendix 2: Gradient program for 1D profile acquisition

{ (0) | (0) | (3.112469) }

{ (0) | (0) | (0) }

{ (0) | (0) | (-6.738582) }

{ (0) | (0) | (0) }

Appendix 3: Parameters for 1D profile acquisition

Current Data Parameters

NAME	gradshim1d1h	name of current data set
EXPNO	1	Experiment number
PROCNO	1	processed data number
DU	u	disk unit
USER	demo	Owner of data

F2 - Acquisition Parameters

PULPROG	imgegs1d	AQ_mod	qsim
TD	512	SOLVENT	D2O
NS	1	DS	0
SWH	40000.000 Hz	FIDRES	78.125000 Hz
FW	201600.00 Hz	AQ	0.0032500 sec
RG	8	DW	12.500 usec
DWOV	3.125 usec	DECIM	1
DIGTYP	HRD16	DIGMOD	digital
DR	16	DDR	1
DE	5.5 usec	TE	300.0 K