ShimIt

User Manual

Automated Shimming Software
VNMR Client

Version 0.8

U.S. Patents
5,218,299 And 5,572,125

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Copyright ShimIt Software

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Trademarks and Acknowledgments

CHAPTER 0

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ShimIt User Manual

CHAPTER 1 *Introduction*

The ShimIt auto-shimming system was written in 1990 as a side-product of the NMRanalyst software. With further improvements in user interface and documentation as well as patent protection[1] ShimIt is now ready for the first public release of the software.

Running ShimIt is similar to manual shimming based upon the shape of a displayed NMR signal. ShimIt runs "inside" the spectrometer software (here: VNMR) so all commands and displays of the spectrometer software remain user accessible. For the interactive shimming on a displayed lineshape a spectroscopist acquires a spectrum, changes the shim values, and repeats this cycle until a satisfactory homogeneity is obtained. In contrast, ShimIt only needs to be told which shim values to optimize and then loops through changing these shim values and acquiring new spectra without the need for further user interaction. The difference between manual and ShimIt optimization of the lineshape is that ShimIt evaluates the lineshape in a way which has been mathematically proven to lead to the optimal homogeneity without the risk of getting trapped with sub-optimal shim values.

There are two competing approaches for automated shimming. Automated lock-level optimization is based on special lock hardware and is quite fast and effective for "touching up" low-

1. U.S. Patent No. 5,218,299 and 5,572,125.

order z shims. However, like the manual lineshape optimization the lock-level optimization is plagued by local optima in the optimization criterion. So ShimIt should be used for every major homogeneity adjustment. However, for minor low-order z shim adjustments, such as between sample changes, the lock-level optimization currently has a speed advantage over ShimIt.[2] The second class of competing auto-shimming methods involves the determination of the actual three-dimensional field strength through imaging or special Nuclear Magnetic Resonance (NMR) mapping probes. The problem of such techniques is that they require the use of special probes and have sensitivity problems, limiting their applications to proton (normally water) samples. ShimIt has none of these limitations. In fact, knowledge of the three-dimensional field strength is not needed for shimming and in the time needed to acquire and reconstruct a single image, ShimIt can acquire and analyze several Free Induction Decays (FIDs). Hence, after integration of ShimIt into a spectrometer system the software could favorably compete even in cases where imaging techniques are applicable.

Another strength of ShimIt is that the method is independent of the spectrometer and magnet used. In practice however, ShimIt has to cooperate with spectrometer software and know at least what shims are available on the magnet used. To reflect this complexity ShimIt is currently implemented as a server process incorporating the general shimming method and additional client software incorporating the spectrometer and magnet specific information. The strength of the current server-client implementation of ShimIt is the flexibility to adjust the software to different spectrometer systems and to experiment with different user interfaces.

Since shimming is such a fundamental problem in NMR, each spectrometer system should be delivered with a *reliable* auto-shimming system. Due to the cost of spectrometer time ShimIt should be ultimately integrated into each spectrometer system to achieve maximum shimming speed. Currently the only ShimIt client available is for Varian VNMR 4.3 or newer systems. Development of client software for other spectrometer systems is planned for future releases of ShimIt. The VNMR client recognizes all seven “shim sets” understood by VNMR 4.3. Despite extensive testing, the ShimIt client software probably still has deficiencies. Please report all problems and suggestions for improvement to me at the contact information given earlier. Please note that this software is protected by copyright and the underlying shimming method is patented.

2. With minor hardware changes it would be possible to acquired complete FIDs through the lock channel. These FIDs could then be used for the ShimIt optimization of the magnet homogeneity.

CHAPTER 2

The Need For Magnet Shimming

Magnet shimming remains one of the few areas of NMR where automated procedures have failed to replace the tedious manual optimization of experimental conditions. Even experienced spectroscopists spend a significant amount of spectrometer time on "touching up" shims before each data acquisition. In cases where a good starting set of shims is not available, such as when bringing up a magnet or installing a new probe, the magnet shimming can take hours or even days to complete. Shimming is often regarded as a "black art"[1] requiring a good knowledge of the particular magnet and extensive experience with magnet shimming in general.

The field distortions of an NMR magnet over the sample volume should be no greater than a fraction of the natural linewidth of the slowest relaxing nucleus to be observed. For a 750 MHz magnet and a 0.1 Hertz proton resonance linewidth this calls for a field accuracy of better than 1:7,500,000,000. Raw magnetic fields are typically several orders of magnitude less homogeneous. Hence shim coils of different shape are placed inside the raw magnet to produce additional magnetic fields to compensate for remaining inhomogeneities. State-of-the-art

1. Chmurny, G.N.; Hoult, D.I.; "The Ancient and Honourable Art of Shimming"; *Concepts in Magnetic Resonance* **1990**, *2*, 131-149.

NMR super-conducting magnets have typically between 10 and 40 room temperature shim coils.

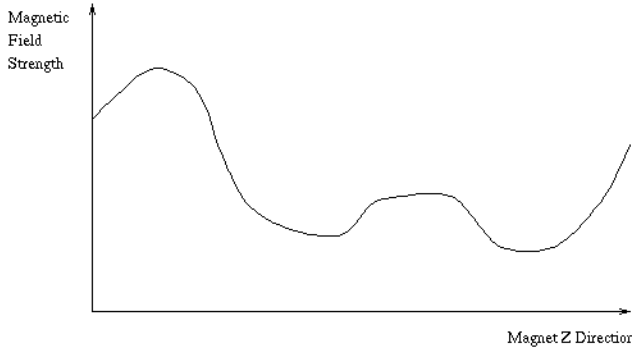
The best shim setting could be determined analytically if the shape of the raw magnetic field, the shape of all shim fields, and the field distortions caused by probe and sample were known. In NMR imaging (MRI) the shape of the magnetic field can be approximately determined through the use of field gradients. In the absence of field gradients, fields would have to be mapped mechanically using specially designed probes. In either case, shimming through field determination is both expensive and of limited accuracy.

Most shim coil sets are build to produce fields which resemble spherical harmonics. The shape of a magnetic field produced by a shim coil should hence be known and the effect of different shim fields should be independent. In practice however, every coil produces higher order effects and, due to design compromises and winding imperfections, lower order effects as well. So the design of the shim set might be used as a guiding principle during the shimming process but the final shim result should not depend on any assumed functional form of the shim coils.

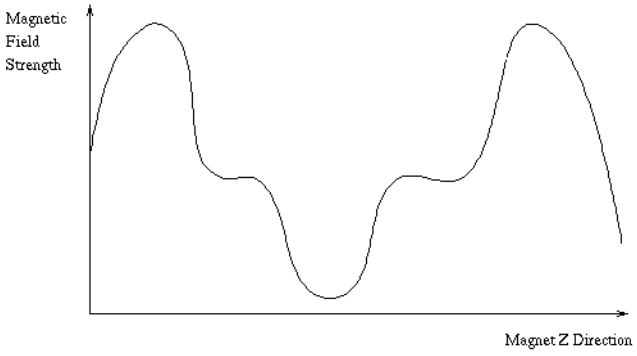
CHAPTER 3

How ShimIt Works

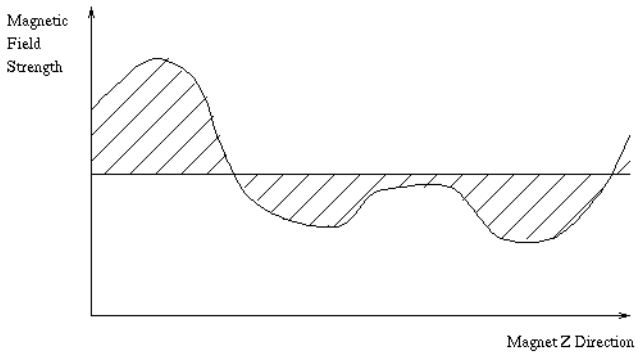
Shimming is the optimization of shim coil currents to maximize the magnet homogeneity in a volume of interest. The crucial question for this multi-parameter optimization which makes the difference between a “black art” and a reliable shimming method is how the current magnet homogeneity is determined.



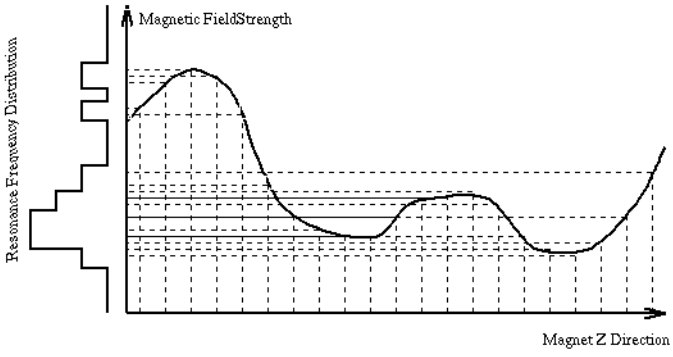
The most widely used criterion for magnet homogeneity is the “lock-level” which can be thought of as the height of the (deuterium) lock signal. The graphic shows a hypothetical magnetic field plot along the z direction of the magnet. The goal of shimming is to obtain a constant magnetic field. Suppose the shim coil currents are changed and the following (hypothetical) magnetic field plot is obtained.



The homogeneity obviously worsened but a lock-level indicator would show an improvement because the magnetic field strength is constant over a wider z range than before causing the height of the lock signal to improve. At the same time the lineshape of the signal worsened, but this is of no relevance to the lock-level height. Choosing the lock-level as homogeneity criterion turns shimming into a highly nonlinear optimization problem resulting in a response surface which has numerous local minima likely to trap any human or automated uphill optimization approach. It is crucial however to notice that the complexity of the response surface is a function of the chosen optimization criterion and does not allow any conclusions about the intrinsic complexity of the shimming problem.



ShimIt approaches this problem as follows: Suppose we calculate the average magnetic field strength and determine the absolute-value area between the observed and average field strength as shown in the figure. In contrast to the lock-level this area is a true representation of the remaining field inhomogeneity. But such field plots are not easy to obtain. Fortunately, such areas can be determined from the observed lineshape. Consider a sample along the magnet z axis. Each spin in the sample resonates corresponding to the experienced magnetic field strength.



Hence the field plot can be translated into a distribution of resonance frequencies as shown for a coarse grid of positions inside the magnet. This operation does not preserve the positional information of a field plot and hence is not reversible. But the distortion area in the one-dimensional examples above as well as the three-dimensional distortion integrals in real magnets are always proportional to the first absolute-value central moment of the resonance frequency distribution obtained from the resulting NMR line.

The remaining problem is to determine this resonance frequency distribution from an observed NMR line. Unfortunately, dispersion mode signals as well as all phase insensitive methods of displaying NMR data (e.g., absolute-value mode) cause lineshapes whose first absolute-value central moment is infinite rendering them unusable for shimming based on lineshape moments. ShimIt determines the resonance frequency distribution from the analysis of the spectral signal using a decomposition model. See U.S. Patent 5,218,299 for details.

The “magic” of the moment criterion is that its associated response surface can be proven to be describable by a linear set of equations. Since a linear set of equations cannot have local minima, ShimIt’s inhomogeneity minimization cannot get trapped with a set of shim values far from the best possible homogeneity. Instrumental instabilities determine how close ShimIt can approach this best possible homogeneity in a reasonable amount of time. Notice that the moment criterion makes no assumptions about the number of shims to be adjusted, whether or not a shim coil works, or what the actual shape of a shim’s produced magnetic field is. Hence, ShimIt itself does not depend on such factors either.

CHAPTER 4

VNMR ShimIt Installation

The VNMR 4.3 ShimIt software consists of macros, menus, and help files. These files need to be placed in directories recognized by VNMR as described in SECTION 4.1: "Installing Macros, Menus, and Help Files". ShimIt was written to work with all seven shim sets recognized by VNMR 4.3. Unfortunately, for some magnets Varian chose to generate the current for one magnet coil from two parameters, a coarse shim and a fine shim. Based on the setting of the VNMR shimset variable ShimIt knows which coarse shims are available. But the sensitivity ratio between coarse and fine shim varies between spectrometers and Varian failed to make these ratios accessible through software or even to document them. Hence, these sensitivity ratios might need to be determined and specified during the ShimIt software installation, as described in SECTION 4.2: "Magnet Specific Customization".

4.1 Installing Macros, Menus, and Help Files

The ShimIt macros should be placed in a VNMR recognized `maclib` directory, the menus in a `menulib` directory, and the help files in a `help` directory. To install ShimIt temporarily or for only one user the `maclib`, `menulib`, and `help` directories in `$HOME/vnmrsys` should be used. For the permanent installation for all users the `maclib`, `menulib`, and

help directories in /vnmr should be used. The last possibility is to place the software anywhere in the filesystem and to set the UNIX PATH variable and various VNMR parameters accordingly.

The ShimIt software is distributed as a compressed tar file named shimit.tar.Z. The file contains the following directories and files:

```
help/ShimIt_Manual.ps
     main2
     params
     shimit
     shims

maclib/parse_shims
       remove_shims
       shimit_SunOS
       shimit_all
       shimit_client
       shimit_display
       shimit_finish
       shimit_init
       shimit_non_z
       shimit_start
       shimit_z
       shimit_z_fine
       usleep_SunOS

menulib/main2
        params
        shimit
        shims
```

First load the file shimit.tar.Z from the distribution medium. Consult your system administrator in case of problems. To simplify the following discussion it is assumed that

`shimit.tar.Z` is loaded in the directory `/tmp`. Now install the software in one of the following three ways:

System-Wide Installation

To install the ShimIt software system-wide obtain root privileges using ("`%`" symbolizes the user prompt):

```
% su
```

and specify the password. Then change the current directory to `/vnmr` ("`#`" symbolizes the `root` prompt) by typing:

```
# cd /vnmr
```

and uncompress (`zcat`) and untar (`tar xvf`) the `shimit.tar.Z` file in the current directory by entering:

```
# zcat /tmp/shimit.tar.Z | tar xvf -
```

This command installs all files in their intended places.

Single User Installation

To install the ShimIt software only for the current user issue the following commands:

```
% cd $HOME/vnmrsys
% zcat /tmp/shimit.tar.Z | tar xvf -
```

Installation In Unsupported Directory

To install the ShimIt software in an unsupported directory (here assumed to be /tmp) issue the following UNIX commands:

```
% cd /tmp
% zcat /tmp/shimit.tar.Z | tar xvf -
```

Notice that in contrast to the previous examples three new directories are created (help, maclib, menulib). The fastest approach to using an unsupported directory for the ShimIt installation is to link all files in the created directories to the corresponding VNMR directories which completes the installation of ShimIt files:

```
% ln -s /tmp/help/* $HOME/vnmrsys/help
% ln -s /tmp/maclib/* $HOME/vnmrsys/maclib
% ln -s /tmp/menulib/* $HOME/vnmrsys/menulib
```

If links for these files are not desired the installation becomes more tedious. To increase the efficiency of the ShimIt software the "macros" shimit_SunOS and usleep_SunOS are actually binary programs. The ShimIt software is configured to search for these executables in the directories in the user's PATH variable, in $HOME/bin, $HOME/vnmrsys/maclib, /vnmr/bin, and /vnmr/maclib.

For UNIX to find the binary program in a non-standard directory either extend the PATH variable with:

```
% PATH=/tmp:$PATH; export PATH  (Borne and Korn shell)
% set path = (/tmp $path)        (C shell)
```

or copy, move or link both files to a recognized directory (here: the user's bin directory)

```
% ln -s /tmp/maclib/shimit_SunOS $HOME/bin
% ln -s /tmp/maclib/usleep_SunOS $HOME/bin
```

or modify the maclib/shimit_start and maclib/shimit_client macros to include the chosen directory in the PATH variable before calling shimit_SunOS and usleep_SunOS.

Finally VNMR has to be told where to search for the new `menus`, `macros`, and `help` files. So inside VNMR issue the following commands (ignore VNMR create warnings about already existing variables):

```
create('helppath','string','global')
create('maclibpath','string','global')
create('menulibpath','string','global')
helppath='/tmp/help'
maclibpath='/tmp/maclib'
menulibpath='/tmp/menulib'
```

Known ShimIt Incompatibilities

In order to make the ShimIt submenus accessible from the VNMR menu system, a `[ShimIt]` button has to be placed in one of the existing menus. The ShimIt software contains a modified VNMR 4.3 `main2` menu which allows one to start the ShimIt menu system. For VNMR sites using an already modified `main2` menu both `main2` files will have to be merged manually.

For reasons of speed all ShimIt computations are done in a binary program called (for Sun SPARC computers) `shimit_SunOS` and for timing purposes the binary program `usleep_SunOS` is used. These executables were build on a Sun SPARC running SunOS 4.1. In order to run the executables under Solaris 2.3 (SunOS 5.3) the "Binary Compatibility Package" which is part of the Solaris 2.3 environment has to be installed.

