EDPROSOL

Manual

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1 Introduction

1.1 About this manual

This manual is a reference to **TopSpin** edprosol tool. **Edprosol** is a module designed for editing the probe and solvent dependent parameters.

The complete **Edprosol** tool will be described.

The definition of probe, solvent and nucleus dependent aquisition parameters with the ***edprosol*** command is used for more than 10 years. Due to new hardware developments a redesign of this tool was required, so changes to former versions will be explained.

1.2 Conventions

Font conventions

edprosol - commands to be entered in the command line are in Courier bold italic

apply – commands to be clicked are in Times New Roman bold italic

fid – filenames are in Courier

name – any name which is not a file name is in Times New Roman italic

1.3 Getting started

1.3.1 Basic Program features

The **edprosol** tool allows editing the probe and solvent dependent aquisition parameters for both, observe and decouple nuclei and channels. These parameters are pulse width and power levels.

This is typically done during the installation of the spectrometer for all probes and solvents you want to use. However, edprosol can be repeated anytime for adding and/or changing parameters of existing or new probes and/or solvents.

Edprosol offers a common mode and an individual mode for the parameter setting. Using the common mode you only have to select the nuclei for your chosen probe.This modus is the recommended one. For expert users the individual mode still offers the possibility to edit parameters for an individual routing.

A Solid State modus is also be availabe.

1.3.2 How to start Edprosol

As **edprosol** is part of **TopSpin,** it will be installed with this program without requiring a special licence.

You start **edprosol** by typing ***edprosol*** into the command line of the **TopSpin** main window. A new window as shown in Figure 1.1 will be displayed.

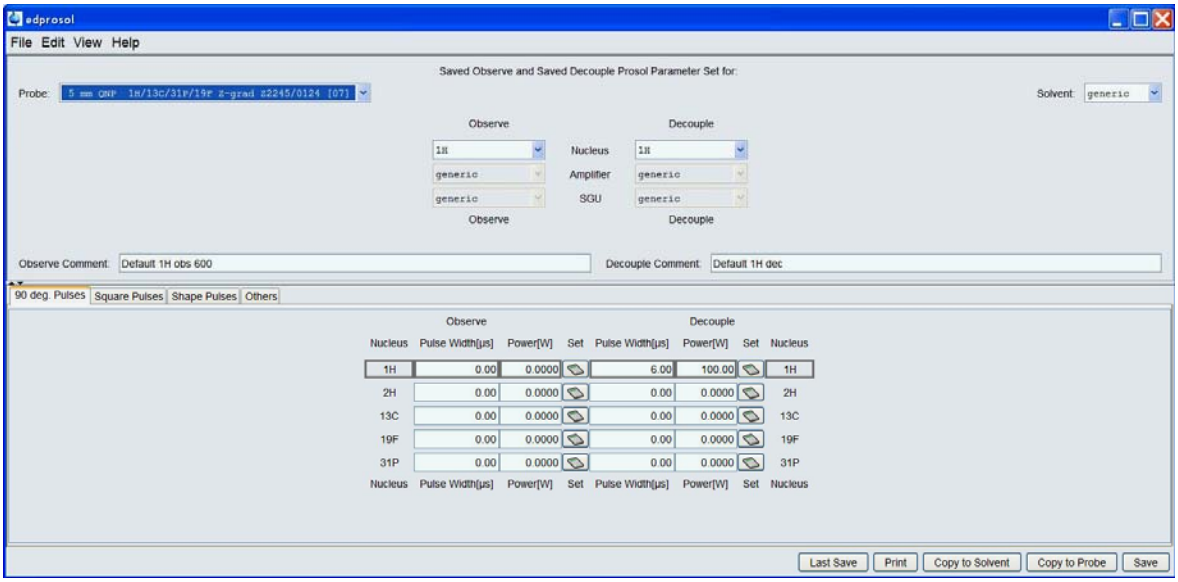

Figure 1.1: edprosol window in the 'Common Mode'

The **edprosol** window has its own menu bar on top of the window and five buttons for quick access of the most important features at the bottom. The window itself is divided into two parts.

In the upper part you have to select your desired probe, the solvent and the observe and decouple nuclei. The lower part of the window allows to define the pulse widths and power levels for the nuclei corresponding to the chosen probe.

Figure 1.1 displays the **edprosol** window in the common mode. Therefore in the upper part only probe, nuclei and solvents can be chosen.

