TopSpin

Edlock/Edsolv Guide

User Manual

Version 002

Innovation with Integrity

NMR

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Contents

Contents

1 Introduction

1.1 About this Manual

This manual is a reference to the TopSpin edlock/edsolv tool. Edlock/edsolv is a new module designed for creating and editing solvent and lock dependent parameters and now combines the former seperate modules edsolv and edlock.

The definition of solvent and lock dependent parameters with the two modules edlock and edsolv has been used for more than 10 years. Due to new hardware developments a redesign of this tool was required and it was decided to combine the two modules into one. It is now no longer necessary to use two routines to define a new solvent (edsolv) and to setup its lock parameters (edlock). Both can now be done in the new module.

In previous edlock versions parameters had to be defined for each probe. The new module provides generic parameters, which should cover most standard probes. A specific probe is only necessary if you need to adapt the lock parameters to the probe.

1.2 Font and Format Conventions

Type of Information	Font	Examples
Shell Command, Commands, "All what you can enter"	Arial bold	Type or enter **fromjdx zg**
Button, Tab, Pane and Menu Names "All what you can click"	Arial bold, initial letters capitalized	Use the **Export To File** button. Click **OK**. Click **Processing**…
Windows, Dialog Windows, Pop-up Windows Names	Arial, initial letters capitalized	The Stacked Plot Edit dialog will be displayed.
Path, File, Dataset and Experiment Names **Data Path Variables** **Table Column Names** **Field Names (within Dialog Windows)**	Arial Italics	*$tshome/exp/stan/nmr/lists* *expno, procno,*
Parameters	Arial in Capital Letters	VCLIST

Program Code
Pulse and AU Program Names
Macros
Functions
Arguments
Variables
	Courier	`go=2`
		`au_zgte`
		`edmac`
		`CalcExpTime()`
		`XAU(prog, arg)`
		`disk2, user2`

AU Macro	Courier in Capital Letters	`REX` `PNO`

Table 1.1: Font and Format Conventions

1.3 Getting Started

1.3.1 Basic Program Features

The edlock/edsolv tool allows editing of solvent and lock dependent parameters. A default list of solvents is provided with all necessary properties and suitable lock parameters. New solvents can be added, existing solvents can be edited anytime. Solvent and probe dependent lock parameters might be adjusted for individual needs. It is no longer possible to directly rename a solvent. This has been replaced by copying with a new name, so the previous version needs to be deleted explicitly.

1.3.2 Supported Hardware

Edsolv and edlock in TopSpin 3.1 support only AV II (BSMS 2 equipped with LCB Board) and AV III spectrometers (BSMS2 equipped with ELCB Ethernet Lock Control Board and optionally L-TRX board). The BSMS2 is located at the bottom of the console. Use the following pictures as a guide to determine the boards (red arrows).

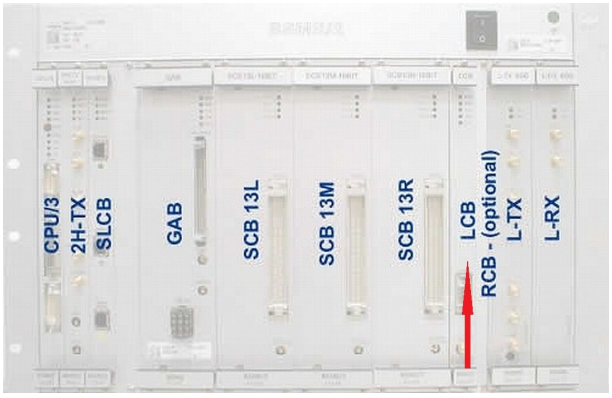


Figure 1.1: BSMS2 with LCB Board

Figure 1.2: BSMS2 with ELCB board, L-TX/L-RX Boards or L-TRX Board

Alternatively you might check the contents of the file:

<TOPSPINHOME>/conf/instr/<Spectrometername>/uxnmr.info.

It will list information if an LCB or ELCB and L-TRX board are present. Or check the BSMS Webpage (Main -> Setup).

1.3.3 Hardware Dependent New Features

The new edsolv/edlock module supports several new features:

- Automatic field adjustment.
- New Autophase function.
- Multi-peak locking function.

These functions will be described in detail in *The Lock Tab [▷ 14]*.

The new features are only available for the BSMS 2 with ELCB Lock Control Board (automatic field adjustment) and an L-TRX board (Autophase, multi-peak locking). ONLY with this hardware, a manual field update is no longer necessary. So the field update is still necessary for the BSMS 2 equipped with LCB board.

These hardware dependencies will again be mentioned in the respective chapters!

1.3.4 How to Start edlock/edsolv

You start edsolv/edlock by typing one of the two commands into the command line of the TopSpin main window.

For those familiar with the separate **edsolv** and **edlock** commands in previous versions, it was decided to keep these syntax. Typing **edsolv** at the command will open the Solvent tab, while **edlock** will correspondingly open the Lock tab.

The **edsolv/edlock** window has its own menu bar on top of the windows and four tabs for quick switching between Solvent List, Lock Parameters, Spectrum Reference and Solvent Properties.

In the upper part you can switch between the Lock nuclei 2H and 19F, activate the new Autophase mode (ELCB + L-TRX only) and get information about the current probe as selected with the **edhead** command.

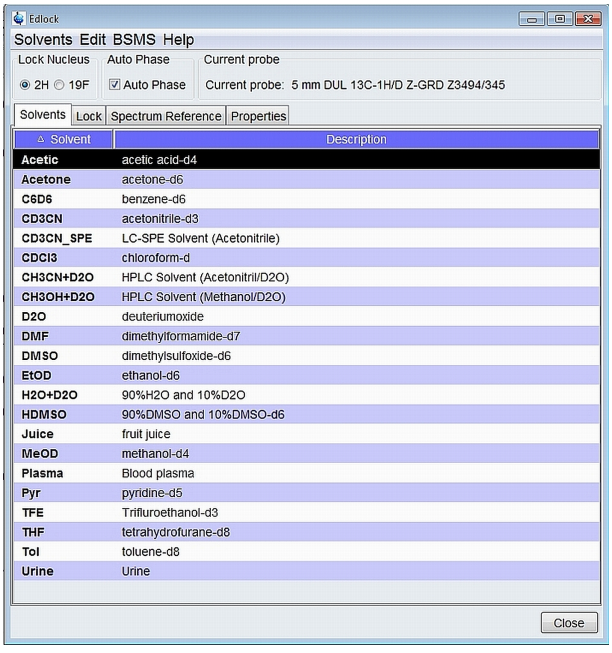


Figure 1.3: Edlock Window (for L-TRX)

1.3.5 Quick Steps to Define a New Solvent

1. Start edlock/edsolv and with the **Solvent** tab active, right click on an existing solvent with properties close to your new solvent. Select **Copy and paste solvent** to copy from this existing solvent to the new solvent. Enter the name of the new solvent and its description.