4.2 Magnet Specific Customization

One of the major strengths of ShimIt is that the software can shim magnets even when no reasonable starting values for the shims are know. To do so requires the knowledge of the range in which shim values can be adjusted, which coarse shims are available, and what the sensitivity ratio of present coarse to fine shims is. ShimIt uses the following global VNMR variables to provide information about the magnet used:

```
sh_range      Maximum +/- range of shim values
z1toz1c       Sensitivity ratio z1 fine to coarse shim
z2toz2c       Sensitivity ratio z2 fine to coarse shim
z3toz3c       Sensitivity ratio z3 fine to coarse shim
z4toz4c       Sensitivity ratio z4 fine to coarse shim
```

VNMR 4.3 recognizes seven shim sets and for each of the recognized shim sets defines the maximum allowable shim range (`sh_range`) and which coarse shims are available for each. So ShimIt sets these variables automatically when the main ShimIt menu is displayed for the first time.[1] For VNMR's shim sets 3, 4, 6, and 7 which have no coarse shims the ShimIt software installation is completed.

Both shim sets 1 and 2 have a `z1c` and `z2c` shim and shim set 5 has all four coarse shims (`z1c`, `z2c`, `z3c`, `z4c`). Varian failed to specify the sensitivity of fine to coarse shim values. So ShimIt sets the `z?toz?c` variables of unavailable coarse shims to minus one and to a default value of 20 for available coarse shims. The value twenty means that the corresponding coarse shim is assumed to have twenty times the effect of the corresponding fine shim.

Unfortunately, the default value is not sufficiently accurate for most spectrometers. The following table of sensitivity ratios was determined from the "Schematics Package" of the corresponding spectrometers:

Spectrometer	shimset	z1toz1c	z2toz2c
Unity-300	1	30.2	46.5
VXR-500	2	24.95	19.55

Additional spectrometers will be added to the table as the corresponding values become available. Since the sensitivity ratio of coarse and fine shims is determined by the shimming hardware, the spectrometer vendor (Varian) should be able to provide missing values.[2] This table

1. To have ShimIt recognize a so far unknown shim set or to customize an already defined shim set the macro `shimit_init` and the menu file `shims` have to be customized accordingly.
2. ShimIt can be configured to ignore a coarse shim by setting the corresponding `z?toz?c` variable to -1 or to only use the coarse shims by setting the variable to 1.

is contained in macro `shimit_init` and to activate the appropriate definitions remove the double quotes from the appropriate lines.

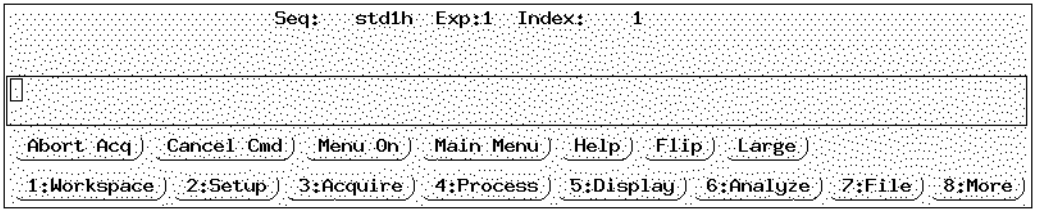
An experimental procedure to estimate these sensitivity ratios is to change a coarse shim by a given number of steps and to determine how many steps of the fine shim are needed to compensate. The corresponding `z?toz?c` shim should be set to the absolute value of the number of determined fine shim steps divided by the number of coarse shim steps. Once these variable values have been determined they should be entered in macro `shimit_init` so each user will get the determined sensitivity ratios by default.

CHAPTER 5

Using The VNMR ShimIt Client Software

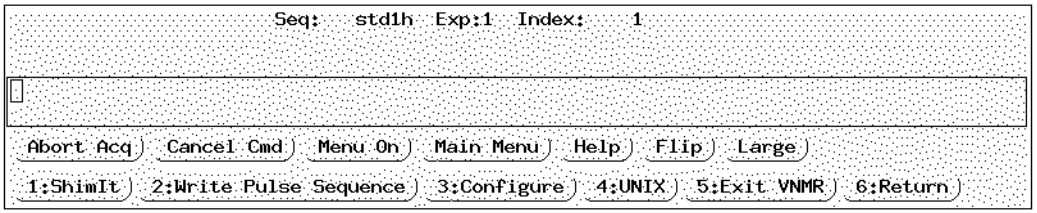
The ShimIt version for VNMR consists of menus, macros, and help files. The user interface consists of three ShimIt menus[1] and a modified "additional main menu" (`main2`) containing a button to show the main ShimIt menu.

The VNMR menu system consists of two rows of buttons. The top row is accessible at all times and is referred to as the permanent menu. The second row can be customized and is used to display the three ShimIt menus. After the start of VNMR or after clicking on the `[Main Menu]` button in the permanent menu the following menus are displayed:



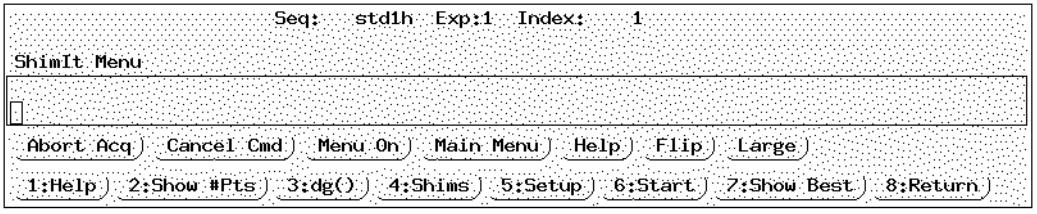
1. The ShimIt menu files are called `shimit`, `shims`, and `params`. Unfortunately, the menu name `setup` was already in use in VNMR 4.3.

Click on the [More] button to start the modified “additional main menu” containing the button to start the ShimIt main menu:



5.1 *ShimIt Main Menu*

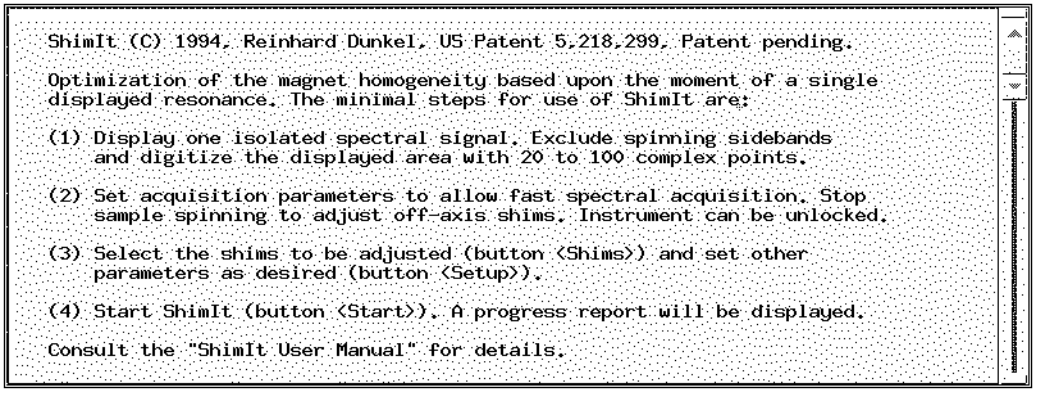
The ShimIt main menu can be reached from the modified “additional main menu” (discussed above) by clicking on the [ShimIt] button:



All functions of ShimIt are available from this menu. To aid in the editing of ShimIt parameters the Shims and Setup submenus are provided and are accessible from this menu, see SECTION 5.2: "Shims Submenu" and SECTION 5.3: "Setup Submenu" for details. To display a short description of the function of a ShimIt menu click on the [Help] button in the permanent menu while the menu of interest is displayed.

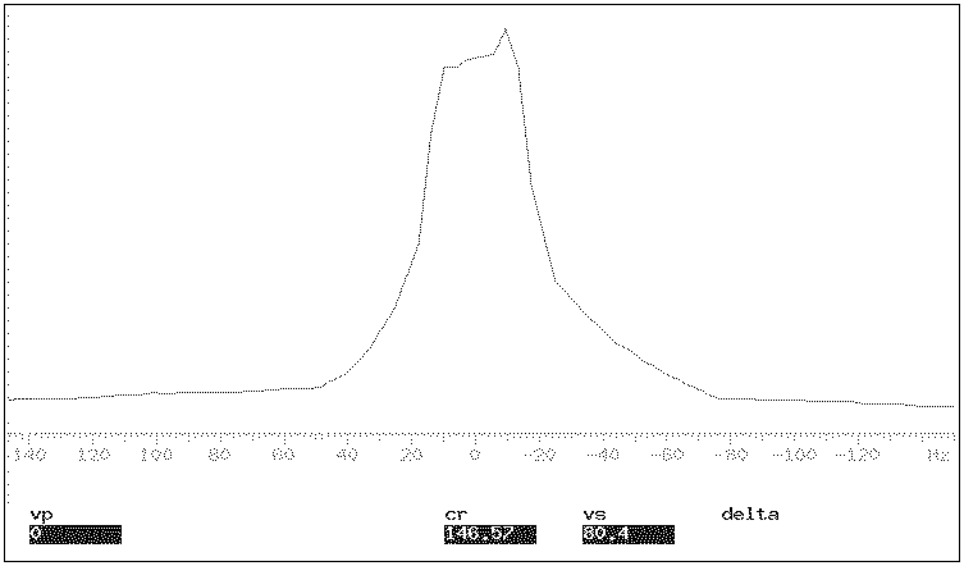
[Help] Button

The [Help] button in the permanent menu explains the function of the menu buttons. This main ShimIt menu [Help] button displays the following short description of the use of ShimIt:



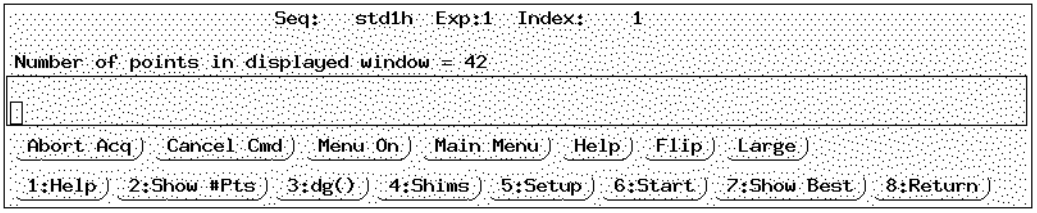
[Show #Pts] Button

The ShimIt software adjusts the magnet homogeneity based on the shape of an isolated NMR signal. So before optimizing shim values the user needs to display an isolated signal with a small amount of baseline on the screen for the ShimIt optimization:



Manual lineshape shimming tends to focus on making the upper part of the line Lorentzian in shape. A main focus might be to minimize the width at half-height of the line. ShimIt focuses on optimizing the base of the signal which eventually leads to a minimization of the width of the signal as well. Selecting a reasonably good range around the signal for the ShimIt optimization is demonstrated in CHAPTER 6: "Automated Shimming Example".

A major concern for the use of ShimIt is the number of points in the displayed spectral area which ShimIt has to analyze for each acquired FID. This `[Show #Pts]` button causes the current number of complex spectral points in the displayed spectral area to be shown in the VNMR status line:

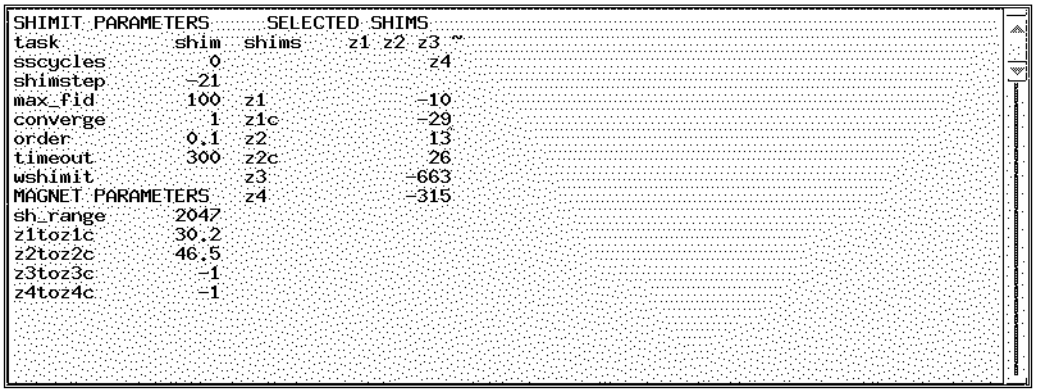


So the spectral area shown contains 42 complex-valued spectral points. The time ShimIt spends on analyzing each FID is normally small compared to the overhead of the Varian software for acquiring a spectrum.[2] However, an excessive number of points in the selected spectral area can lead to a noticeable slow-down of ShimIt. So this number should be kept as small as possible. On slow workstations the number should be around 50 and faster workstations can normally handle 100 points without causing significant delays. To decrease the number of points in the spectral area decrease the acquisition time, re-acquire the spectrum, and use the `[Show #Pts]` button to check the current number of complex points again.

[dg()] Button

Several parameters are provided to customize ShimIt's behavior. All ShimIt parameters can be displayed in a data group (`dg`) using this `[dg()]` button. The button action is equivalent to issuing `dg('dg_shimit')` from the command line:

2. Currently VNMR and ShimIt read the acquired FIDs and FFT the data separately. This inefficiency causes most of the ShimIt response time for analyzing an FID.



All displayed parameter values can be changed from the command line. The `SELECTED SHIMS` group is described in SECTION 5.2: "Shims Submenu". The Shims menu started by the `[Shims]` button allows one to change the selection of shims to be optimized. The `SHIMIT PARAMETERS` are described in SECTION 5.3: "Setup Submenu". These parameters can be interactively changed from the Setup menu started by the `[Setup]` button. Finally, the `MAGNET PARAMETERS` group values should be set during the software installation and should not require further customization. See SECTION 4.2: "Magnet Specific Customization" for details.

[Shims] Button

The `[Shims]` button starts the Shims submenu of ShimIt. This submenu provides a convenient way to specify the shims to be optimized during the shimming process. See the discussion of this submenu in SECTION 5.2: "Shims Submenu" for details.

[Setup] Button

The `[Setup]` button starts the Setup submenu of ShimIt. This submenu provides a convenient way to interactively specify the ShimIt parameters controlling the iterative shimming process. See the discussion of this submenu in SECTION 5.3: "Setup Submenu" for details.

[Start] | [Stop] Button

This button can be used to start the shimming process once an isolated NMR signal is displayed and the ShimIt parameters are set as desired. On start of ShimIt the button label toggles from `[Start]` to `[Stop]`. The `[Stop]` button can then be used to terminate the running ShimIt program. The `[Stop]` button only terminates the ShimIt run but does not terminate an acquisition in progress. To terminate an acquisition click on the `[Abort Acq]` button in the permanent menu. The `[Stop]` button changes back to `[Start]` whenever ShimIt terminates due to a user request, the set maximum number of iterations is reached, the convergence criterion is satisfied, or the response from spectrometer or ShimIt exceeds the set time-out period.

VNMR provides several means of automatic processing which slow down or even interfere with ShimIt. To make ShimIt easy to use, the automatically called MAGICAL macro `shimit_start` switches all automatic VNMR features off before beginning an auto-shimming run. Should this behavior be undesirable, comment out the corresponding lines in this macro:

```
"No automatic VNMR processing"
"============================"
load = 'n'        "Don't load shim values from experiment yet"
wshim = 'n'       "No automatic shimming besides ShimIt"
alock = 'n'       "Leave lock in its current state"
spin = 'n'        "Leave spin rate at currently used value"
gain = 'y'        "No automatic adjustment of receiver gain"
hdwshim = 'n'     "No hardware z1 shimming"
in = 'n'          "No interlock: don't adjust lock level or spin rate"
wexp = ''         "No action yet when experiment completes"
werr = ''         "No action for acquisition error"
wbs = ''          "No action after bs transients"
wnt = ''          "No action after nt transients"

"Delay acquisition until new shim values stabilize"
"================================================="
IF (pad + d1 < 1) THEN
   d1 = 1 - pad
ENDIF"
```

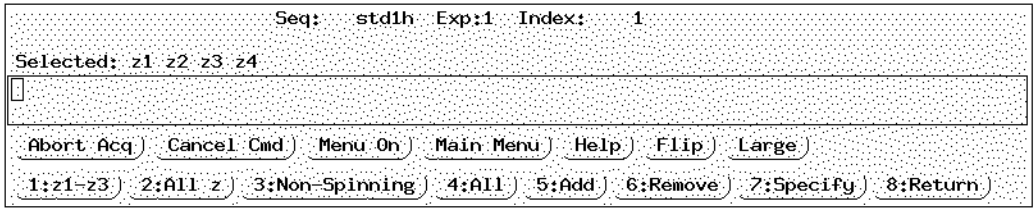
[] | [Show Best] Button

ShimIt improves the magnet homogeneity iteratively. As a result several FIDs might be acquired with a homogeneity worse than previous FIDs. On start of ShimIt the `[Show Best]` button is only displayed if a Best spectrum from a previous ShimIt run is still available. After the requested steady-state FIDs are completed, ShimIt saves the starting spectrum and the `[Show Best]` button is displayed. Whenever ShimIt is stopped manually or stops due to a time-out this `[Show Best]` button should be used to retrieve the best acquired FID and its shim values. If ShimIt terminates normally (either by converging or by reaching the maximum number of iterations) the best spectrum is retrieved automatically at the end of the shimming run.

[Return] Button

The `[Return]` button in the main ShimIt menu causes the menu system to return to the "additional main menu" (menu file `main2`).