In the individual mode the upper part of the **edprosol** window looks different to the common mode if in the lower part the '90 deg Pulses' table is the current one. In addition to probe, nuclei and solvent, you are also allowed to select/combine SGU and Amplifier, thus to select an individual routing. The lower part of the window is the same as in the common mode. Figure 1.2 shows the appearance of the edprosol window in the individual mode.

When starting **edprosol**, by default the common mode will be chosen. If you like to work in the individual mode click ***Edit*** from the menu bar and chose 'Enable the Individual Mode'. Doing the same again will disable this mode.

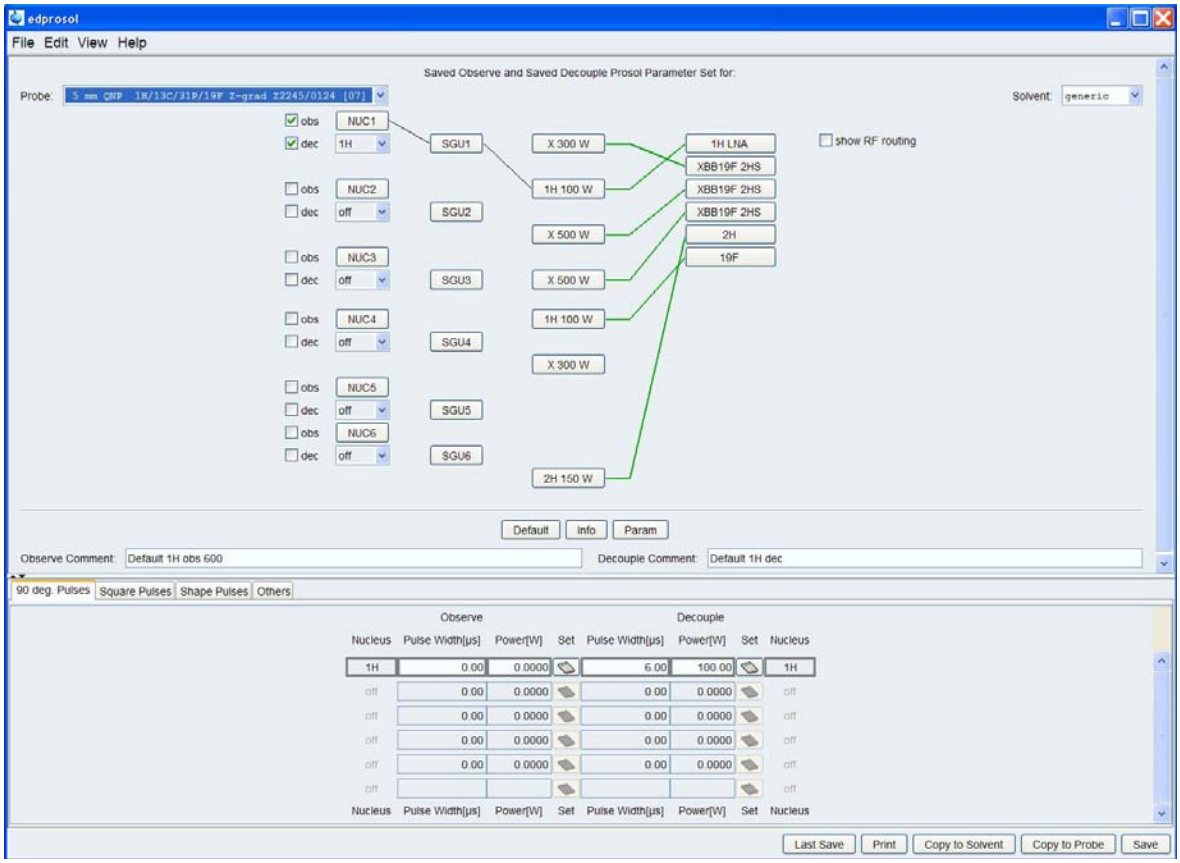

Figure 1.2: edprosol window in the 'Individual Mode'

This chapter only gives a short introduction about **edprosol**, starting the tool and appearance of the **edprosol** window.

Chapter 2 shows in detail how to use the **edprosol** window to set up your parameters. The menu bar will be explained elaborately.

1.3.3 Updating edprosol version 2.1

If the **TopSpin** Version 3.0 with the new **edprosol** tool is an upgrade to the existing version 2.1 you have the possibility to transfer your old 90° pulses to this new tool. At the end of the **expinstall** tool the 'Prosol Import Dialog' window (see Figure 1.3) will be displayed.