   Example: For a new solvent CD_2Cl_2 right click on $CDCl_3$, which has similar properties. Enter the name of the new solvent CD_2Cl_2 and in the description field, enter dichloromethane-d2.

2. Change to the Lock Parameters by clicking the Lock tab, select the new solvent and right click to select **Edit Lock parameters**. You'll find all parameters of the solvent used for copy and paste in the first step.
   - In the 'Signals' part, change the shift in ppm according to the signal used for locking in your new solvent. For the CD_2Cl_2 example, change the shift of the dichloromethane resonance to 5.33 ppm.
   - You might want to optimize further lock parameters as described in *Optimizing Lock Parameters [▷ 17]*.

3. On the spectrum reference tab, right click the new solvent to select **Edit spectrum reference parameters**. Adjust the reference shift and search width according to your needs. For the most common TMS just leave the reference shift at 0 ppm and the search width at 0.5 ppm. In this case the search range is +/- 0.25 ppm around 0 ppm, which is suitable for TMS.

   For the CD_2Cl_2 example, enter 176K for the melting point and 312K for the boiling point. These two values are just reference for now, but might be used in future.

2 The Edlock/Edsolv Window

The edsolv/edlock has its own menu bar on top of the windows and four tabs for quick switching between Solvent List, Lock Parameters, Spectrum Reference and Solvent Properties.

In the upper part you can switch between the Lock nuclei 2H and 19F, activate the new Auto phase mode (ELCB and L-TRX only!) and get information about the current probe as selected with edhead routine.

2.1 The Solvent Tab

The solvent tab will be displayed when typing **edsolv** at the command line and shows the Bruker default solvent list. It consists of the most common NMR solvent and solvent mixtures with the solvent name or abbreviation on the left side and its description on the right side. Existing solvents can be edited / deleted or hidden / shown. New solvents can be added in the following ways:

Right click anywhere in the solvent list opens a new selection window, as displayed below:

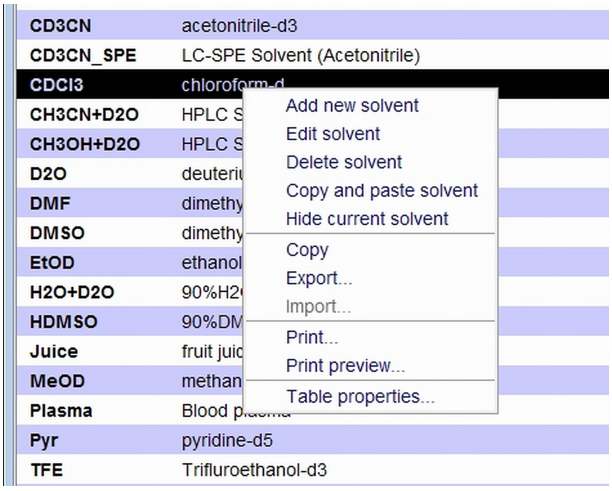


Figure 2.1: Popup Window after Right Click on a Solvent

The following features are available:

Add a new solvent

Clicking **Add a new solvent** opens a window shown:

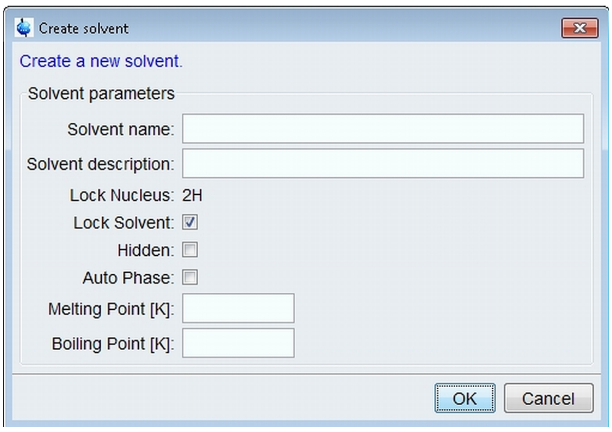


Figure 2.2: Create Solvent Window

Enter the solvent name and description into the empty fields. The displayed lock nucleus corresponds to the selection in the upper part of the edsolv/edlock window. You can define the solvent as hidden, specify if this solvent is used as lock solvent, activate the autophase mode (ELCB + L-TRX only) and optionally enter it's melting point and boiling point (might be used in future versions).

Please note, all solvents not marked as lock solvents will only appear in the list if the **Show no locking solvents** is active in the Solvents pull down menu. These solvents cannot be used with the lock command.

Edit a Solvent

Clicking **Edit a solvent** displays the highlighted solvent in a window identical to *Add a new solvent*, just the solvent name and its description are correspondingly filled and cannot be changed.

Delete a Solvent

Clicking this feature deletes the highlighted solvent after entering the NMR Superuser password and further confirmation. In case of a Bruker default solvent a restore is possible using the pull down menu entry **Solvents**, then **Restore default solvents**.

Copy and paste an existing solvent

This selection copies all parameters from a highlighted existing solvent to a new solvent. Just enter the name and description of the new solvent. This can also be used to rename a solvent.

Hide the current solvent

You can hide the current solvent to protect it from accidental deletion or modification. These solvents will only appear in the list if the **Show hidden solvent** feature is activated in the **Solvents** pull-down menu. The hide function is also recommended to make unused solvents temporarily invisible, so it can be avoided to delete them.

The following features are standard functionality for every Bruker table:

Copy

Clicking **Copy** copies name and description of the highlighted solvent. This can be used to paste the contents in an editor or spreadsheet.