5.2 Shims Submenu



The `[Shims]` button in the ShimIt main menu starts the Shims submenu shown above. The purpose of this submenu is to aid in the selection of shim variables to be adjusted by ShimIt. On start of this submenu the ShimIt parameters are displayed in the VNMR alpha window using the `dg` command. The current selection of shim values is displayed both in the alpha window as well as in the status line as shown in the figure above. As the selection of shims is changed using these menu functions both the `dg` display in the alpha window as well as the status line are updated accordingly.

The current selection of shims is stored in the `shims` variable as a list of shim names separated by blanks. To specify a list of shim values, the shim names can be separated by a blank, comma, semicolon, colon, or any non-empty combination thereof. In principle the list can contain all shims recognized by VNMR except for the `z0` shim[3] and the coarse shims.[4] The macro `parse_shims` also verifies that the specified shims are contained in the selected shim set.[5] The default value of `shims` are all z shims in the selected shim set.

Using these menu functions provides several advantages over setting the shims variable directly from the command line: From the VNMR `shimset` variable the available shims are already known and can be specified in groups, e.g. “all z shims” and “all non-spinning shims”. The menu also allows one to conveniently add and remove shims from the current selection. Finally, all user input is parsed directly and so input errors are discovered immediately. When setting the `shims` variable from the command line possible errors are only detected at the start of ShimIt.

[z1-z3] Button

This button selects the `z1`, `z2`, and `z3` shims to be optimized during the automated shimming. The low-order z shims are related to quite visible lineshape distortions and tend to be adjusted after every sample change. Notice that the moment optimization used by ShimIt is very sensitive to high-order z shims allowing ShimIt to be quite effective in their optimization. So the `[All z]` button should be used if high-order shims might be able to correct some of the observed distortions of the spinning lineshape.

[All z] Button

This button selects all z (axial) shims in the current shim set to be optimized during the automated shimming. For the optimization of the z shims the sample should in general be spinning and the displayed spectral area should not contain the spinning sidebands. Should a clear sep-

3. The `z0` shim is used to compensate for magnetic field drifts, a process called “locking”. This shim should not change the signal lineshape and hence is irrelevant for shimming.
4. If a fine shim is specified in the list the corresponding coarse shim is automatically adjusted if the corresponding `z?toz?c` variable is set to a value greater than zero.
5. As magnets using new shim sets become available this check mechanism will have to be extended or disabled.

aration of center resonance and spinning sidebands not be possible use the [All] button instead. To decrease the height of spinning sidebands stop the sample spinning and use the [Non-Spinning] button instead.

[Non-Spinning] Button

This button selects all non-spinning shims (also called non-axial shims) in the current shim set to be optimized during the automated shimming. For a spinning sample the non-spinning shims influence the height of the spinning sidebands. For the optimization of non-spinning shims the sample spinning has to be stopped so that the moment of the center line is influenced by the off-axis homogeneity. Some magnets show a strong interaction between spinning and non-spinning shims. Hence the spinning shims might need to be readjusted after the optimization of the non-spinning shims.

[All] Button

This button selects all shims in the current shim set to be optimized during the automated shimming. Selecting the optimization of all shims is only necessary when the magnet homogeneity is too bad for the sample spinning to baseline separate the spinning sidebands from the center resonance. Otherwise optimizing the non-spinning shims first followed by the optimization of the spinning shims will in general yield a better spinning lineshape.

[Add] Button

This button starts an interactive input request for the specification of shim names to be added to the current shim selection. Duplicate shim names are deleted from the resulting list.

[Remove] Button

This button starts an interactive input request for the specification of shim names to be deleted from the current shim selection.

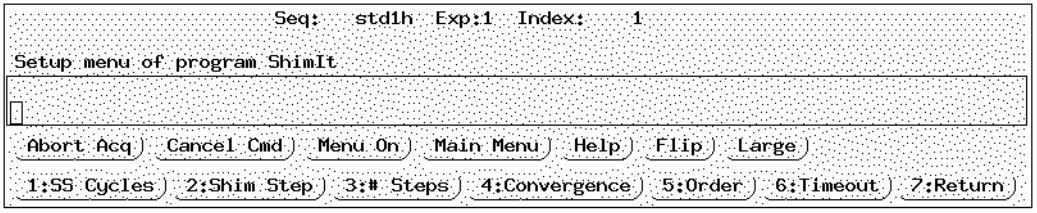
[Specify] Button

This button starts an interactive input request for the specification of a new list of shim names to be optimized during the automated shimming.

[Return] Button

This `[Return]` button causes the menu system to return to the main ShimIt menu.

5.3 Setup Submenu



The `[Setup]` button in the main ShimIt menu starts the Setup submenu shown above.[6] There are three groups of parameters which influence the way ShimIt performs the auto-shimming of a magnet. The magnet specific parameters[7] are set during the installation of ShimIt as described in SECTION 4.2: "Magnet Specific Customization". The shims to be adjusted can be chosen from the Shims submenu described in SECTION 5.2: "Shims Submenu". The final group of parameters determines how the auto-shimming is performed and these parameters can be set from this submenu. Note that all ShimIt parameters can also be set from the VNMR command line.

6. The menu file for the Setup submenu is called `params` since the name `setup` is used by VNMR 4.3 for other purposes.
7. Strictly speaking, splitting a magnet shim into a coarse and fine “dial” is a function of both the software and the DACs used to generate the shimming currents and is not really a function of the magnet.

[SS Cycles] Button

ShimIt acquires FIDs in rapid succession during shimming. If the relaxation time of the resonance selected for shimming is longer than the repetition time of ShimIt, the sample progressively saturates during the shimming run. A time-consuming method to avoid this problem is to increase the pre-acquisition delay (`d1`) and thereby to slow down the data acquisition.

A faster approach is to decrease the amount of sample saturation and to auto-shim on the partly saturated sample. The amount of sample saturation during the shimming run can be decreased by lowering the 90 degree pulse width provided the signal-to-noise (S/N) ratio of the spectrum is sufficient. The `[SS Cycles]` button allows one to set the `sscycles` variable interactively. ShimIt performs the specified number of `sscycles` steady-state cycles of acquiring and analyzing an FID to reach the steady-state sample saturation before starting the auto-shimming process.

ShimIt will normally recover from a partial sample saturation occurring during the auto-shimming. However, specifying a few steady-state cycles to be performed before the analysis of a partially saturating signal can improve the speed of the shimming process. Frequently, `sscyles`=3 is sufficient to approximate the final level of sample saturation. The default value of `sscycles` is zero.

[Shim Step] Button

ShimIt does not perform a sensitivity analysis of the individual shims specified for optimization. Using this button the `shimstep` variable can be set interactively. This variable specifies the initial shim change for ShimIt to be used for the auto-shimming process. During the shimming the step size of each shim is automatically adjusted as needed. The default value of `shimstep` is 256.

The value for `shimstep` should be chosen so that each shim adjusted by the specified value causes a visible change in the shape of the displayed line. After ShimIt is started the program shows the starting spectrum and a spectrum for each selected shim with the requested initial shim change applied. If the effect of the shim change is either too small or too large the shimming process can be stopped with the `[Stop]` button in the main ShimIt menu, the best shim settings found so far can be recalled with the `[Show Best]` button in the main ShimIt

menu, the shimstep variable can be adjusted using this [Shim Step] button, and the auto-shimming process can be restarted.

[# FIDs] Button

Using this button the max_fid variable can be set interactively. For an unattended shimming run this variable is useful to limit the time spend by ShimIt for auto-shimming. ShimIt works in logical iteration steps and each step can result in the acquisition of several FIDs. So when the specified maximum number of FIDs are acquired, ShimIt finishes the current logical iteration step and then terminates. Hence, the acquired number of FIDs can slightly exceed the number of FIDs specified by the max_fid variable. The default value of max_iter is 100 and the recommended value for fast shimming is eight times the number of selected shims to be optimized.

[Convergence] Button

ShimIt optimizes the moment of the displayed line. This [Convergence] button allows one to interactively specify the converge variable. This variable causes termination of the auto-shimming process when the smallest determined moment is estimated to lie within converge percent of its optimal value.

Notice that the stability of an NMR instrument and the finite S/N ratio of the spectrum limit the accuracy of determined moments. The default value of converge is 1%. A value for the order parameter of less than one decreases the fluctuation of the determined moment and the converge value should be decreased accordingly. Setting this variable to much less than the default value can significantly delay the convergence of ShimIt without further improvements in the magnet homogeneity.

[Order] Button

Lock-level shimming concentrates on maximizing the height of the lock signal. As a result the lock-level is quite effective for “touching up” the low-order z shims. Unfortunately, in all other cases lock-level optimization tends to run astray and to result in less than optimal lock-level maxima. ShimIt on the other hand optimizes the absolute-value (normally first) central

moment of an observed line. This reliably minimizes the width of the base of a signal and minimizes remaining baseline distortions. Given an imperfect shim set, the maximum height and the best narrow base of a signal can frequently not be obtained simultaneously.

Many spectroscopists favor an improved signal height at the expense of a deterioration of the baseline and width of the signal base. The [Order] button allows one to interactively set the order parameter. This parameter determines the order of the (absolute-value) lineshape moment which ShimIt optimizes. Large order values favor flatter baselines and narrower signal bases while smaller order values lead to higher signals with generally smaller width-at-half-height values.

The default value of order is one, corresponding to the minimization of the first absolute-value central moment. The order parameter should be kept between 1 and 0.1. There seems to be no advantage of choosing an order parameter value above one. The second central moment of an absorption-mode Lorentzian line (order=2) is already infinite (for an infinite spectral width) causing instabilities of the shimming algorithm. Setting the order parameter to a negative value causes ShimIt to destroy rather than improve the magnet homogeneity.

It should be noted that only for order values of one (and higher) has it been proven that moment minimization always leads to the best magnet homogeneity. So order=1 should always be used until a good homogeneity has been found. If so desired the value of the order parameter can then be decreased (but kept above zero) to cause ShimIt to more strongly weight the height of the displayed resonance for the optimization.

[Timeout] Button

The VNMR client software of ShimIt was written solely based on the user documentation of the Varian spectrometer system. Besides an avoidable runtime overhead this also resulted in an asynchronous communication of ShimIt with both the spectrometer and the VNMR software.

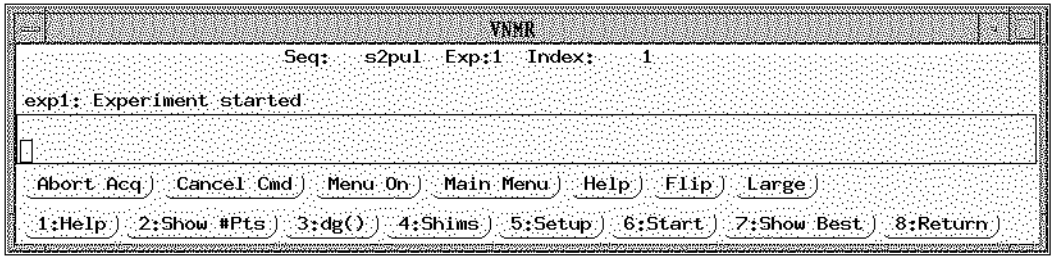
Using the [Timeout] button the timeout variable can be set interactively. If the spectrometer has not successfully acquired a spectrum requested by ShimIt within timeout seconds or ShimIt has not analyzed an FID within this time frame the auto-shimming is aborted. The default value of timeout is 300 seconds.

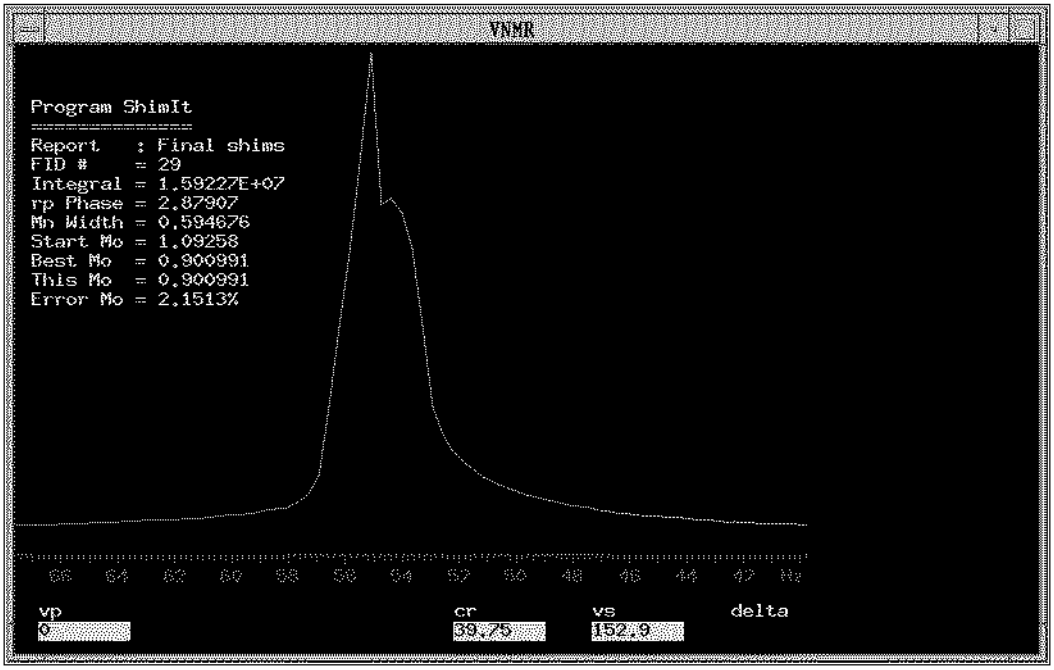
[Return] Button

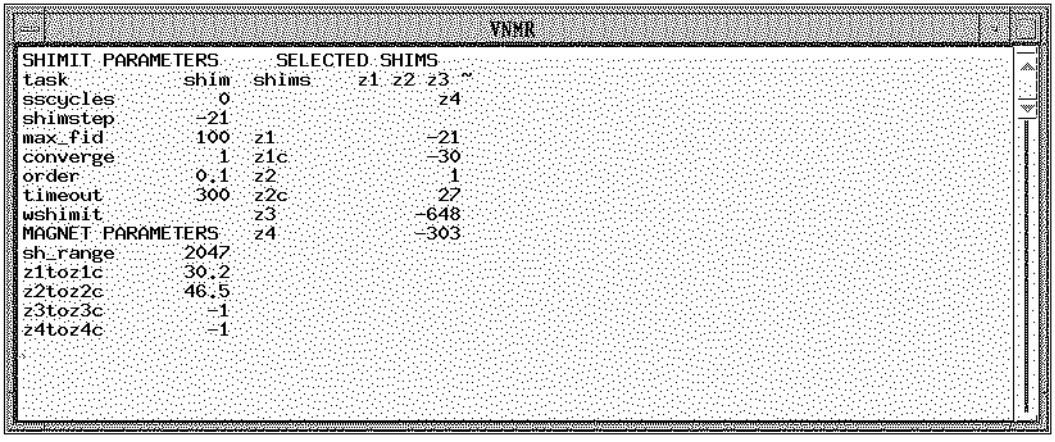
The `[Return]` button causes the menu system to return to the main ShimIt menu.

5.4 Displayed Shimming Results

During a shimming run ShimIt displays all variable settings, acquired spectra, and obtained analysis results. For further speed improvement, future versions of ShimIt will likely provide an option to reduce the amount of displayed information. While the ShimIt homogeneity optimization is in progress the VNMR display typically shows the following components:




VNMR
Program ShimIt
Report : Final shims
FID # = 29
Integral = 1.59227E+07
rp Phase = 2.87907
Hz Width = 0.594676
Start Mo = 1.09258
Best Mo = 0.900991
This Mo = 0.900991
Error Mo = 2.1513%
66 64 62 60 58 56 54 52 50 48 46 44 42 Hz
vp
0
cr
39.75
vs
152.9
delta


VNMR
SHIMIT PARAMETERS
task
sscycles 0
shimstep -21
max_fid 100
converge 1
order 0.1
timeout 300
wshimit
MAGNET PARAMETERS
sh_range 2047
z1toz1c 30.2
z2toz2c 46.5
z3toz3c -1
z4toz4c -1
SELECTED SHIMS
shims z1 z2 z3 z4
z1 -21
z1c -30
z2 1
z2c 27
z3 -648
z4 -303

The status line of the Menu window shows messages like “Experiment started”. The graphic window is used to display the area of the current spectrum used for auto-shimming. Both phasing and current position of the analyzed spectral region are updated for every acquired FID. ShimIt does however not adjust the width of the displayed spectral area or the number of points in the analysis range. These changes can be automatically performed from macros which use ShimIt as their basic shimming engine, see CHAPTER 6: "Automated Shimming Example".

The values listed at the left side of the spectrum are ShimIt’s analysis results of this spectrum. The `Report` line lists remarks from ShimIt about the currently displayed spectrum, such as the “Best Shims So Far” message displayed above. The `FID #` line shows the number of the current FID acquired for this shimming run. The displayed number is counted from minus the number of requested steady-state cycles (`sscycles` variable), over zero for the starting spectrum, to the number of acquired FIDs for the shim optimization.