In the upper part of this window you will find all necessary information about the importing process. Then you only have to choose the probe for which the 90° pulses should be transfered and click **OK**.

You also have the possibility to skip this process here and import your pulses later out of the **edprosol** tool. For more information see Chapter 2.1, the **EDIT** button of the menu bar. You will find an 'Import old 90°pulses' command there.

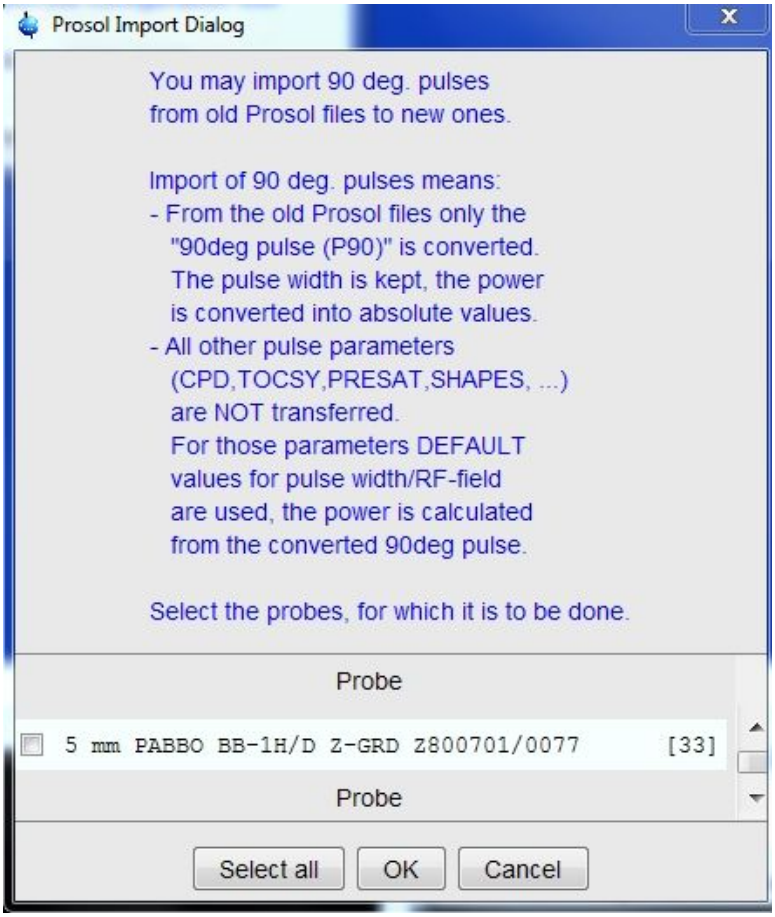

Figure 1.3: 'Prosol Import Dialog' Window

2 The edprosol window

When starting the **edprosol** tool by typing ***edprosol*** in the command line of the **TopSpin** main window, the edprosol window as shown in Figure 1.1 will be displayed.

This window contains a menu bar on top of the window and a toolbar on the lower right side. For setting your specific parameters there are two separated areas called upper and lower area in the following paragraphs and chapters.

In this chapter the functionality of menu bar and the toolbar will be described in detail.

2.1 The menu bar of the edprosol window

The menu bar encloses four buttons. Clicking a button will open a popup menu with detailed functions you can chose from.

The first button is the **File** button. Clicking this button opens the following popup menu:

Figure 2.1: Popup menu after clicking the **File** button

First of all you have the possibility to save the current parameters by clicking **Save**.

If you have done changes in the lower part of the **edprosol** window and want to get back to the former values, click **Last Save**. The values which have been most recently saved for the current dependency will be restored.

To delete a prosol parameter set or parts of it click the **Remove** button.

First you will be prompted to type the administrator password. Demanding for the administrator password always occurs when writing to the disk or deleting from the disk for the first time of an **edprosol** session.

Now a 'Prosol Parameter Set Selection' window is displayed as shown in Figure 2.2.