Export

This selection exports the entire solvent list to be used with spreadsheets (.csv or .xls for Microsoft Excel).

Print

This function prints the entire solvent list after optionally adjusting your print and printer setup.

Print preview

This feature offers a graphical printout feature after optionally adjusting your print and printer setup.

Table properties

Use this to adjust the general display properties of the tables. You can adjust columns, colors, spacing and miscellaneous such as shaded row backgrounds for printouts.

Add, **Edit**, **Delete**, **Copy** and **Paste** are also available via the **EDIT** pull down menu.

2.1.1 Autophase

The new edlock module offers a new sophisticated Autophase handling if your BSMS is equipped with an ELCB and L-TRX board.

Important: If your BSMS is equipped with an LCB board or with ELCB board and without L-TRX board, the Autophase behaviour remains unchanged. Therefore, the Autophase selection is NOT available in edlock! Of course you can still activate Autophase via BSMSDISP or BSMS keyboard, but it uses the old algorithm.

Autophase and lock are treated differently. The behavior of the lock command with respect to Autophase handling can be controlled independently with a checkbox in the edlock window. Autophase during lock can be switched on or off. When turned on, the FFA algorithm (Spectrum) is used. The default behavior is no Autophase during lock and **lock level default** for the algorithm, which corresponds to the old behavior. In this state the table will contain the lock phase column. With Autophase turned on, the lock phase column is not needed and therefore unavailable.

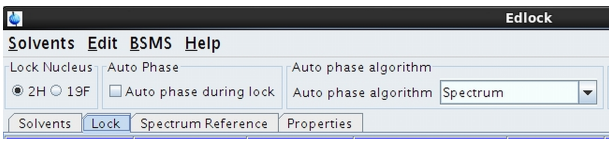


Figure 2.3: Autophase and Algorithm Selection in the Lock Window

There are three selections for the Autophase algorithm:

- **Lock level default**: This uses the old algorithm, optimization via lock level.
- **Enhanced lock level**: This also uses the old algorithm, but with wider range. It will therefore need more time.
- **Spectrum**: This is the new algorithm (FFA). It will also take longer, but not that much, because a spectrum is measured anyway during locking. This is the recommended selection if Autophase is activated for the L-TRX and execution time is not critical, e.g. in case of high throughput samples.

Calibration of the Autophase offset

This calibration is mandantory if **Autophase** is selected and spectrum selected for the algorithm. It can be selected via the pull down menu entry **BSMS** -> **Calibrate Autophase offset**. This control can also be added to the BSMS Display (bsmsdisp) if needed. The following window will be displayed:

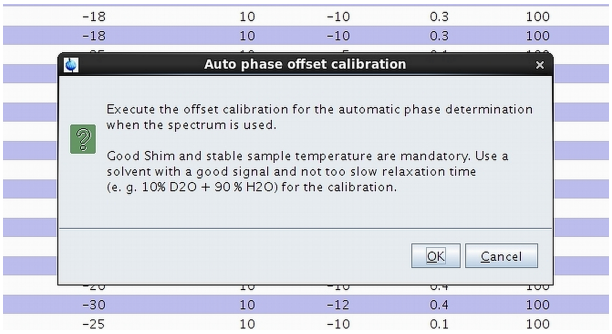


Figure 2.4: Autophase Offset Calibration

Please follow the instructions, insert the recommended sample and click **OK** when finished.

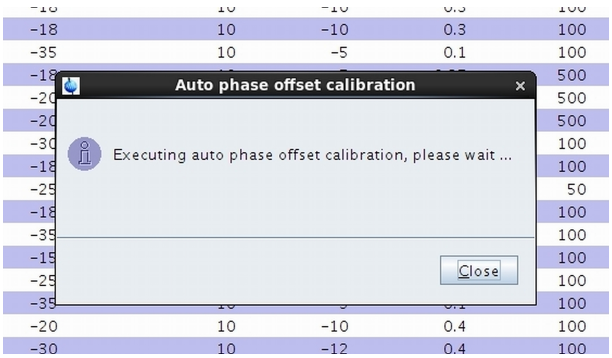


Figure 2.5: Autophase Offset Calibration During Execution

Please wait until the offset calibration is ready (approximately 1½-2 minutes). The result can be checked on the ELCB Webpage. Click **LOCK** -> **LOCK Conf.** -> **Autolock Conf.** and check **Phase offset FFA to Lock**.

Figure 2.6: ELCB Webpage, Check of Phase Offset Value.

The ELCB Webpage can also be used to activate the Phase offset calibration. Use the BSMS Service Page -> *Lock Parameter and Commands* and click the **Auto Phase Calibration** button in the Auto area. Again use a suitable sample as outlined in the Auto Phase Calibration Info field.