The determined area of the displayed spectral region is listed in the `Integral` line. A decrease of the listed integral during a ShimIt run is normally due to progressive sample saturation. If the selected spectral area initially did not contain the complete signal intensity the integral might slightly increase as the magnet homogeneity improves. ShimIt always normalizes the absolute-value integral of the analyzed spectral area before determining the line moment and hence is fairly insensitive to modest integral changes.

Every acquired FID is phase corrected by adjusting the Varian zero-order phase parameter `rp`.[8] The `rp Phase` line shows the currently used phase parameter. The shape of an NMR line is determined by the T_2 relaxation time of the observed nucleus and the inhomogeneity of the current magnetic field. The `Mn Width` line shows ShimIt’s estimate of what the width of the displayed line would be without magnetic field inhomogeneities.

The following three lines in the graphic window show the lineshape moment at start of ShimIt (`Start Mo` line), the best moment found so far (`Best Mo` line), and the moment of the currently displayed spectral area (`This Mo` line). Notice that ShimIt uses an iterative shimming approach and the moment of the currently displayed spectrum might in fact be worse than the best moment or even the starting moment. The `Error Mo` line provides an estimate of the

8. ShimIt does not modify the user-set frequency dependent first-order phase parameter `lp`.

percent uncertainty in the best moment determined so far. The error value is given after ShimIt has probed the sensitivity of the shims to be optimized and the value is then updated after each acquired FID. The listed error will decrease during shimming and hence is used in conjunction with the `converge` parameter as a termination criterion. The nonlinear nature of the optimization algorithm, and instabilities in both the instrumental response and the spectral analysis can cause the listed error value to fluctuate somewhat.

The bottom window ("alpha window") in the above figure lists the current ShimIt parameters and the values of the shims to be optimized for the displayed spectrum. For an explanation of the displayed parameters, see SECTION 4.2: "Magnet Specific Customization", SECTION 5.1: "ShimIt Main Menu", and SECTION 5.3: "Setup Submenu".

Created Files

ShimIt generates several files during a shimming run and stores them in directory `$HOME/vnmrsys/ShimIt`. When ShimIt is started all files from a previous shimming run are deleted. The first file generated is called `start` and contains all ShimIt and VNMR parameters relevant to the shimming run. In the file `ShimIt.log` written next are stored during a shimming run the spectrometer commands issued and the shimming results obtained. Finally, each FID acquired which constitutes an improvement in magnet homogeneity over all previous FIDs is stored in a directory called `Best??.fid` in `$HOME/vnmrsys/ShimIt`. Directory `Best01.fid` contains the starting FID and the `Best??.fid` directory with the highest number contains the best FID acquired so far.

CHAPTER 6

Automated Shimming Example

The biggest challenge for manual and automated shimming alike is to shim a magnet starting without knowing initial shim values. Using a 300 MHz Varian UNITY spectrometer with an NCC Z*Spec probe this shimming example demonstrates how ShimIt can shim such a magnet in less than an hour starting from all shim values set to zero. The examples were run using a Sun SPARC II computer. The speed of ShimIt is compute limited and faster workstations obtain a significant speed-up. Experienced spectroscopists typically need at least a day to shim a magnet from scratch.

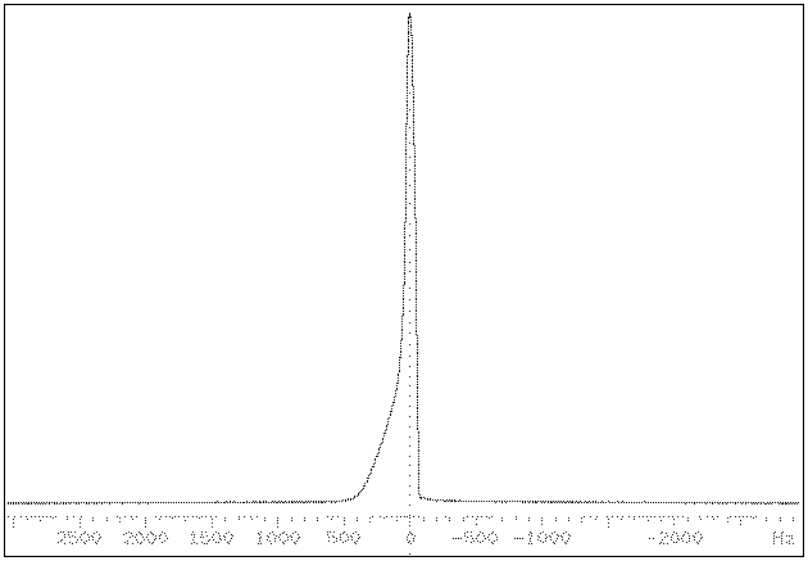
Currently the phasing module of ShimIt assumes that the signal in both the real and imaginary part of the displayed spectrum arises from the resonance to be optimized. So the shimming should be based on an isolated line in the spectrum.[1] Another requirement for fast shimming is a short relaxation time of the observed resonance to avoid an excessive sample saturation. For the following example a plain water sample is used.

ShimIt contains a software lock which shifts the position of the analysis region in the acquired spectrum to compensate for resonance frequency shifts between FIDs. Therefore, the Vari

1. Some research samples might not have a sufficiently isolated signal for use by the current version of ShimIt. Future ShimIt versions will address this issue.

autolock should be set to off. Even for samples which (in contrast to the water sample used) contain a lock substance the Varian autolock mechanisms should normally be turned off, at least during coarse shimming. The danger of using Varian's autolock is that when the lock signal is lost during the auto-shimming the lock mechanism wildly changes the field to search for the lock signal - even if an acquisition is in progress. ShimIt performs the software locking whether or not the spectrometer locking system is active.

For the UNITY-300 spectrometer used for this example the spectrum of the proton lineshape sample with all shims set to zero and no locking or sample spinning looks as follows:

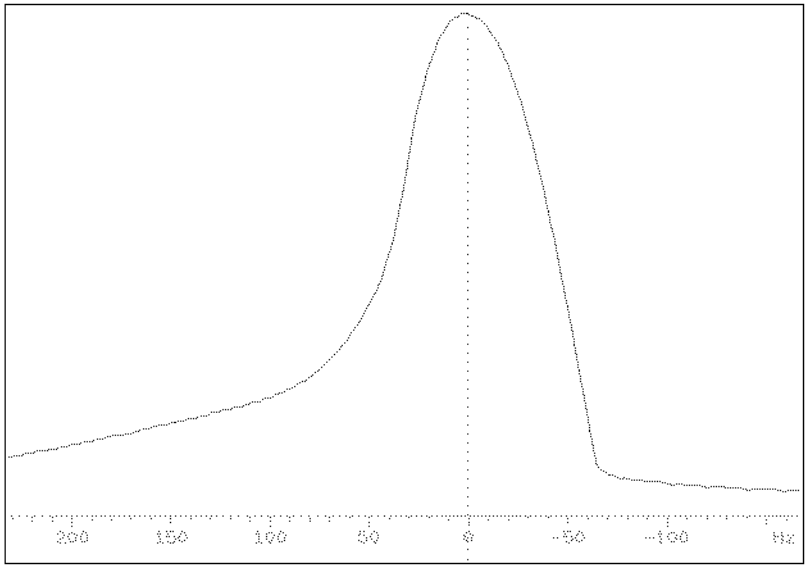


Even though the shimming will only be based on the center resonance, the acquired spectral width should be chosen wider. For speed reasons ShimIt performs locking not by adjusting `z0` but by shifting the analysis window over the acquired spectrum to compensate for constant offsets in impure shims.[2] On the other hand the acquired spectral width should only be chosen as large as necessary. During a ShimIt run a large number of FIDs are acquired and a large

2. ShimIt can indeed also shift the field by adjusting `z0`. A currently disabled feature of ShimIt is to function as a software lock for data acquisitions where the normal deuterium hardware lock is not applicable.

spectral width has to be digitized by a large number of points which slows down the Fast Fourier Transform (FFT) of the FIDs.

The next step in preparation of the autoshimming is to reduce the displayed spectral region to be analyzed for the auto-shimming. The goal here is to include the signal and its tails but hardly any baseline. For this example the chosen area is:



Admittedly, the chosen spectral range does not completely include the signal tails as assumed for the mathematical derivation of the method. However, ShimIt was found to be very forgiving in this regard.

The ShimIt analysis parameters can now be set from the ShimIt menus and the shimming process can be started using menu buttons as discussed in previous chapters. However, the complete shimming of the room temperature shims from scratch involves several steps with increasing spectral resolution and some steps should be performed with a spinning sample and others without sample spinning. This general process can be done conveniently using macros instead of the menu buttons. In this chapter the parameters for the auto-shimming are set from a series of MAGICAL macros. Besides convenience there is no difference between issuing the commands manually vs. issuing them from macros.

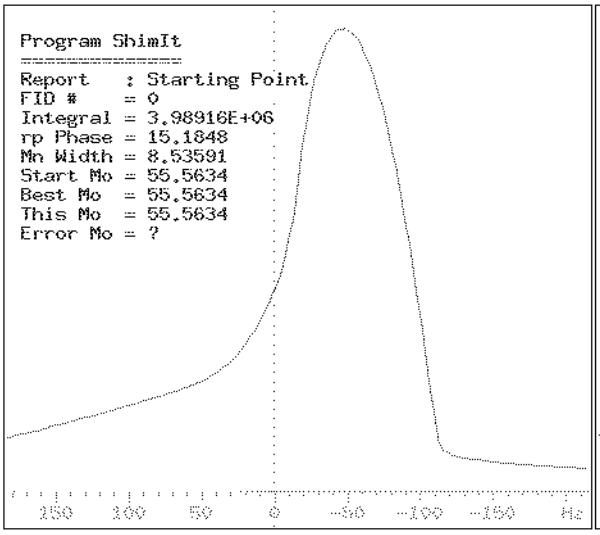
The series of macros is started using the `shimit_all` command. The `shimit_all` macro optimizes all shims using a non-spinning sample as described in SECTION 6.1: "Optimization Of All Shims". On completion of the `shimit_all` macro the `shimit_z` macro starts and optimizes the z shims using sample spinning as described in SECTION 6.2: "Optimization Of Spinning (z) Shims". After `shimit_z` the `shimit_non_z` macro starts and optimizes the non-spinning shims as described in SECTION 6.3: "Optimization Of Non-Spinning Shims". Finally macro `shimit_z_fine` starts and further improves the z shims as described in SECTION 6.4: "Further Optimization Of Spinning (z) Shims". Each section shows the macro used and the spectra representing the successive improvements in magnet homogeneity.

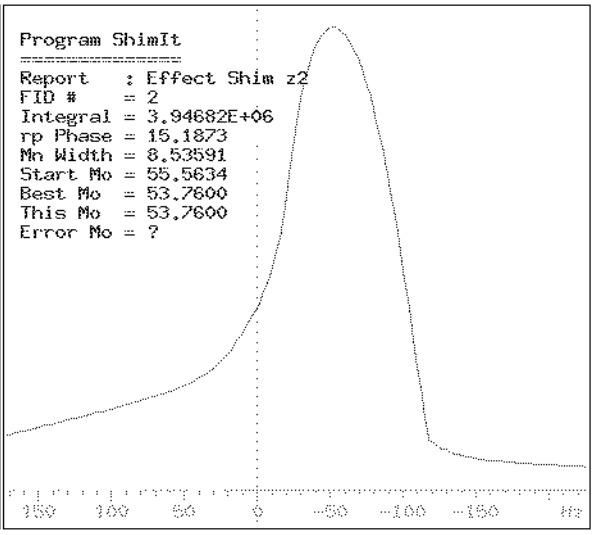
Notice that an auto-shimming run can also be started from the other macros if the magnet homogeneity is already sufficiently high. While the shimming macros are assumed to be generally applicable it is quite instructive to at least once shim a magnet using ShimIt without additional macros. The macros themselves don't try to provide much of a user interface and should at this point be regarded as a demonstration of what ShimIt can do and how to integrate ShimIt in other software systems.

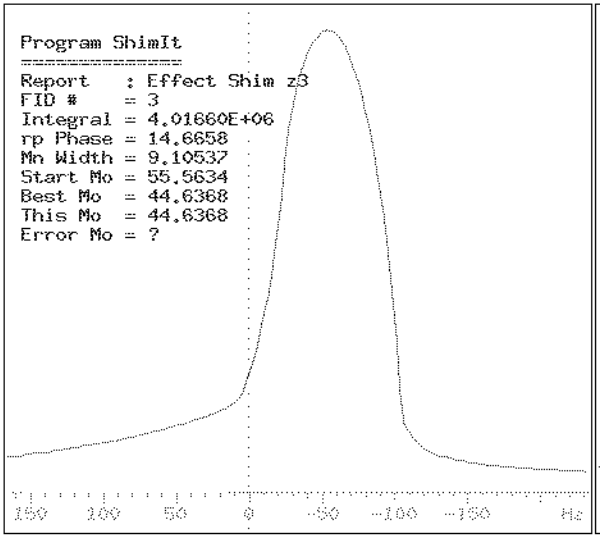
6.1 Optimization Of All Shims

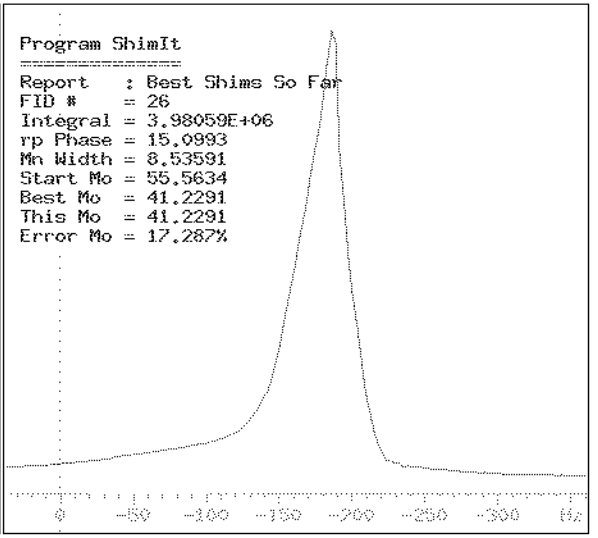
```
"*************************************************************************"
"*                                                                       *"
"*    MAGICAL macro shimit_all                                           *"
"*                                                                       *"
"*    Optimize all shims using non-spinning sample with auto-shimming    *"
"*    software ShimIt.                                                   *"
"*                                                                       *"
"*    (C) Reinhard Dunkel                              Nov 29, 1994      *"
"*                                                                       *"
"*************************************************************************"

spin = 0                                "No sample spinning"
spin                                    "Stop spinning now"
alock = 'u'                             "No Varian locking"
lockpower = 0                           "No power for lock channel"
lockgain  = 0                           "Don't detect lock signal"
in = 'n'                                "No checking of lock or spin"
```

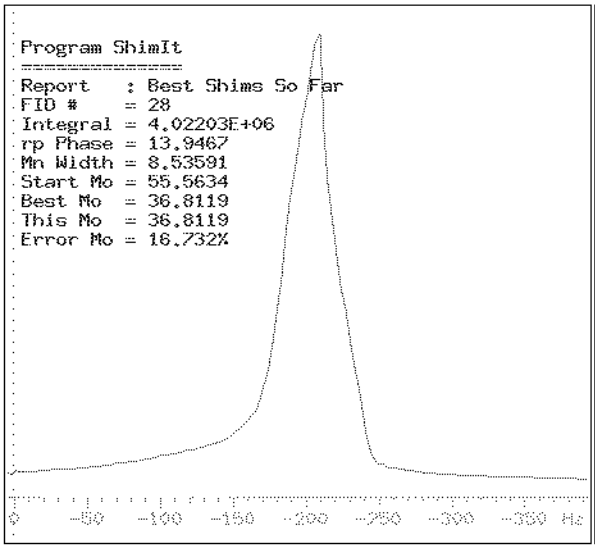
```
shimit_init                                "Create ShimIt variables"
shims = axial_shims+' '+radial_shims       "Optimize all available shims"
shimit_init                                "Initialize ShimIt"
task = 'shim'                              "Set ShimIt to auto-shimming"
sscycles = 0                               "No sample saturation expected"
shimstep = trunc(-sh_range/2)              "Shims completely unknown"
order = 1                                  "Minimize first central moment"
converge = 1.0 * order                     "Termination by max_fid"
timeout = 300                              "Time-out after 5 minutes idle"
$iWord = -1                                "Count number of selected shims"
REPEAT
  $current_shim = ''
  $iWord = $iWord + 1
  substr(shims, $iWord+1):$current_shim
UNTIL $current_shim = ''
max_fid = $iWord * 8                       "Coarse shim adjustment"
cr = sp + wp/2                             "Cursor to middle of display"
$rflrfp = rfl - rfp                        "Assign 0 Hz to cursor position"
rfp = 0
rfl = cr + $rflrfp
sp = sp - cr + rfp
cr = rfp
$oldtof = tof                              "Center display area in spectrum"
tof = $oldtof - sw/2 - rfp + rfl
rfl = rfl + $oldtof - tof                  "Fix spectral referencing"
IF sw > sfrq * 20 THEN                     "Limit spectral width to 20 ppm"
   $oldsw = sw
   sw = sfrq * 20
   rfl = rfl - $oldsw/2 + sw/2             "Fix spectral referencing"
ENDIF
at = 75 * at*sw*2/wp/np                    "Use 75 points for display"
nt = 1                                     "No time for signal averaging"
rm(userdir+'/ShimIt_all')                  "Delete old ShimIt directory"
wshimit = 'mv(userdir+"/ShimIt",'+\
          'userdir+"/ShimIt_all")'+\
          ' shimit_z'                      "Finished? Save & start z shimming"
menu('shimit')                             "Show main ShimIt menu"
shimit_start                               "Start ShimIt"
```