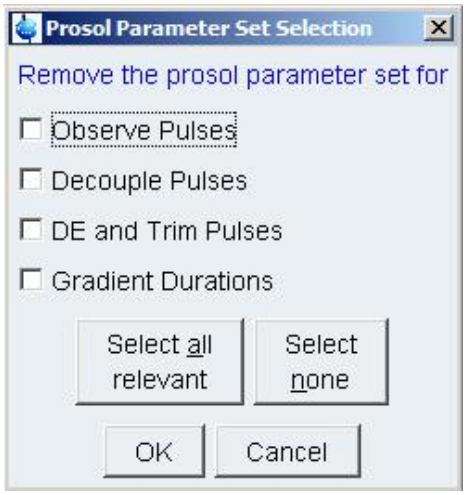

Figure 2.2: 'Prosol Parameter Set Selection' window for removing prosol parameter sets

You have the possibility to choose one or more parameter sets for removing. Clicking the **Select all relevant** button will tag all parameter sets. Using the **Select none** button will untag all parameter sets. Now clicking **OK** will remove all selected sets from your disk. With clicking **Cancel** you may leave this window without any changes.

Clicking the **Copy to** button offers the possibility to save prosol parameter sets for a specific probe or for a solvent.

If necessary you will be prompted to enter the administrator password, then again a 'Prosol Parameter Set Selection' window will be displayed. (see Figure 2.3)

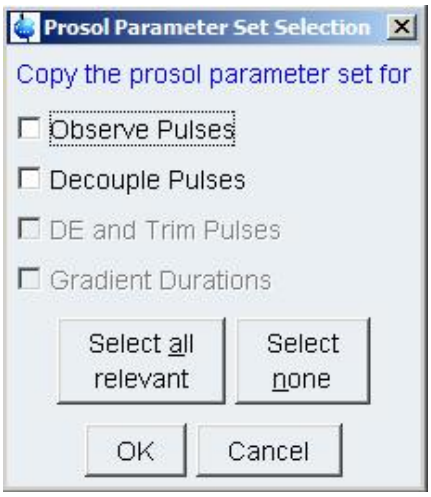

Figure 2.3: 'Prosol Parameter Set Selection' window for copying prosol parameter sets

Now you may copy the parameter set for observe pulses or decouple pulses or both to a probe. The same procedure can be performed for solvents.

Copy to a probe/solvent means to copy the parameter sets to a directory which contains all prosol data sets concerning the chosen probe. Its location is

<TopSpinHome>/conf/instr/<spectrometer>/prosol/

Here you will find a directory for each probe of your system. The directories are named with the number in brackets at the end of the Probe definition in the **edprosol** window (see Figure 1.1). In a later version of this tool it shall be the name of the probe.

In the directories for each probe you will find a directory named generic, which contains parameter sets for the nuclei performed with 'generic' solvent. If you have specific parameter sets for certain solvents, then choose the solvent instead of generic in the upper part of the **edprosol** window (see Figure 1.1) and the parameter set is copied to a directory with this solvent name.

If you like to have a summary of your parameter sets click **Print -> Sets** and a 'Preview of Prosol Parameter Set Table' window is displayed (see Figure 2.4).

This window just represents a simple editor which summarizes your probes and solvent parameter sets in a clear layout. You may save this summary to a file or directly print it. Besides you can edit the file (For more information look at the menu bar of this window).