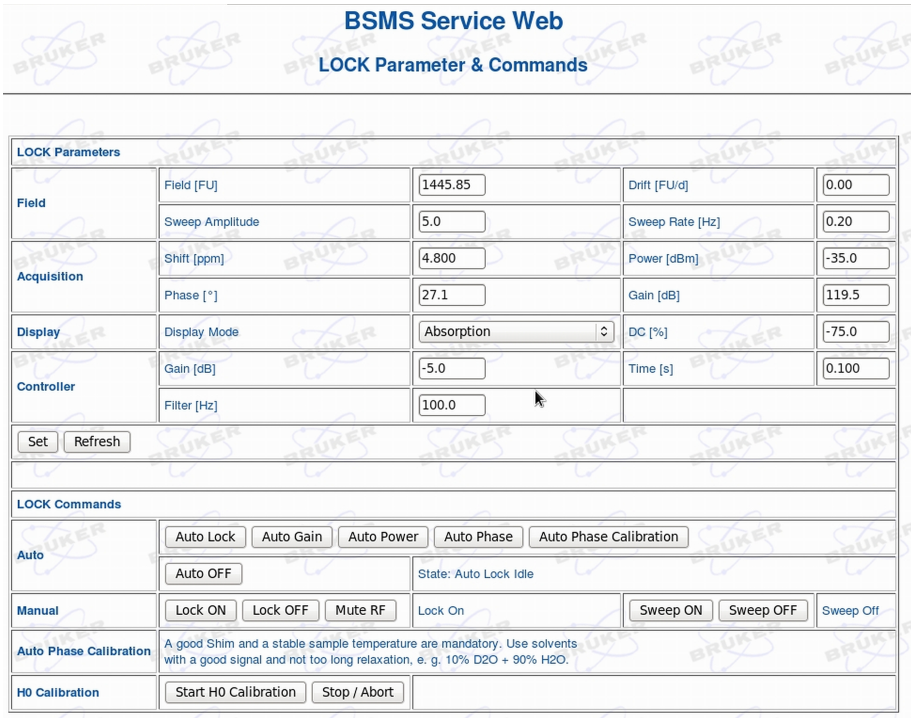
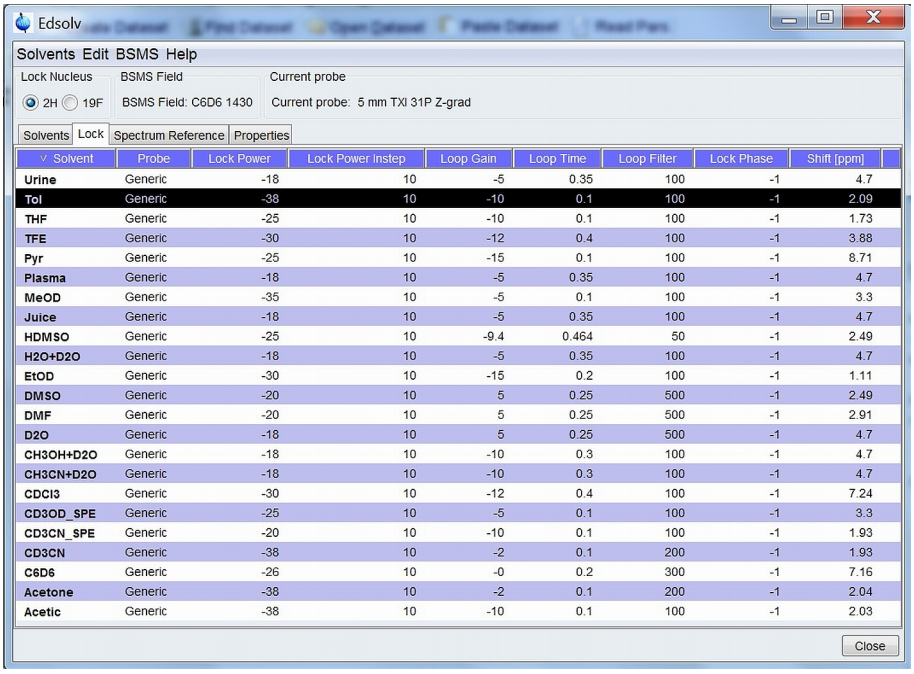


Figure 2.7: BSMS Service Web, Lock Parameter and Commands Page

Important: The phase offset calibration should be repeated if the 2H Preamplifier is exchanged.

2.2 The Lock Tab

Typing **edlock** at the command line or clicking the **Lock** tab opens the default list of lock parameters for the default solvents:



Solvent	Probe	Lock Power	Lock Power Instep	Loop Gain	Loop Time	Loop Filter	Lock Phase	Shift [ppm]
Urine	Generic	-18	10	-5	0.35	100	-1	4.7
Tol	Generic	-38	10	-10	0.1	100	-1	2.09
THF	Generic	-25	10	-10	0.1	100	-1	1.73
TFE	Generic	-30	10	-12	0.4	100	-1	3.88
Pyr	Generic	-25	10	-15	0.1	100	-1	8.71
Plasma	Generic	-18	10	-5	0.35	100	-1	4.7
MeOD	Generic	-35	10	-5	0.1	100	-1	3.3
Juice	Generic	-18	10	-5	0.35	100	-1	4.7
HDMSO	Generic	-25	10	-9.4	0.464	50	-1	2.49
H2O+D2O	Generic	-18	10	-5	0.35	100	-1	4.7
EtOD	Generic	-30	10	-15	0.2	100	-1	1.11
DMSO	Generic	-20	10	5	0.25	500	-1	2.49
DMF	Generic	-20	10	5	0.25	500	-1	2.91
D2O	Generic	-18	10	5	0.25	500	-1	4.7
CH3OH+D2O	Generic	-18	10	-10	0.3	100	-1	4.7
CH3CN+D2O	Generic	-18	10	-10	0.3	100	-1	4.7
CDCl3	Generic	-30	10	-12	0.4	100	-1	7.24
CD3OD_SPE	Generic	-25	10	-5	0.1	100	-1	3.3
CD3CN_SPE	Generic	-20	10	-10	0.1	100	-1	1.93
CD3CN	Generic	-38	10	-2	0.1	200	-1	1.93
C6D6	Generic	-26	10	-0	0.2	300	-1	7.16
Acetone	Generic	-38	10	-2	0.1	200	-1	2.04
Acetic	Generic	-38	10	-10	0.1	100	-1	2.03

Figure 2.8: Edlock Window, Lock Tab

Initially the table consists of the following columns:

- Lock Power - shows the lock power in dB.
- Lock Power Instep - displays the Initial Step for the Lock Power.

  This value is used for the Initial Lock Step, to be added to the Lock Power. Example: For CDCl3, the Lock Power is -28, the InStep is +10, so the Initial Lock Power Step will be done with -18 dB.
- Loop Gain - value for the Loop Gain.

  This lock regulator gain can be set to value between -80 and 0 dB. It is set at the end of the acquisition to the loop gain currently set on the BSMS unit. This usually, but not necessarily corresponds to the value of the Loop Gain in the table. If lock-in was performed with the command **Lock**, the loop gain is first read from the table and set on the BSMS unit. However, using autolock or Lock on/off in bsmsdisp or the BSMS keyboard, performs lock-in without first reading the table!
- Loop Time - value for the Loop Time.

  The lock regulator time constant can be set to a value between 0.001 and 1.0 seconds.
- Loop Filter - value for the Loop Filter.

  This is the lock regulator cut-off frequency of the low pass filter, its range is between 1-200 Hz
- Shift [ppm] - chemical shift value for the signal to be locked.

The following table summarizes the lock parameters and their ranges.