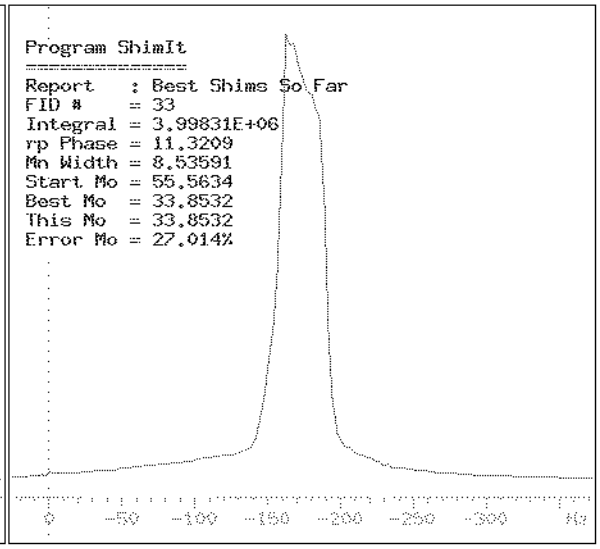

Program ShimIt
Report : Starting Point
FID # = 0
Integral = 3.98916E+06
rp Phase = 15.1848
Mn Width = 8.53591
Start Mo = 55.5634
Best Mo = 55.5634
This Mo = 55.5634
Error Mo = ?
150 100 50 0 -50 -100 -150 Hz

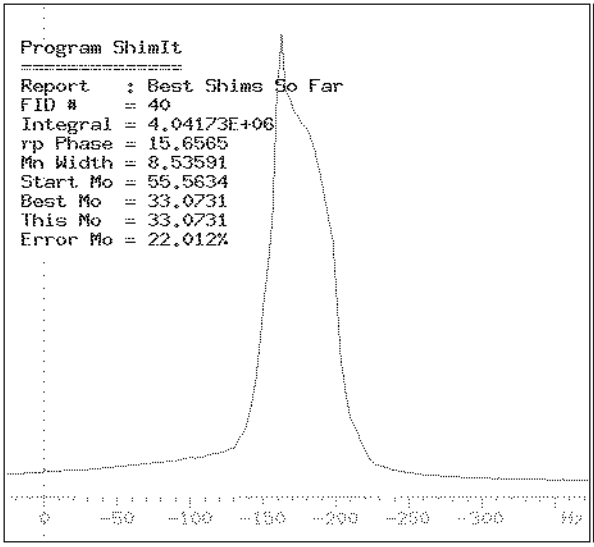

Program ShimIt
Report : Effect Shim z2
FID # = 2
Integral = 3.94682E+06
rp Phase = 15.1873
Mn Width = 8.53591
Start Mo = 55.5634
Best Mo = 53.7600
This Mo = 53.7600
Error Mo = ?
150 100 50 0 -50 -100 -150 Hz

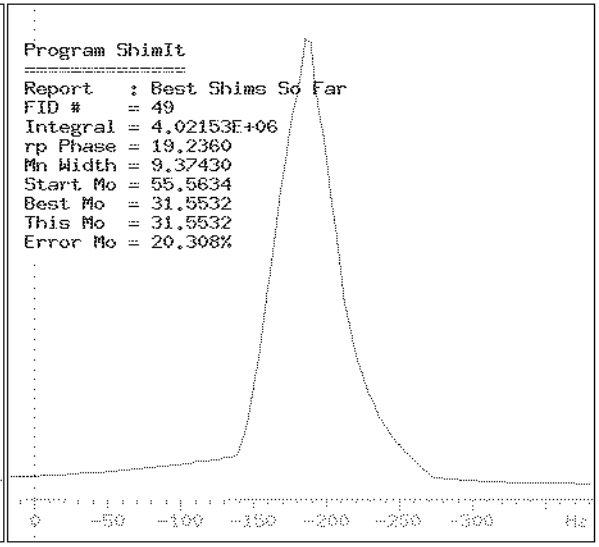

Program ShimIt
Report : Effect Shim z3
FID # = 3
Integral = 4.01660E+06
rp Phase = 14.6658
Mn Width = 9.10537
Start Mo = 55.5634
Best Mo = 44.6368
This Mo = 44.6368
Error Mo = ?
150 100 50 0 -50 -100 -150 Hz

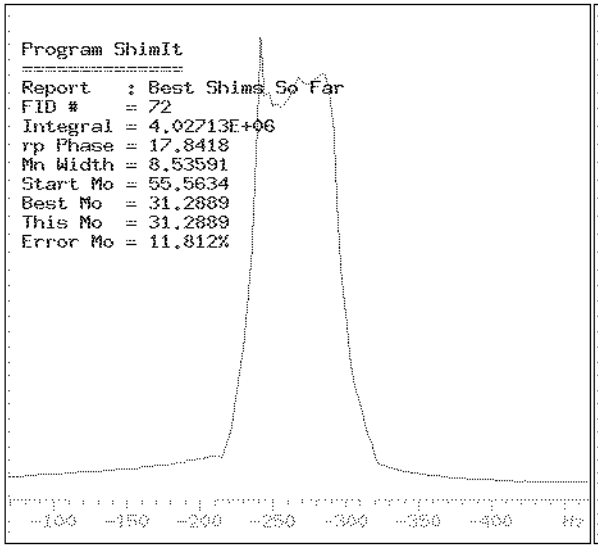

Program ShimIt
Report : Best Shims So Far
FID # = 26
Integral = 3.98059E+06
rp Phase = 15.0993
Mn Width = 8.53591
Start Mo = 55.5634
Best Mo = 41.2291
This Mo = 41.2291
Error Mo = 17.287%
0 -50 -100 -150 -200 -250 -300 Hz

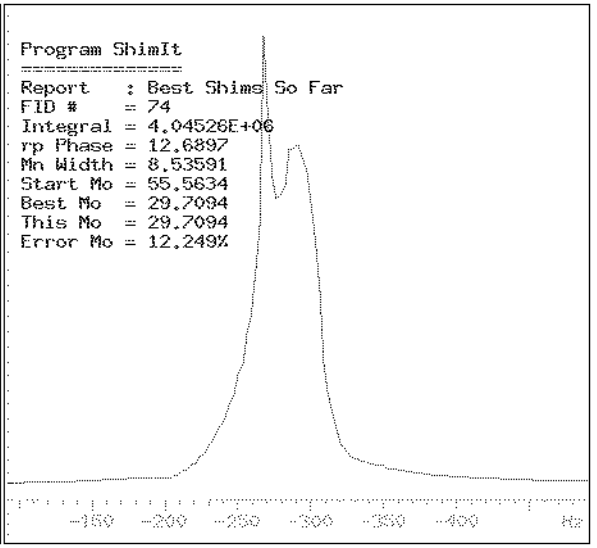

Program ShimIt
Report : Best Shims So Far
FID # = 28
Integral = 4.02203E+06
rp Phase = 13.9467
Mn Width = 8.53591
Start Mo = 55.5634
Best Mo = 36.8119
This Mo = 36.8119
Error Mo = 16.732%
0 -50 -100 -150 -200 -250 -300 -350 Hz

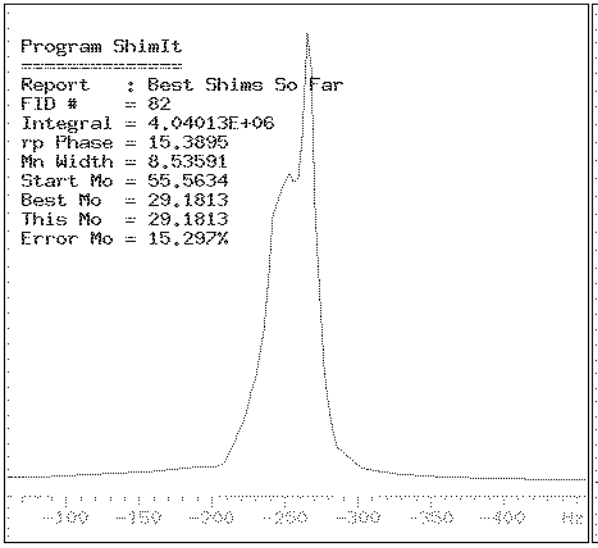

Program ShimIt
Report : Best Shims So Far
FID # = 33
Integral = 3.99831E+06
rp Phase = 11.3209
Mn Width = 8.53591
Start Mo = 55.5634
Best Mo = 33.8532
This Mo = 33.8532
Error Mo = 27.014%
0 -50 -100 -150 -200 -250 -300 Hz

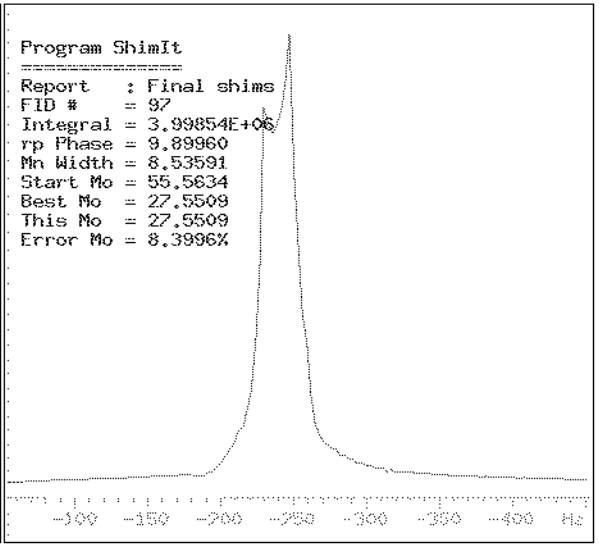

Program ShimIt
Report : Best Shims So Far
FID # = 40
Integral = 4.04173E+06
rp Phase = 15.6565
Mn Width = 8.53591
Start Mo = 55.5634
Best Mo = 33.0731
This Mo = 33.0731
Error Mo = 22.012%
0 -50 -100 -150 -200 -250 -300 Hz


Program ShimIt
Report : Best Shims So Far
FID # = 49
Integral = 4.02153E+06
rp Phase = 19.2360
Mn Width = 9.37430
Start Mo = 55.5634
Best Mo = 31.5532
This Mo = 31.5532
Error Mo = 20.308%
0 -50 -100 -150 -200 -250 -300 Hz


Program ShimIt
Report : Best Shims So Far
FID # = 72
Integral = 4.02713E+06
rp Phase = 17.8418
Mn Width = 8.53591
Start Mo = 55.5634
Best Mo = 31.2889
This Mo = 31.2889
Error Mo = 11.812%
-100 -150 -200 -250 -300 -350 -400 Hz


Program ShimIt
Report : Best Shims So Far
FID # = 74
Integral = 4.04526E+06
rp Phase = 12.6897
Mn Width = 8.53591
Start Mo = 55.5634
Best Mo = 29.7094
This Mo = 29.7094
Error Mo = 12.249%
-150 -200 -250 -300 -350 -400 Hz

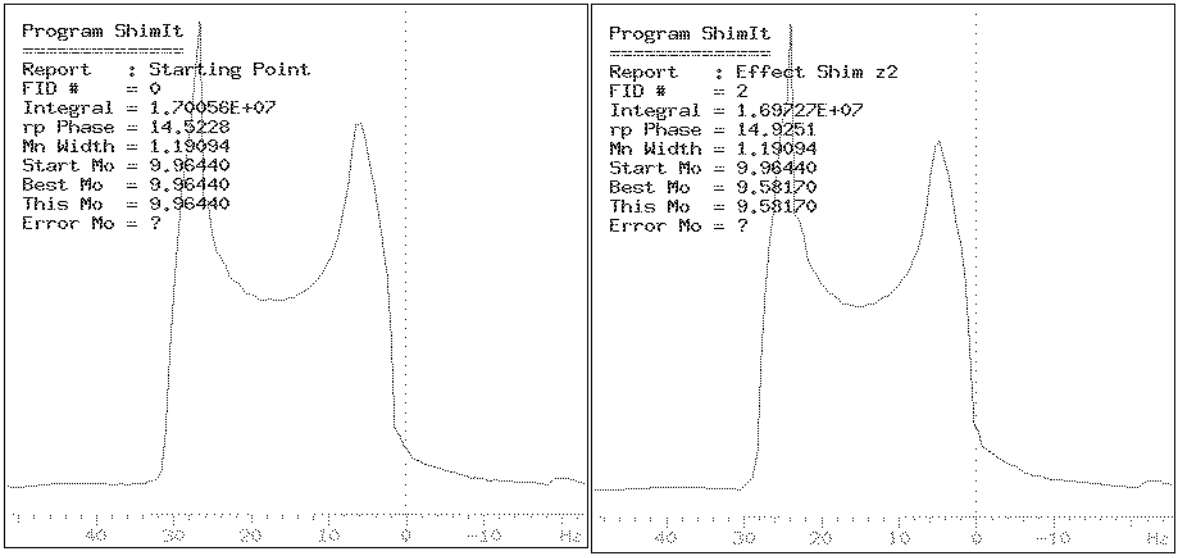

Program ShimIt
Report : Best Shims So Far
FID # = 82
Integral = 4.04013E+06
rp Phase = 15.3895
Mn Width = 8.53591
Start Mo = 55.5634
Best Mo = 29.1813
This Mo = 29.1813
Error Mo = 15.297%
-100 -150 -200 -250 -300 -350 -400 Hz

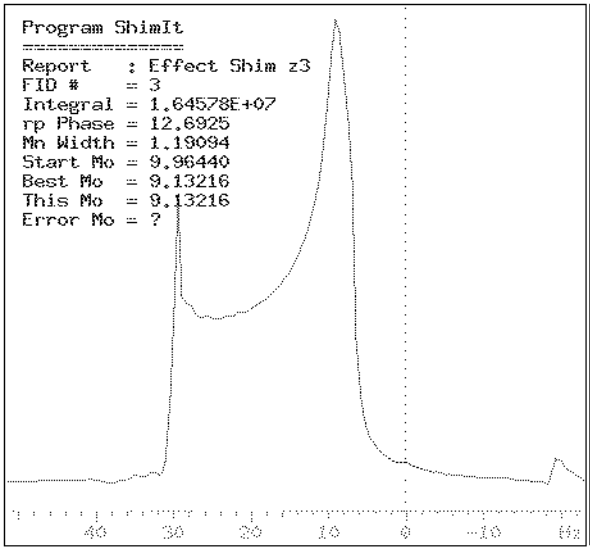

Program ShimIt
Report : Final shims
FID # = 97
Integral = 3.99854E+06
rp Phase = 9.89960
Mn Width = 8.53591
Start Mo = 55.5634
Best Mo = 27.5509
This Mo = 27.5509
Error Mo = 8.3996%
-100 -150 -200 -250 -300 -350 -400 Hz

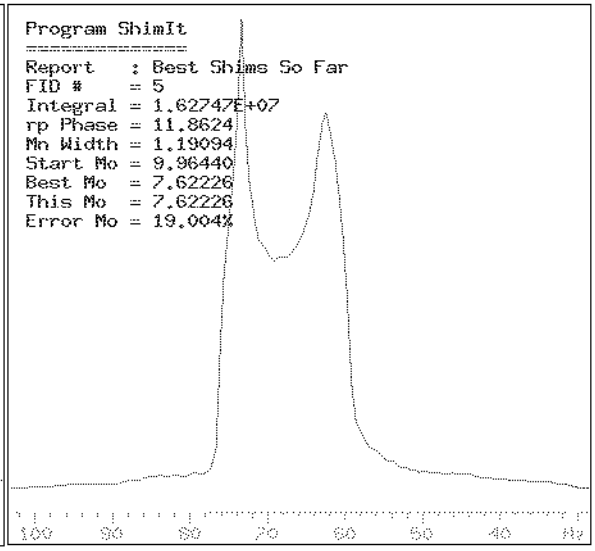
6.2 Optimization Of Spinning (z) Shims

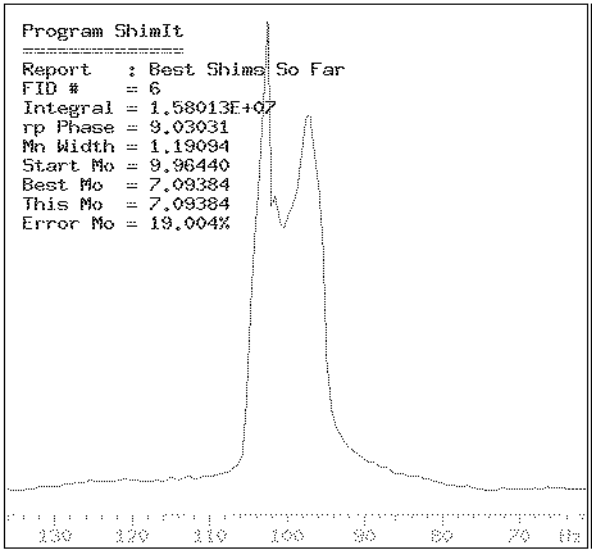
```
"*************************************************************************"
"*                                                                       *"
"*    MAGICAL macro shimit_z                                             *"
"*                                                                       *"
"*    Optimize spinning shims using spinning sample with auto-shimming   *"
"*    software ShimIt.                                                   *"
"*                                                                       *"
"*    (C) Reinhard Dunkel                                 Nov 29, 1994   *"
"*                                                                       *"
"*************************************************************************"

spin = 50                                   "Spin sample at 50 Hz"
spin                                        "Regulate spinning now"
alock = 'u'                                 "No Varian locking"
lockpower = 0                               "No power for lock channel"
lockgain  = 0                               "Don't detect lock signal"
in = 'n'                                    "No checking of lock or spin"
shimit_init                                 "Create ShimIt variables"
shims = axial_shims                         "Optimize spinning shims"
shimit_init                                 "Initialize ShimIt"
task = 'shim'                               "Set ShimIt to auto-shimming"
sscycles = 0                                "No sample saturation expected"
shimstep = trunc(sh_range/4)                "z shims partly optimized"
order = 1                                   "Minimize first central moment"
converge = 1.0 * order                      "Termination by max_fid"
timeout = 300                               "Time-out after 5 minutes idle"
sp = sp + (wp - spin*1.5)/2                 "Exclude spinning sidebands"
wp = spin * 1.5                             "Narrow displayed spectral area"
$iWord = -1                                 "Count number of selected shims"
REPEAT
  $current_shim = ''
  $iWord = $iWord + 1
  substr(shims, $iWord+1):$current_shim
UNTIL $current_shim = ''
max_fid = $iWord * 8                        "Coarse shim adjustment"
cr = sp + wp/2                              "Cursor to middle of display"
$rflrfp = rfl - rfp                         "Assign 0 Hz to cursor position"
rfp = 0
rfl = cr + $rflrfp
sp = sp - cr + rfp
cr = rfp
$oldtof = tof                               "Center display area in spectrum"
```