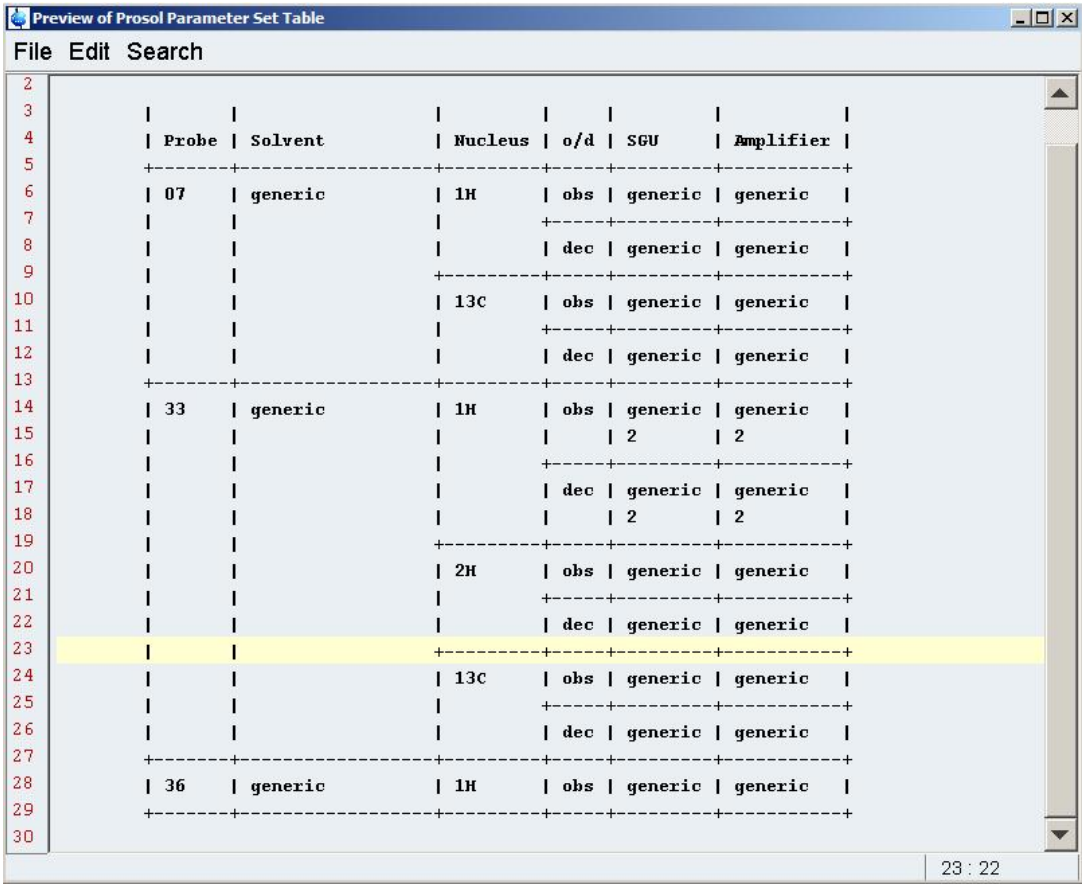

Figure 2.4: 'Preview of Prosol Parameter Set Table' window

If you like to have a summary of the parameters click **Print -> Parameters.** A 'Prosol Parameter Set Selection' window will be displayed where you can select Observe or Decouple Pulses or both. Clicking OK opens a 'Preview of the Parameter Table' window. It is comparable to the one for parameters sets.

Clicking **Exit Prosol Editor** will close the **edprosol** window. If there are unsaved changes you will be prompted to save/leave with a 'Prosol Parameter Set Selection' window.

The second button of the menu bar is the **Edit** button. Clicking this button opens the following pop up menu:

Figure 2.5: Popup menu after clicking the **Edit** button

By default **edprosol** starts in the common mode as shown in Figure 1.1.

Selecting **Enable the Individual Mode** you can switch to the Individual mode (see Figure 1.2), where you may set the routing.

- **This should only be used by experienced users!**

Clicking **Enable the Individual Mode** again disables this mode and **edprosol** can be used in the common mode.

Selecting **Enable the Solid State Mode** supports your solid state equipment and experiments.

Selecting **Set Default Puls Widths** or **Set Default Pulse Description** opens the now well-known 'Prosol Parameter Set Selection' window. You only have to choose for which pulses the default values/descriptions should be set.

Clicking **Save Pulse Descriptions** will save your changes to this topic.

These three selections can only be used if the administrator password is known. You will be prompted to type it when one of these actions is the first writing/setting action for a session. This also relevant for the next two selections, **Edit Tunefile** and **Import old 90^{o} Pulses**.

Selecting **Edit Tunefile** opens the 'Select tunfile' window (Figure 2.6).

Figure 2.6: 'Select tunefile' window

Choose a tunefile by clicking on it or create a new one. Type the name of your new file in the designated box and click the **Edit** button to open the editor. Now create the new file.

If you have chosen an existing tunefile it will be displayed by clicking the **Edit** button. Now you may write corrections, additions etc to it.

Besides editing, all chosen tunefiles can be executed, deleted or just cancelled by clicking the corresponding button from the button bar at the bottom of the window.

Clicking the **Edit probe tunefile** button you will open a tunefile which is use in automation.

In former setups for each probe such a tunefile was available. Now there is one basic tunefile for all probes used in automation, but you may adjust this with different solvents. **Edprosol** allows you to save this 'probe tunefile' to a desired solvent directory of your probe(s).

Finally the **Edit** menu offers the possibility to import old 90° pulses. You can select between a Default Mode and a Custumized Mode. Both will import 90° pulses from the old **edprosol** tool for the current probe.

Clicking **Import Old 90° Pulses -> Default Mode** will open the following dialog window:

Figure 2.7: 'Prosol Import Dialog' window

Pressing the OK button starts the import of the old files. If one or more files already exist you will be asked if you like to override the file(s). When the import is finished a protocol as shown in Figure 2.8 will be displayed.