Parameter	Meaning	Range
Lock Power	Lock power.	-60 - 0 dB
Lock Gain	Lock gain.	-80 - 0 dB
Loop Gain	Lock regulator gain.	-80 - 0 dB
Loop Time	Lock regulator time.	0,001 -1 sec.
Loop Filter	Lock regulator cut-off frequency.	1 - 200 Hz

Table 2.1: Lock parameters and their ranges

Right clicking on the blue tab header leads to more column options such as lock phase and additional options like **More** for table display options.

Please note, for the ELCB/L-TRX the lock phase is only selectable if the Autophase function is inactive.

Double clicking anywhere in a solvent line or clicking the '**+**' box to the left of the solvent opens the expanded view with all signals listed. This new multi peak locking feature is especially relevant for solvents with multiple signals such as MeOD ot EtOD.

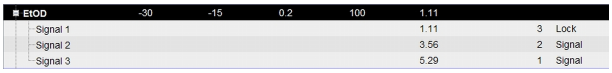


Figure 2.9: Expanded Solvent Line

2.2.1 Editing Lock Parameters

In the default state the list of standard lock parameters are valid for all probes. Thus, in the Probe column will always appear *generic*. It is possible though to customize the lock parameters for individual needs. The editing mode can be selected by right clicking in the solvent line and selecting **Edit lock parameters** if the **Lock** tab is active. Depending on your hardware the appearing window will display only lock parameters (LCB) or lock parameters and signals (ELCB).

The following parameters can be edited after entering the NMR Superuser password:

Lock parameters

- Probe description
- Lock power
- Loop gain
- Loop Time
- Loop Filter
- Lock Phase (-1 means the previously active value will be used)
- Lock power instep

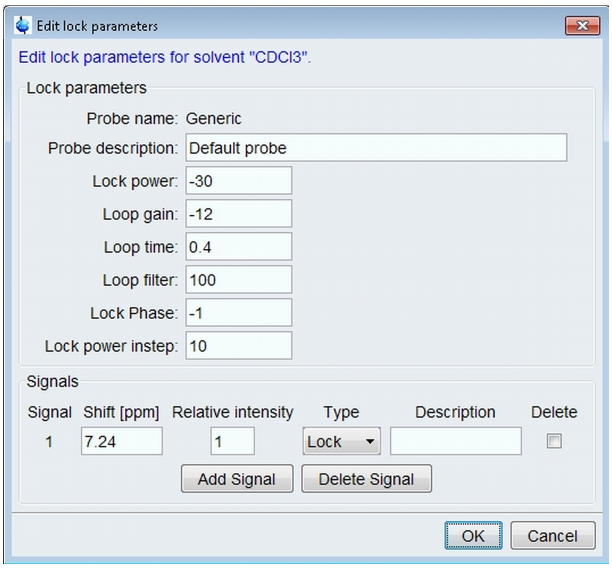


Figure 2.10: Edlock Parameters Window

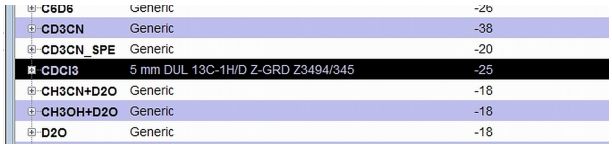
Signals

Using the **Add** button, up to 10 signals can be entered (1 for Lock, 9 signals) with their shift [ppm], relative intensity, type (**Lock** or **Signal**) and description.

The signals can be marked for deletion, clicking the **Delete** button will finally delete them.

Please note: One signal must have the type *Lock*! The other signals will be used for solvent detection, mainly to ensure locking on the correct signal, e.g. in case of MeOD.

Important: If editing is confirmed using the ‚OK' button, these parameters will be stored for the current probe and for the selected probe only. This current probe (as defined in edhead) will then also appear in the Lock parameters list. Parameters for the other probes will remain unchanged and remain visible as probe type *generic*.



After changing and storing lock parameters using the **OK** button.

The pull down menu entry **Delete Probe** deletes a probe (created by editing edlock parameters of the generic probe) from the current solvent or all solvents respectively.

After highlighting the edited solvent, using the pull down menu function **Edit**, then **Copy probe to all solvents** will copy the changes to all solvents! For copying the lock phase to all solvents, **Edit**, then **Copy lock phase to all solvents** can be used alternatively.

For changing parameters for the generic probe, right clicking in the solvents list will provide the function **Edit parameters of generic probe**.

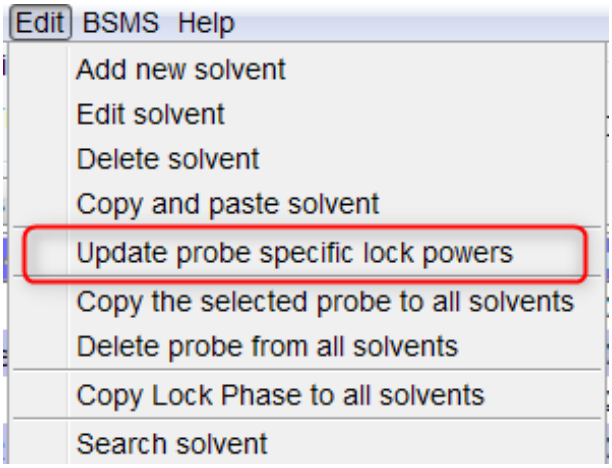
2.2.2 Optimizing Lock Parameters

Lock Power

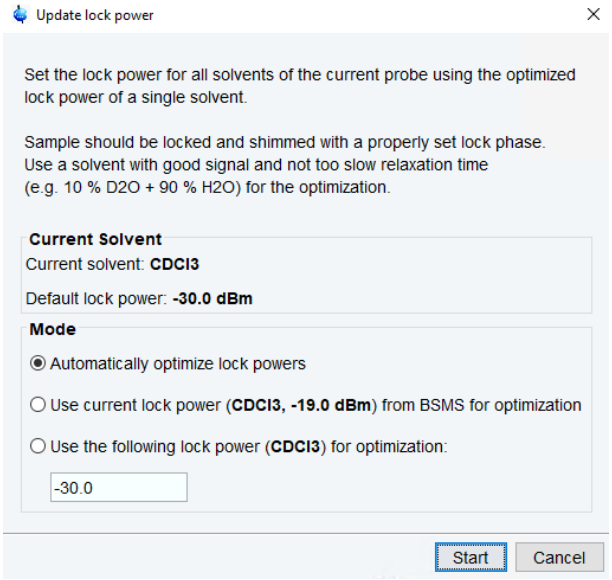
After the sample has been locked and shimmed, start the auto-power routine from the **bsmsdisp** module or if available, from the BSMS keyboard. For lock solvents with long T1 relaxation times (e.g. CDCl3), auto-power might take an unacceptably long time. In this case a manual optimization of the lock power is recommended. Increase the lock power until the lock signals begins to oscillate (until saturation!), and then reduce the power level slightly (approximately 3 - 6 dB). Do not reduce too much, as this will affect the field stability.