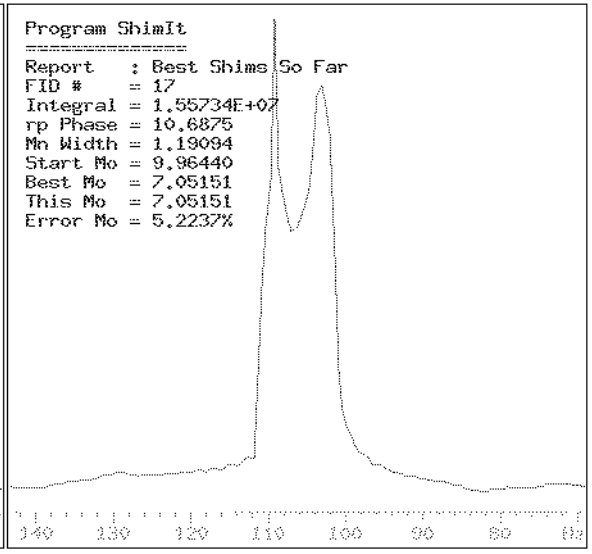
```
tof = $oldtof - sw/2 - rfp + rfl
rfl = rfl + $oldtof - tof                "Fix spectral referencing"
IF sw > sfrq * 15 THEN                   "Limit spectral width to 15 ppm"
   $oldsw = sw
   sw = sfrq * 15
   rfl = rfl - $oldsw/2 + sw/2           "Fix spectral referencing"
ENDIF
at = 100 * at*sw*2/wp/np                 "Display 100 points (.75 Hz/pt)"
nt = 1                                   "No time for signal averaging"
rm(userdir+'/ShimIt_z')                  "Delete old ShimIt directory"
wshimit = 'mv(userdir+"/ShimIt",'+\
          'userdir+"/ShimIt_z")'+\
          ' shimit_non_z'                "Finished? Save & start non-z shimming"
menu('shimit')                           "Show main ShimIt menu"
shimit_start                             "Start ShimIt"
```

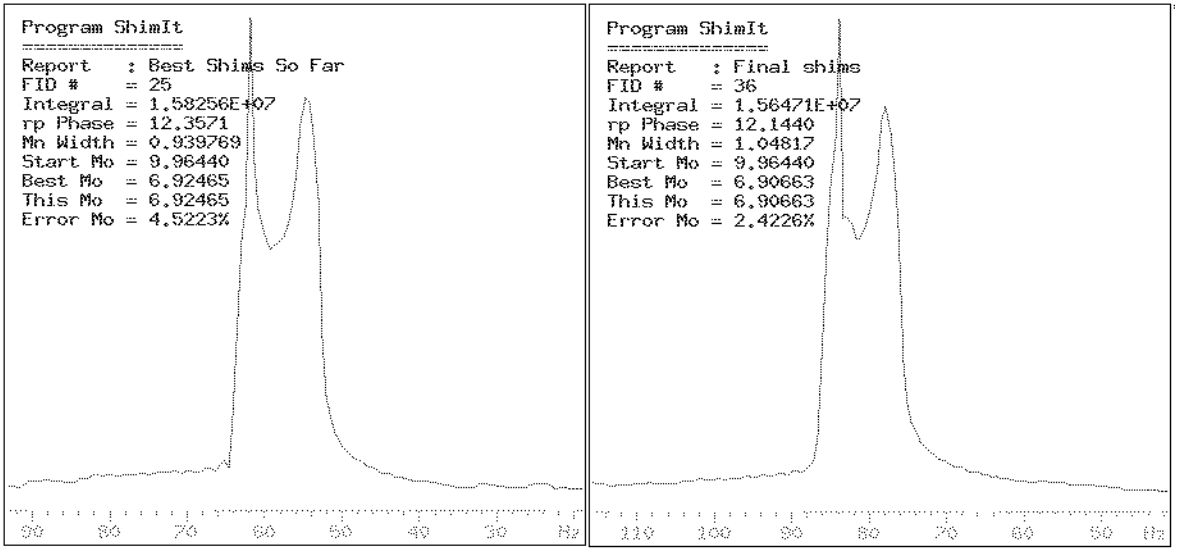



Program ShimIt
Report : Effect Shim z3
FID # = 3
Integral = 1.64578E+07
rp Phase = 12.6925
Mn Width = 1.19094
Start Mo = 9.96440
Best Mo = 9.13216
This Mo = 9.13216
Error Mo = ?
40
30
20
10
0
-10
Hz


Program ShimIt
Report : Best Shims So Far
FID # = 5
Integral = 1.62747E+07
rp Phase = 11.8624
Mn Width = 1.19094
Start Mo = 9.96440
Best Mo = 7.62226
This Mo = 7.62226
Error Mo = 19.004%
100
90
80
70
60
50
40
Hz


Program ShimIt
Report : Best Shims So Far
FID # = 6
Integral = 1.58013E+07
rp Phase = 9.03031
Mn Width = 1.19094
Start Mo = 9.96440
Best Mo = 7.09384
This Mo = 7.09384
Error Mo = 19.004%
130
120
110
100
90
80
70
Hz

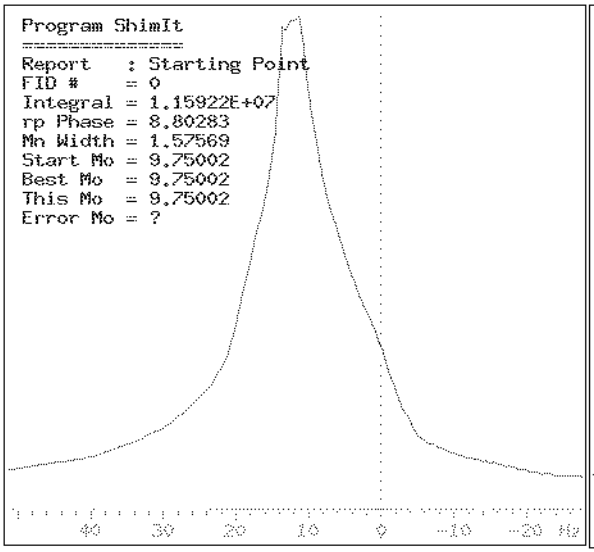

Program ShimIt
Report : Best Shims So Far
FID # = 17
Integral = 1.55734E+07
rp Phase = 10.6875
Mn Width = 1.19094
Start Mo = 9.96440
Best Mo = 7.05151
This Mo = 7.05151
Error Mo = 5.2237%
140
130
120
110
100
90
80
Hz

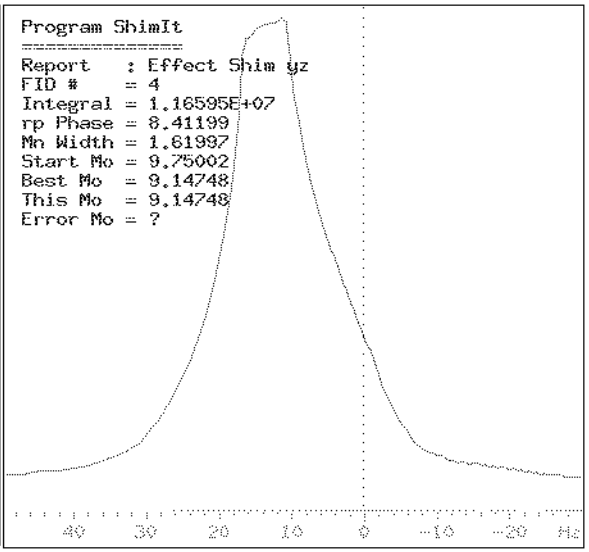


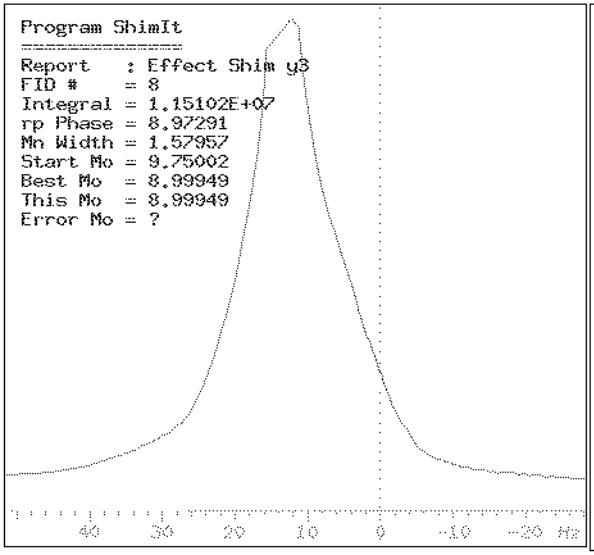
6.3 Optimization Of Non-Spinning Shims

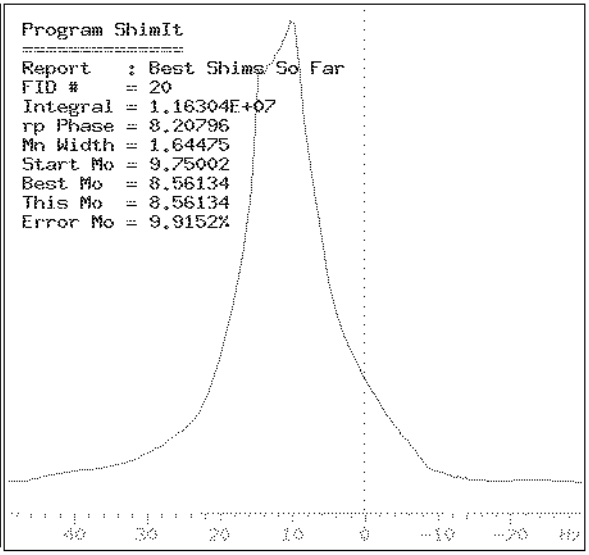
```
"*************************************************************************"
"*                                                                       *"
"*    MAGICAL macro shimit_non_z                                         *"
"*                                                                       *"
"*    Optimize non-spinning shims using non-spinning sample using        *"
"*    auto-shimming software ShimIt.                                     *"
"*                                                                       *"
"*    (C) Reinhard Dunkel                              Nov 29, 1994      *"
"*                                                                       *"
"*************************************************************************"

spin = 0                                "No sample spinning"
spin                                    "Stop spinning now"
alock = 'u'                             "No Varian locking"
lockpower = 0                           "No power for lock channel"
lockgain  = 0                           "Don't detect lock signal"
in = 'n'                                "No checking of lock or spin"
shimit_init                             "Create ShimIt variables"
```

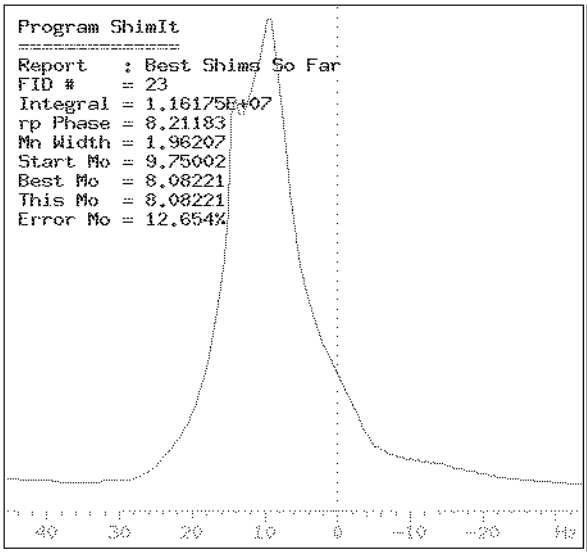
```
shims = radial_shims                        "Optimize spinning shims"
shimit_init                                 "Initialize ShimIt"
task = 'shim'                               "Set ShimIt to auto-shimming"
sscycles = 0                                "No sample saturation expected"
shimstep = trunc(-sh_range/8)               "z shims partly optimized"
order = 1                                   "Increase weight of signal height"
converge = 1.0 * order                      "Termination by max_fid"
timeout = 300                               "Time-out after 5 minutes idle"
sp = sp + (wp - 100)/2                      "Display +/-40 Hz around signal"
wp = 80
$iWord = -1                                 "Count number of selected shims"
REPEAT
  $current_shim = ''
  $iWord = $iWord + 1
  substr(shims, $iWord+1):$current_shim
UNTIL $current_shim = ''
max_fid = $iWord * 8                        "Coarse shim adjustment"
cr = sp + wp/2                              "Cursor to middle of display"
$rflrfp = rfl - rfp                         "Assign 0 Hz to cursor position"
rfp = 0
rfl = cr + $rflrfp
sp = sp - cr + rfp
cr = rfp
$oldtof = tof                               "Center display area in spectrum"
tof = $oldtof - sw/2 - rfp + rfl
rfl = rfl + $oldtof - tof                   "Fix spectral referencing"
IF sw > sfrq * 15 THEN                      "Limit spectral width to 15 ppm"
   $oldsw = sw
   sw = sfrq * 15
   rfl = rfl - $oldsw/2 + sw/2              "Fix spectral referencing"
ENDIF
at = 75 * at*sw*2/wp/np                     "Display 75 points (1 Hz/pt)"
nt = 1                                      "No time for signal averaging"
rm(userdir+'/ShimIt_non_z')                 "Delete old ShimIt directory"
wshimit = 'mv(userdir+"/ShimIt",'+\
          'userdir+"/ShimIt_non_z") '+\
          'shimit_z_fine'                   "Finished? Save & start z-fine shimming"
menu('shimit')                              "Show main ShimIt menu"
shimit_start                                "Start ShimIt"
```

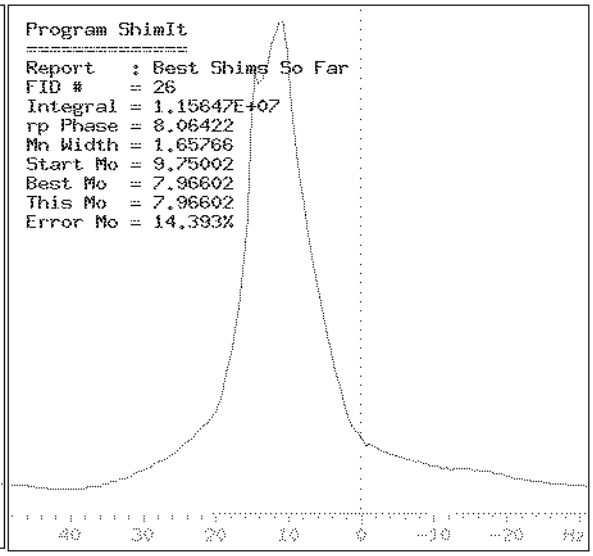

Program ShimIt
Report : Starting Point
FID # = 0
Integral = 1.15922E+07
rp Phase = 8.80283
Mn Width = 1.57569
Start Mo = 9.75002
Best Mo = 9.75002
This Mo = 9.75002
Error Mo = ?
40 30 20 10 0 -10 -20 Hz

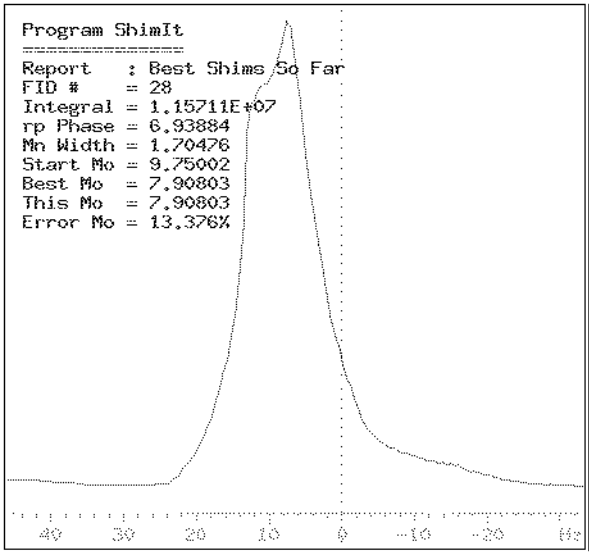

Program ShimIt
Report : Effect Shim yz
FID # = 4
Integral = 1.16595E+07
rp Phase = 8.41199
Mn Width = 1.61997
Start Mo = 9.75002
Best Mo = 9.14748
This Mo = 9.14748
Error Mo = ?
40 30 20 10 0 -10 -20 Hz

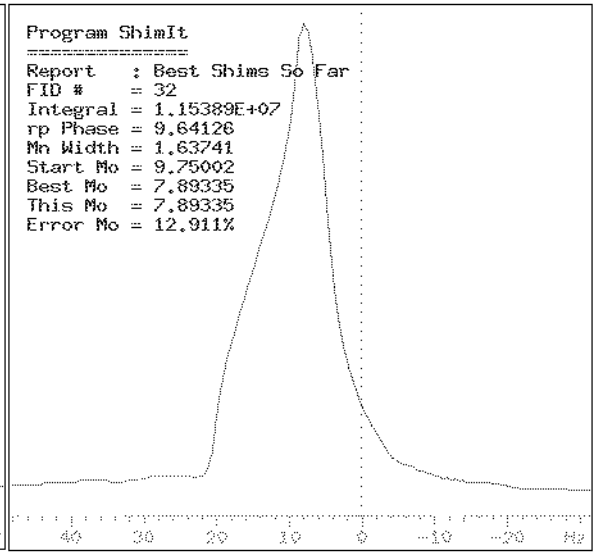

Program ShimIt
Report : Effect Shim y3
FID # = 8
Integral = 1.15102E+07
rp Phase = 8.97291
Mn Width = 1.57957
Start Mo = 9.75002
Best Mo = 8.99949
This Mo = 8.99949
Error Mo = ?
40 30 20 10 0 -10 -20 Hz

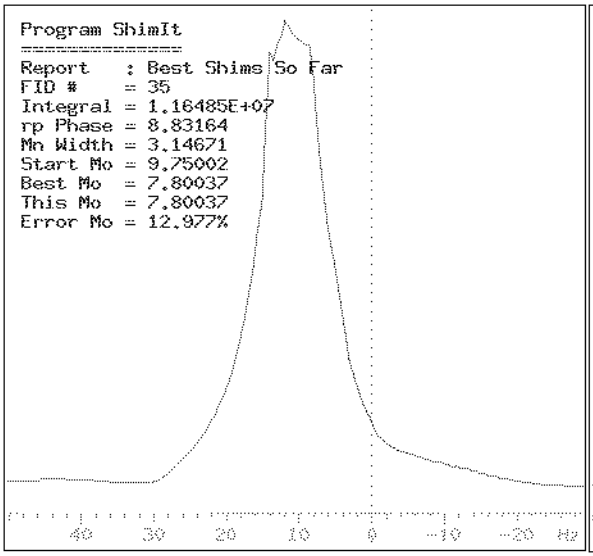

Program ShimIt
Report : Best Shims So Far
FID # = 20
Integral = 1.16304E+07
rp Phase = 8.20796
Mn Width = 1.64475
Start Mo = 9.75002
Best Mo = 8.56134
This Mo = 8.56134
Error Mo = 9.9152%
40 30 20 10 0 -10 -20 Hz

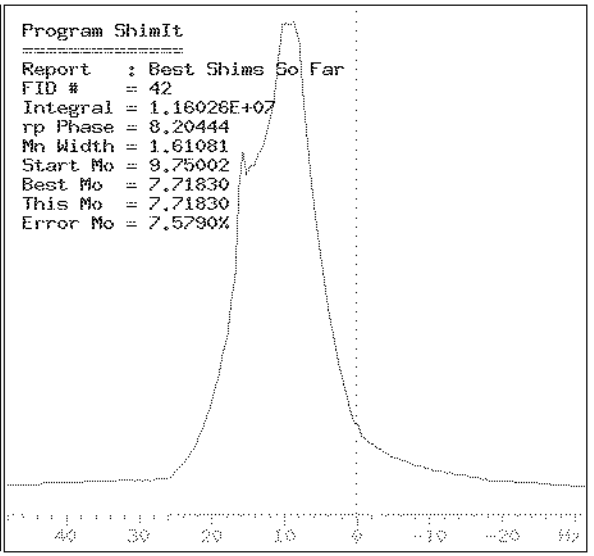

Program ShimIt
Report : Best Shims So Far
FID # = 23
Integral = 1.16175E+07
rp Phase = 8.21183
Mn Width = 1.96207
Start Mo = 9.75002
Best Mo = 8.08221
This Mo = 8.08221
Error Mo = 12.654%
40 30 20 10 0 -10 -20 Hz

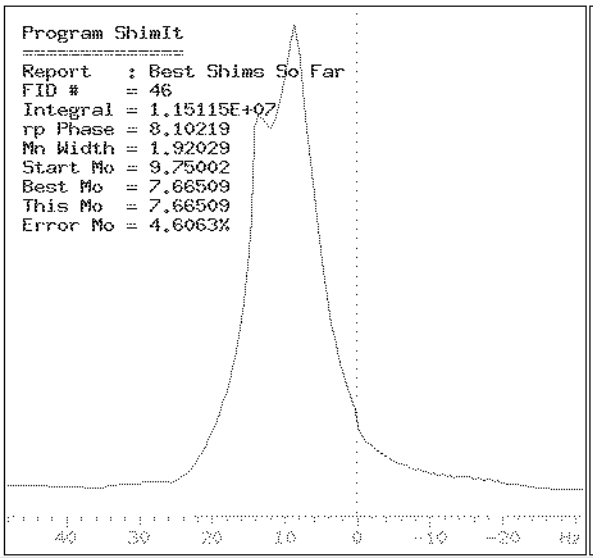

Program ShimIt
Report : Best Shims So Far
FID # = 26
Integral = 1.15847E+07
rp Phase = 8.06422
Mn Width = 1.65766
Start Mo = 9.75002
Best Mo = 7.96602
This Mo = 7.96602
Error Mo = 14.393%
40 30 20 10 0 -10 -20 Hz

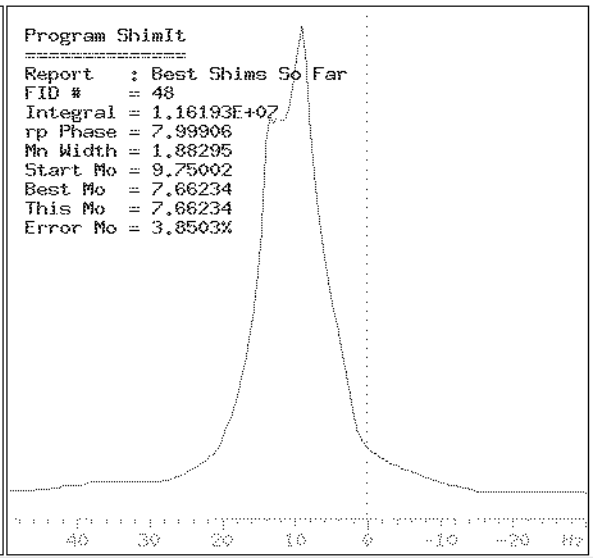

Program ShimIt
Report : Best Shims So Far
FID # = 28
Integral = 1.15711E+07
rp Phase = 6.93884
Mn Width = 1.70476
Start Mo = 9.75002
Best Mo = 7.90803
This Mo = 7.90803
Error Mo = 13.376%
40 30 20 10 0 -10 -20 Hz

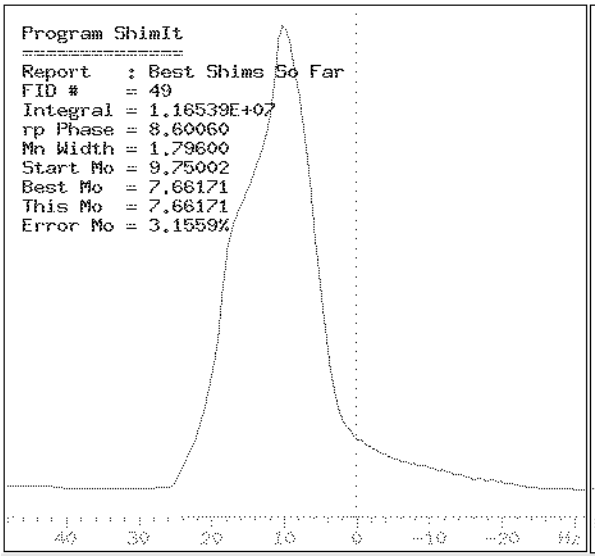

Program ShimIt
Report : Best Shims So Far
FID # = 32
Integral = 1.15389E+07
rp Phase = 9.64126
Mn Width = 1.63741
Start Mo = 9.75002
Best Mo = 7.89335
This Mo = 7.89335
Error Mo = 12.911%
40 30 20 10 0 -10 -20 Hz

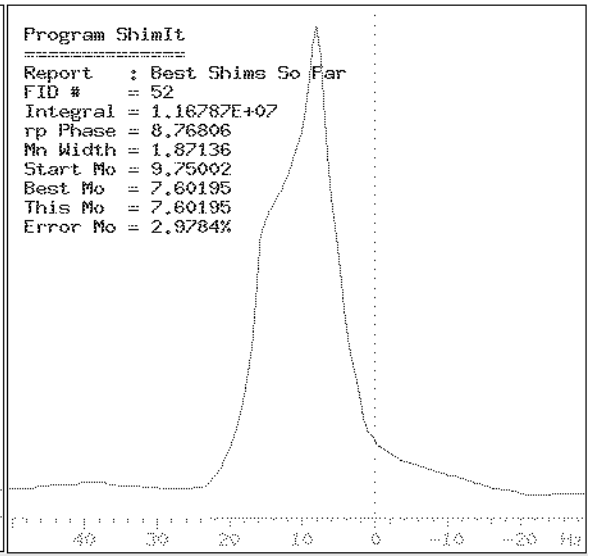

Program ShimIt
Report : Best Shims So Far
FID # = 35
Integral = 1.16485E+07
rp Phase = 8.83164
Mn Width = 3.14671
Start Mo = 9.75002
Best Mo = 7.80037
This Mo = 7.80037
Error Mo = 12.977%
40 30 20 10 0 -10 -20 Hz

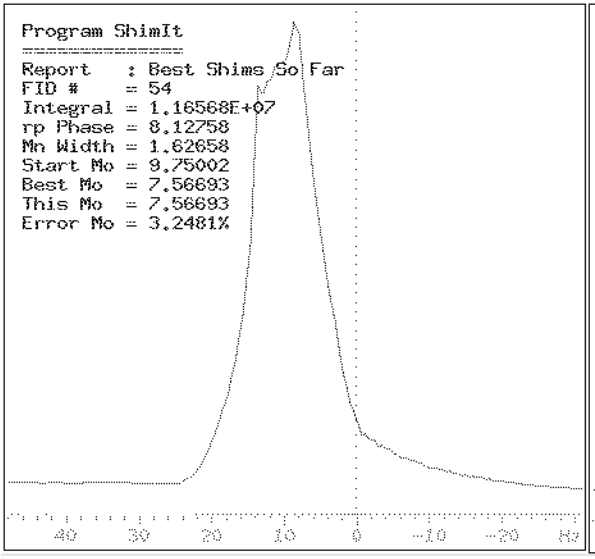

Program ShimIt
Report : Best Shims So Far
FID # = 42
Integral = 1.16026E+07
rp Phase = 8.20444
Mn Width = 1.61081
Start Mo = 9.75002
Best Mo = 7.71830
This Mo = 7.71830
Error Mo = 7.5790%
40 30 20 10 0 -10 -20 Hz

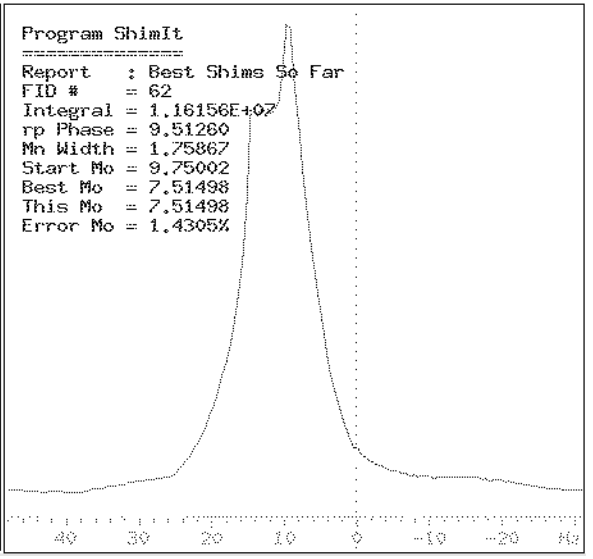

Program ShimIt
Report : Best Shims So Far
FID # = 46
Integral = 1.15115E+07
rp Phase = 8.10219
Mn Width = 1.92029
Start Mo = 9.75002
Best Mo = 7.66509
This Mo = 7.66509
Error Mo = 4.6063%
40 30 20 10 0 -10 -20 Hz

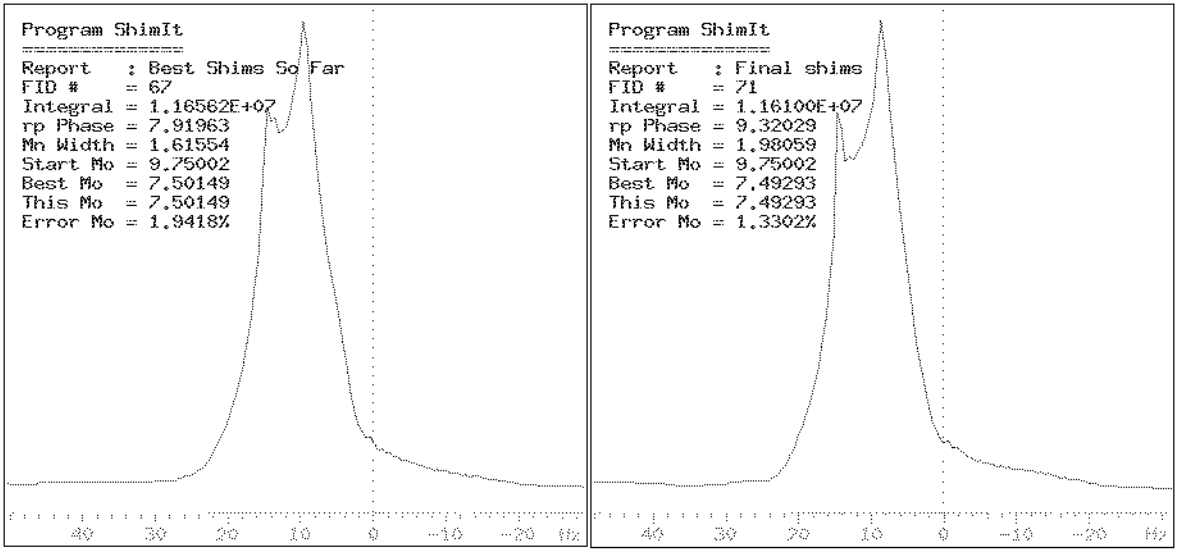

Program ShimIt
Report : Best Shims So Far
FID # = 48
Integral = 1.16193E+07
rp Phase = 7.99906
Mn Width = 1.88295
Start Mo = 9.75002
Best Mo = 7.66234
This Mo = 7.66234
Error Mo = 3.8503%
40 30 20 10 0 -10 -20 Hz


Program ShimIt
Report : Best Shims So Far
FID # = 49
Integral = 1.16539E+07
rp Phase = 8.60060
Mn Width = 1.79600
Start Mo = 9.75002
Best Mo = 7.66171
This Mo = 7.66171
Error Mo = 3.1559%
40 30 20 10 0 -10 -20 Hz


Program ShimIt
Report : Best Shims So Far
FID # = 52
Integral = 1.16787E+07
rp Phase = 8.76806
Mn Width = 1.87136
Start Mo = 9.75002
Best Mo = 7.60195
This Mo = 7.60195
Error Mo = 2.9784%
40 30 20 10 0 -10 -20 Hz


Program ShimIt
Report : Best Shims So Far
FID # = 54
Integral = 1.16568E+07
rp Phase = 8.12758
Mn Width = 1.82658
Start Mo = 9.75002
Best Mo = 7.56693
This Mo = 7.56693
Error Mo = 3.2481%
40 30 20 10 0 -10 -20 Hz