Alternatively you might use a gradient experiment (e.g. Parameter set COSYGPSW, or the pulse program `preempgp2`) to observe the gradients on the lock. In case of optimum lock power the lock signal will return to normal level after the gradient. An overshoot before returning to the normal level is caused by saturation, so reduce the lock power until this overshoot is no longer visible.

Edlock does also offer an automatic way to optimize lock powers for all standard solvents for an installed probe:



The following dialog shows the available options:



Automatically optimize lock powers runs an AU-program to optimize the lock powers for all standard solvents for the currently installed probe; after the optimization, the new lock power value is automatically loaded to the BSMS

Use current lock power from BSMS for optimization uses the current lock power from the BSMS to determine the lock power difference to the standard value for the used solvent, and then also optimizes all lock powers of all standard solvents for the currently installed probe with this value; no new lock power value is loaded to the BSMS during this procedure, so a potential change will take effect only after the next lock command

Use the following lock power does the same thing, but takes a user defined lock power value instead of the current value from the BSMS

Lock Phase

Use the auto-phase feature in bsmsdisp or on the BSMS keyboard (if available) to optimize the Lock Phase.

Lock Gain

Use the auto-gain feature in bsmsdisp or on the BSMS keyboard (if available) to optimize the Lock Gain.

Loop Gain, Loop Time and Loop Filter

Generally these parameters should be already suitable in the default Bruker Solvent list, so there should be no need to change them. However, the AU program `loopadj` can be used to automatically optimize loop gain, loop time and loop filter for optimal long-term stability.

Alternatively the following procedure might be used:

Note the Lock Gain value AFTER the auto-gain routine has optimized it. Using this value, select the appropriate values for the loop filter, loop gain and loop time as shown in the following table.

Lock RX Gain (after auto gain) [dB]	Loop Filter [Hz]	Loop Gain [dB]	Loop Time [sec]
120	20	-17.9	0.681
	30	-14.3	0.589
110	50	-9.4	0.464
	70	-6.6	0.384
	100	-3.7	0.306
100	160	0.3	0.220
	250	3.9	0.158
	400	7.1	0.111
90	600	9.9	0.083
	1000	13.2	0.059
	1500	15.2	0.047
	2000	16.8	0.041

Table 2.2: Lock Regulator Parameters

Example:

Auto-gain determines a lock gain of 100 dB. From the table, the user should set the loop filter to 160 Hz, the loop gain to 0.3 dB and the loop time to 0.220 sec.

This procedure is recommended to use with shielded magnets. For non-shielded magnets a general procedure cannot be given, so the relation between the three parameters should be determined individually. If in doubt, it is recommended to leave the Bruker default parameters unchanged!

2.2.3 BSMS Field Update

For AVII spectrometers with BSMS 2 and LCB board the field should be updated regularly. From the pull down menu, choosing BSMS and 'Field update' will open the field update window as displayed:

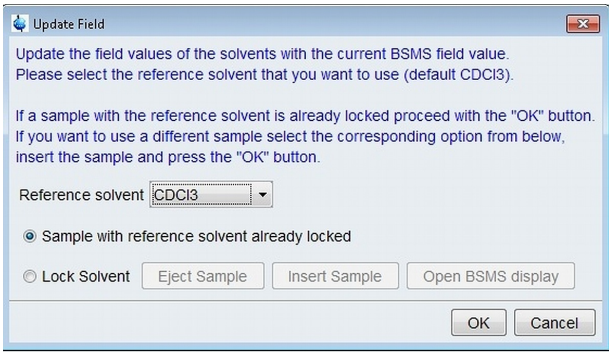


Figure 2.11: Field Update Window

$CDCl_3$ is the default solvent used for field update, but other solvents can be used as well.

If the solvent is already locked, leave the **Sample with reference already locked** selection active. Clicking the **OK** button will update the field.

If the sample is not locked yet, please use the **Lock Solvent** selector and the corresponding **Eject Sample** and then **Insert Sample** buttons to insert your sample into the magnet. Open BSMS display to lock the sample accordingly, than proceed with **OK** as above to update the field.

If no field update has been done for a certain time period (three months), the software will automatically ask you to do so, e.g. when using a lock command. In this case you need to lock a sample manually using the bsmsdisp module (center lock signal and press the **Lock** button) and then proceed with the field update procedure as described above.

Important: For AVIII spectrometers with ELCB the field update is no longer necessary, it will be done automatically during locking according to the reference shift. This also makes definition of solvents used for the field update in the file solvents.fieldupdate (in *<TOPSPINHOME>/exp/stan/nmr/lists*) and in the IconNMR configuration suite obsolete. The corresponding features are no longer available in IconNMR. IconNMR will display a link to edlock instead.

2.3 The Spectrum Reference Tab

Clicking the **Spectrum reference** tab opens the default list of spectrum reference parameters for the default solvents.

The table consists of the following columns:

- Noise (initially 10).
- Reference shift [ppm]: This is the reference shift of the signals used for referencing, usually TMS with 0 ppm.
- Search width [ppm]: This specifies the search width window for the reference signals, e.g. a value of 0.5 ppm will search from -0.25 to 0.25 ppm from the specified reference shift in ppm.