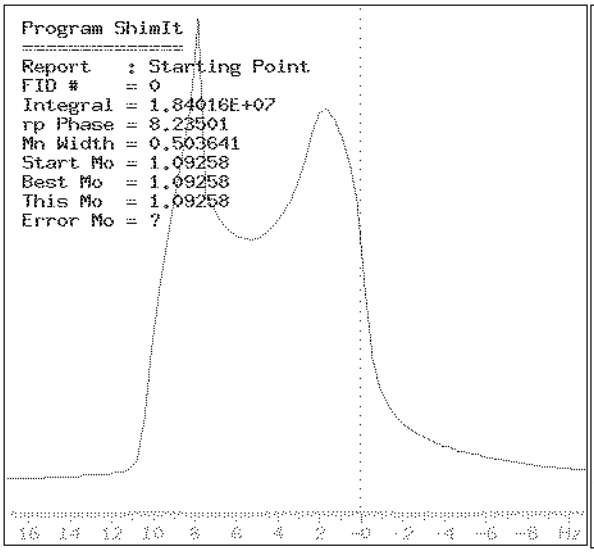

Program ShimIt
Report : Best Shims So Far
FID # = 62
Integral = 1.16156E+07
rp Phase = 9.51260
Mn Width = 1.75867
Start Mo = 9.75002
Best Mo = 7.51498
This Mo = 7.51498
Error Mo = 1.4305%
40 30 20 10 0 -10 -20 Hz

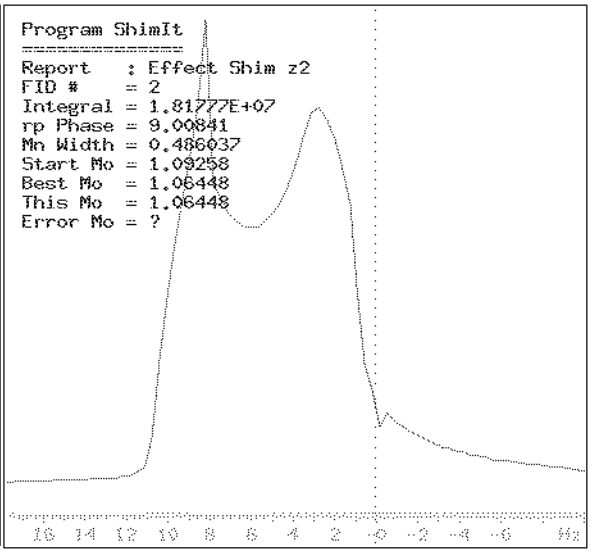


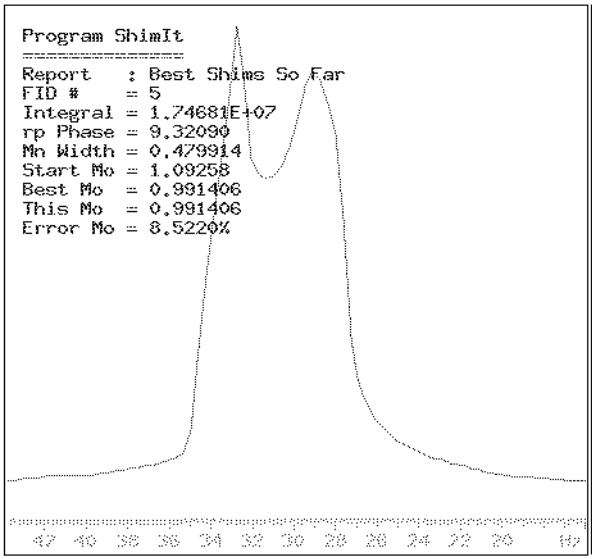
6.4 *Further Optimization Of Spinning (z) Shims*

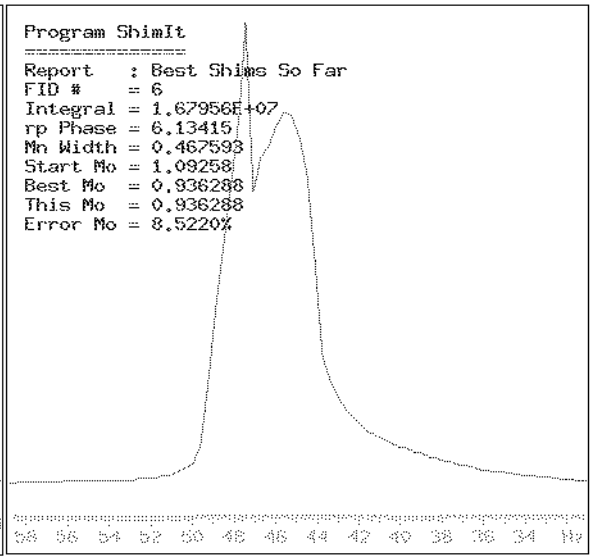
```
"************************************************************************"
"*                                                                      *"
"*    MAGICAL macro shimit_z_fine                                       *"
"*                                                                      *"
"*    Final optimization of spinning shims using spinning sample with   *"
"*    auto-shimming software ShimIt.                                    *"
"*                                                                      *"
"*    (C) Reinhard Dunkel                              Nov 29, 1994     *"
"*                                                                      *"
"************************************************************************"

spin = 35                                "Spin sample at 35 Hz"
spin                                     "Regulate spinning now"
alock = 'u'                              "No Varian locking"
lockpower = 0                            "No power for lock channel"
lockgain  = 0                            "Don't detect lock signal"
in = 'n'                                 "No checking of lock or spin"
shimit_init                              "Create ShimIt variables"
```

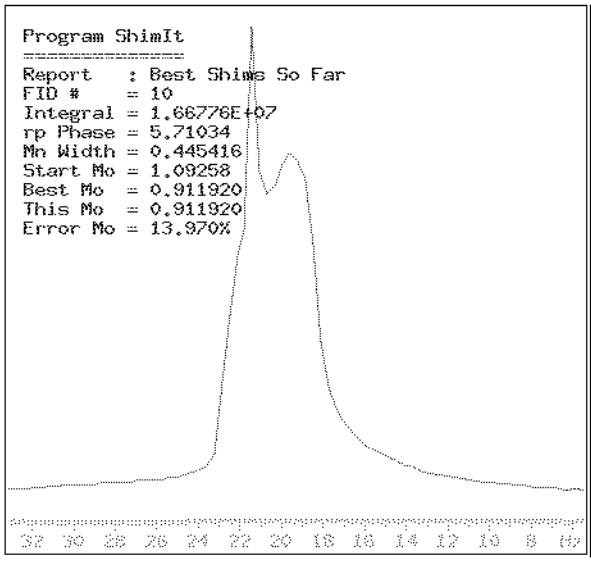
```
shims = axial_shims                         "Optimize spinning shims"
shimit_init                                 "Initialize ShimIt"
task = 'shim'                               "Set ShimIt to auto-shimming"
sscycles = 0                                "No sample saturation expected"
shimstep = trunc(sh_range/8)                "z shims pre-optimized"
order = 0.5                                 "Increase weight of signal height"
converge = 1.0 * order                      "Termination by max_fid"
timeout = 300                               "Time-out after 5 minutes idle"
sp = sp + (wp - spin)/2                     "Exclude spinning sidebands"
wp = spin * 0.8                             "Narrow displayed spectral area"
$iWord = -1                                 "Count number of selected shims"
REPEAT
  $current_shim = ''
  $iWord = $iWord + 1
  substr(shims, $iWord+1):$current_shim
UNTIL $current_shim = ''
max_fid = $iWord * 10                       "Coarse shim adjustment"
cr = sp + wp/2                              "Cursor to middle of display"
$rflrfp = rfl - rfp                         "Assign 0 Hz to cursor position"
rfp = 0
rfl = cr + $rflrfp
sp = sp - cr + rfp
cr = rfp
$oldtof = tof                               "Center display area in spectrum"
tof = $oldtof - sw/2 - rfp + rfl
rfl = rfl + $oldtof - tof                   "Fix spectral referencing"
IF sw > sfrq * 10 THEN                      "Limit spectral width to 10 ppm"
   $oldsw = sw
   sw = sfrq * 10
   rfl = rfl - $oldsw/2 + sw/2              "Fix spectral referencing"
ENDIF
at = 75 * at*sw*2/wp/np                     "Display 75 points (.35 Hz/pt)"
nt = 1                                      "No time for signal averaging"
rm(userdir+'/ShimIt_z_fine')                "Delete old ShimIt directory"
wshimit = 'mv(userdir+"/ShimIt",'+\
          'userdir+"/ShimIt_z_fine")'+\
          ' wshimit=""'                     "On termination: Save output"
menu('shimit')                              "Show main ShimIt menu"
shimit_start                                "Start ShimIt"
```

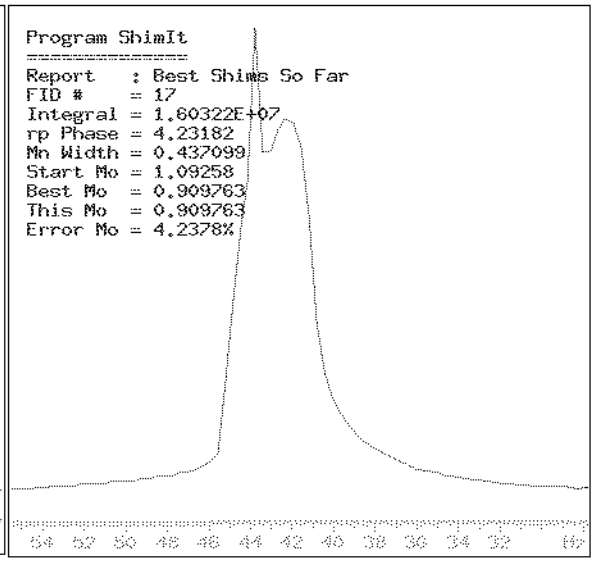

Program ShimIt
Report : Starting Point
FID # = 0
Integral = 1.84016E+07
rp Phase = 8.23501
Mn Width = 0.503641
Start Mo = 1.09258
Best Mo = 1.09258
This Mo = 1.09258
Error Mo = ?
16 14 12 10 8 6 4 2 0 -2 -4 -6 -8 Hz

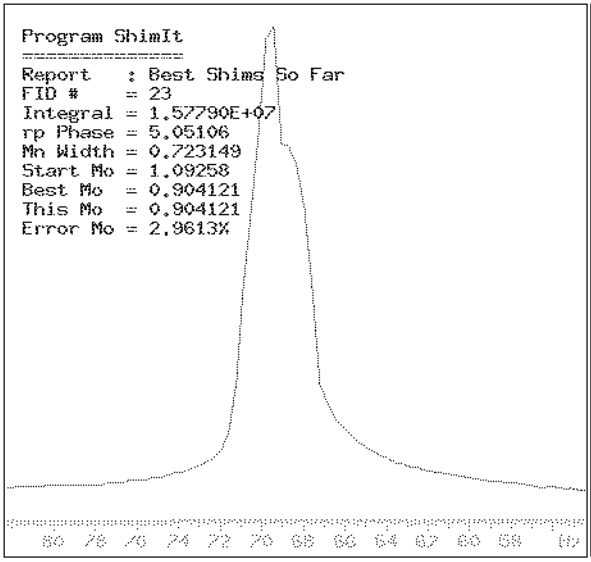

Program ShimIt
Report : Effect Shim z2
FID # = 2
Integral = 1.81777E+07
rp Phase = 9.00841
Mn Width = 0.486037
Start Mo = 1.09258
Best Mo = 1.06448
This Mo = 1.06448
Error Mo = ?
16 14 12 10 8 6 4 2 0 -2 -4 -6 Hz

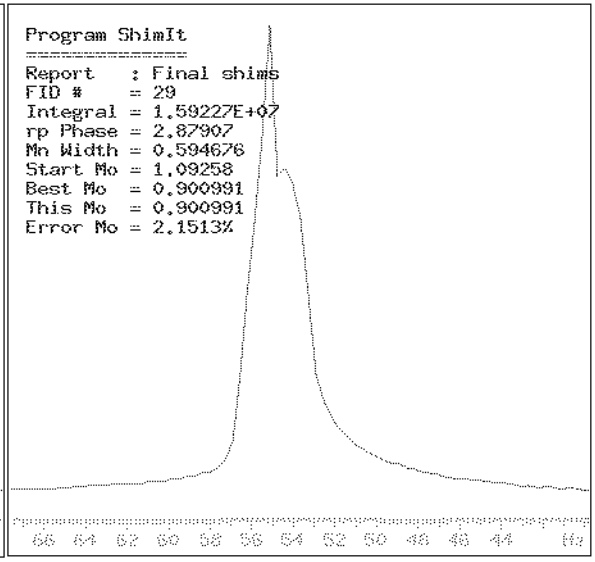

Program ShimIt
Report : Best Shims So Far
FID # = 5
Integral = 1.74681E+07
rp Phase = 9.32090
Mn Width = 0.479914
Start Mo = 1.09258
Best Mo = 0.991406
This Mo = 0.991406
Error Mo = 8.5220%
42 40 38 36 34 32 30 28 26 24 22 20 Hz


Program ShimIt
Report : Best Shims So Far
FID # = 6
Integral = 1.67956E+07
rp Phase = 6.13415
Mn Width = 0.467593
Start Mo = 1.09258
Best Mo = 0.936288
This Mo = 0.936288
Error Mo = 8.5220%
58 56 54 52 50 48 46 44 42 40 38 36 34 Hz

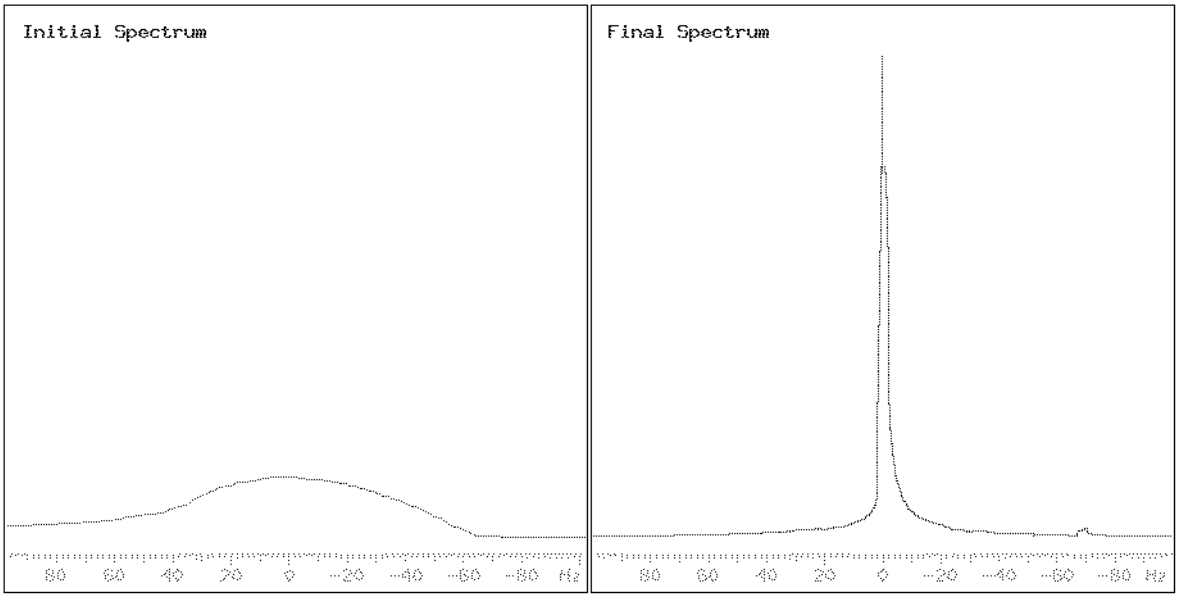

Program ShimIt
Report : Best Shims So Far
FID # = 10
Integral = 1.66776E+07
rp Phase = 5.71034
Mn Width = 0.445416
Start Mo = 1.09258
Best Mo = 0.911920
This Mo = 0.911920
Error Mo = 13.970%
32 30 28 26 24 22 20 18 16 14 12 10 8 (H)


Program ShimIt
Report : Best Shims So Far
FID # = 17
Integral = 1.60322E+07
rp Phase = 4.23182
Mn Width = 0.437099
Start Mo = 1.09258
Best Mo = 0.909763
This Mo = 0.909763
Error Mo = 4.2378%
54 52 50 48 46 44 42 40 38 36 34 32 (H)


Program ShimIt
Report : Best Shims So Far
FID # = 23
Integral = 1.57790E+07
rp Phase = 5.05106
Mn Width = 0.723149
Start Mo = 1.09258
Best Mo = 0.904121
This Mo = 0.904121
Error Mo = 2.9613%
80 76 72 68 64 60 56 52 48 44 40 36 (H)


Program ShimIt
Report : Final shims
FID # = 29
Integral = 1.59227E+07
rp Phase = 2.87907
Mn Width = 0.594676
Start Mo = 1.09258
Best Mo = 0.900991
This Mo = 0.900991
Error Mo = 2.1513%
66 64 62 60 58 56 54 52 50 48 46 44 (H)

Final comparison:



In the final spectrum the first spinning sidebands (35 Hz) cannot even be seen. The visible low frequency second spinning sideband stems from the NCC Z*SPEC probe and is not a shimming problem. The center resonance is not quite Lorentzian in shape yet. Further ShimIt low-order z shimming using a low `order` parameter value would obtain the desired lineshape. However, given the current implementation of ShimIt manual or automated lock-level shimming would likely be faster for this final stage.

CHAPTER 7

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