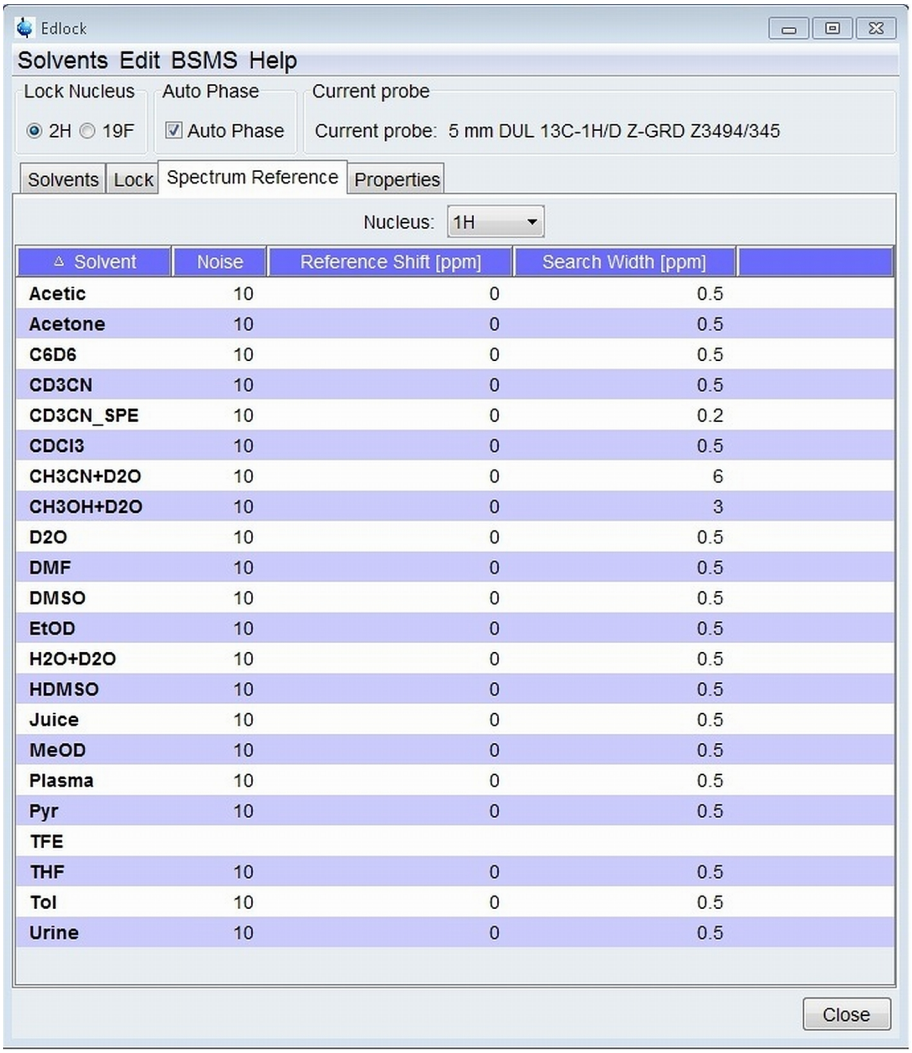


Figure 2.12: Edlock Window with Spectrum Reference Tab Displayed

Double clicking on a solvent while the **Spectrum reference** tab is active or right clicking will open the Spectrum reference editing window:

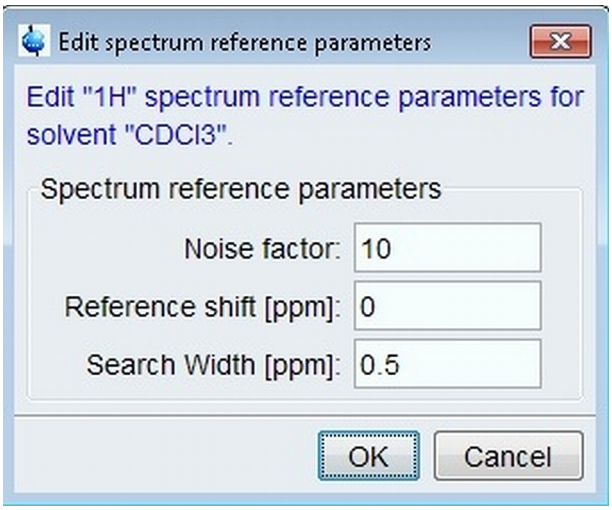
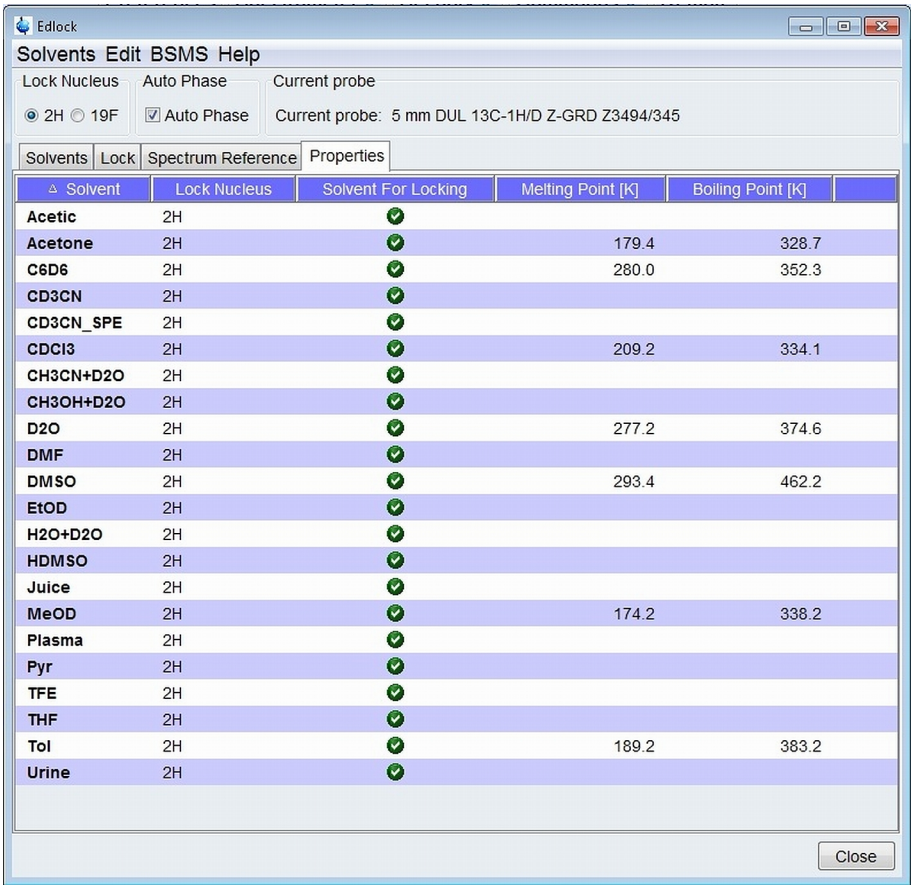


Figure 2.13: Spectrum Reference Editing Window

Noise, Reference shift [ppm] and Search width [ppm] can be customized for individual needs.

2.4 The Properties Tab

Clicking the **Properties** tab opens the default list of properties parameters for the default solvents.



Solvent	Lock Nucleus	Solvent For Locking	Melting Point [K]	Boiling Point [K]
Acetic	2H	✓		
Acetone	2H	✓	179.4	328.7
C6D6	2H	✓	280.0	352.3
CD3CN	2H	✓		
CD3CN_SPE	2H	✓		
CDCl3	2H	✓	209.2	334.1
CH3CN+D2O	2H	✓		
CH3OH+D2O	2H	✓		
D2O	2H	✓	277.2	374.6
DMF	2H	✓		
DMSO	2H	✓	293.4	462.2
EtOD	2H	✓		
H2O+D2O	2H	✓		
HDMSO	2H	✓		
Juice	2H	✓		
MeOD	2H	✓	174.2	338.2
Plasma	2H	✓		
Pyr	2H	✓		
TFE	2H	✓		
THF	2H	✓		
Tol	2H	✓	189.2	383.2
Urine	2H	✓		

Figure 2.14: Default List of Properties Parameters

The table consists of the following columns, depending on your hardware.

1. For the AVIII with ELCB or ELCB/L-TRX:

- Lock nucleus

  As defined in the lock nucleus field in the upper part of the edsolv/edlock window.

- Solvent for locking

  Shows if the solvent is used for locking or not.

- Melting point

  Melting point in °C or K. The unit can be changed via the pull down menu entry **Solvents**, then **Temperature units for solvents**. Currently this entry is only used for information purpose, but it might be used in future versions.

- Boiling point

  Boiling point in °C or K. The unit can be changed via the pull down menu entry **Solvents**, then **Temperature units for solvents**. Currently this entry is only used for information purpose, but it might be used in future versions.

2. For the AVII with LCB

   - Lock nucleus

     As defined in the lock nucleus field in the upper part of the edsolv/edlock window.

   - Field offset

     Values for the field offset.

   - Field update

     Shows if the solvent is available for field update. Please refer to *BSMS Field Update [▷ 19]* for further information.

   - Auto Lock

     Shows if Auto Lock or lock 'on' will be used for the solvent. Lock 'on' instead of Auto Lock is commonly used for solvents with multiple signals like MeOD.

   - Solvent for locking

     Shows if the solvent is used for locking or not.

   - Melting point

     Melting point in °C or K. The unit can be changed via the pull down menu entry **Solvents**, then **Temperature units for solvents**. Currently this entry is only used for information purpose, but it might be used for different purposes in future versions.

   - Boiling point

     Boiling point in °C or K. The unit can be changed via the pull down menu entry **Solvents**, then **Temperature units for solvents**. Currently this entry is only used for information purpose, but it might be used for different purposes in future versions.

Double clicking on a solvent line will open the editor window, here shown for AVII spectrometers:

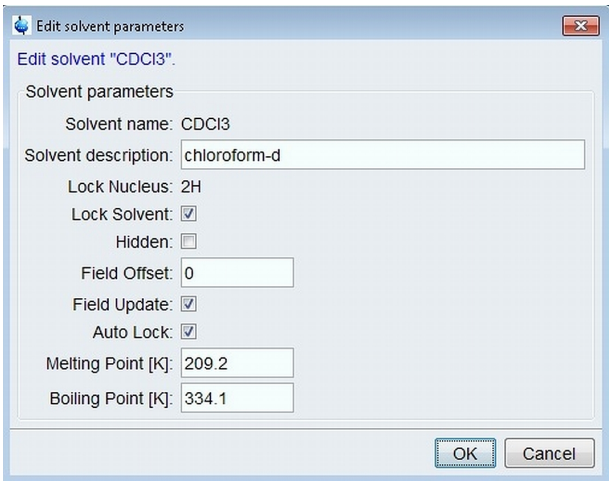


Figure 2.15: Editor Window with Active ‚Properties' tab for AVII Spectrometer

2.5 Miscellaneous Pull-down Menu Functions

These functions are not mentioned in the text above.

- **Solvents** -> **Restore default solvent**

  This restores the Bruker default solvent list and lock parameters. Caution: Any changes to these are overwritten!

- **BSMS** - **Import Loop Parameters**

  Loop parameters defined in previous version might be imported. The values will be taken from *<TOPSPINHOME>/conf/instr/<Spektrometername>/prosol/<Probe-ID>/<Solvent>/bsmspar*, if different from the actual values.

- **Help** -> **Help**

  Opens this manual.

- **Help** -> **About solvents**

  Display information about the last file editing date, its version origin and in case of the AV II with ELCB, again the reference solvent and the current field value.

2.6 FAQ - Frequently Asked Questions

Why is the field update function no longer available on AVIII spectrometers?

The ELCB is capable to always use the correct field, determined from the shift value for the lock signal, as defined in the Lock table. Hence the field update no longer necessary. It is only necessary for AV II spectrometers with LCB board.

Can I change the parameters for the *Generic* probe?

Yes. With the **Lock** tab active, please right click on a solvent line and choose **Edit parameters** of Generic probe.

Is it necessary to define edlock parameters for each probe?

No! Generic parameters are provided, which should work for most standard probes.

How do I create edlock parameters for my probe?

A new entry or the current probe is automatically generated when edlock parameters for a solvent are edited. These parameters can be copied to all other solvents (context menu).

3 Contact

Manufacturer

Bruker BioSpin GmbH
Silberstreifen 4
D-76287 Rheinstetten
Germany

E-Mail: *nmr-support@bruker.com*
http://www.bruker.com
WEEE DE43181702

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List of Figures

List of Figures

List of Tables

List of Tables

Bruker Corporation

info@bruker.com
www.bruker.com

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