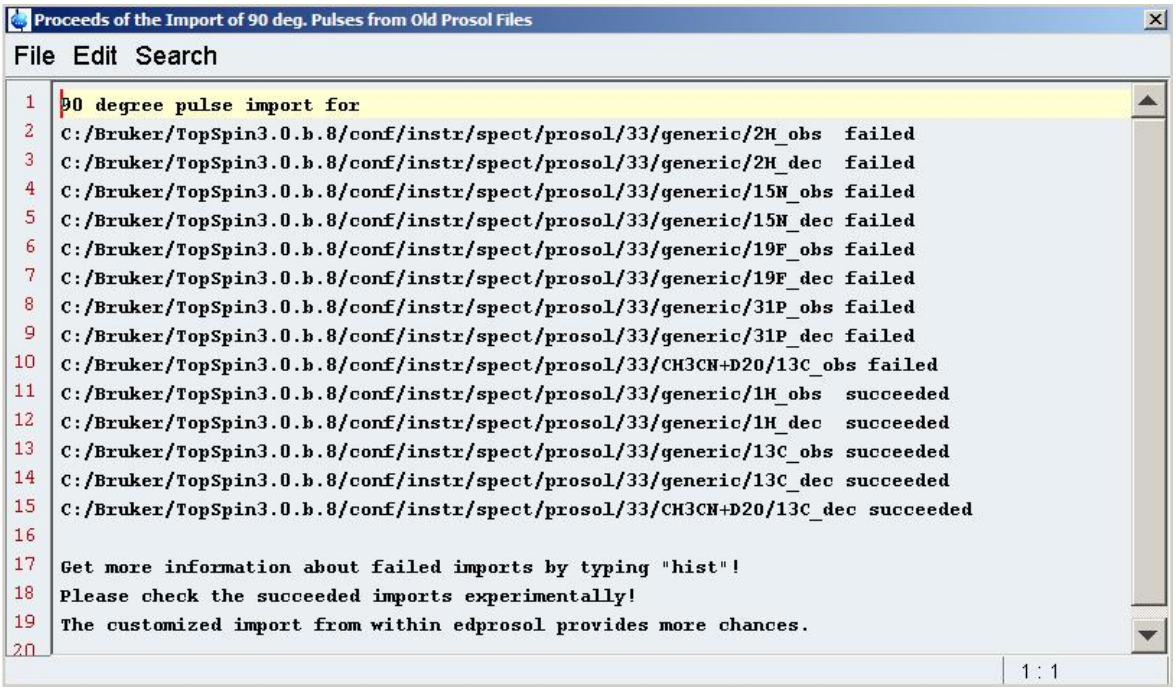

Figure 2.8: Import protocol

Clicking **Import Old 90° Pulses -> Customized Mode** will open the following dialog window:

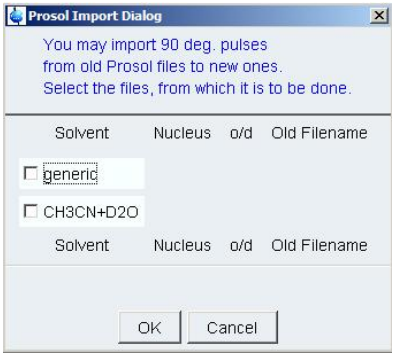

Figure 2.9: 'Prosol Import Dialog' for customized mode

You now may select for which solvent the old pulses should be imported. After marking one or more solvents, the window offers more information about the nuclei and channels for which old data are available (see Figure 2.10)

Figure 2.10: 'Prosol Import Dialog' for customized mode after file seletion

Clicking the **OK** button will import the selected 90° pulses. After finishing this import, again an import protocol comparable to the one in the Default Mode will be displayed.

The third button of the menu bar, the **View** button, opens the following popup window:

Figure 2.11: Popup menu after clicking the **View** button

Every selection from this popup menu will extent or decrease the displayed information in the lower part of the **edprosol** window, where all settings for pulses and power levels are done.

This part of the **edprosol** window consists of 4 tables contaning 90 deg Pulses, Square Pulses, Shape Pulses and Others, which can be selected by clicking on the corresponding tab.

Selecting the **Base View** from the popup menu (Figure 2.11) in all four tables only the relevant pulse widths and power levels are displayed. Activating the **Full View**, in the tables Square Pulses and Shape Pulses flip angles, RF fields and alignments are displayed additionally as shown in Figures 2.12 and 2.13.

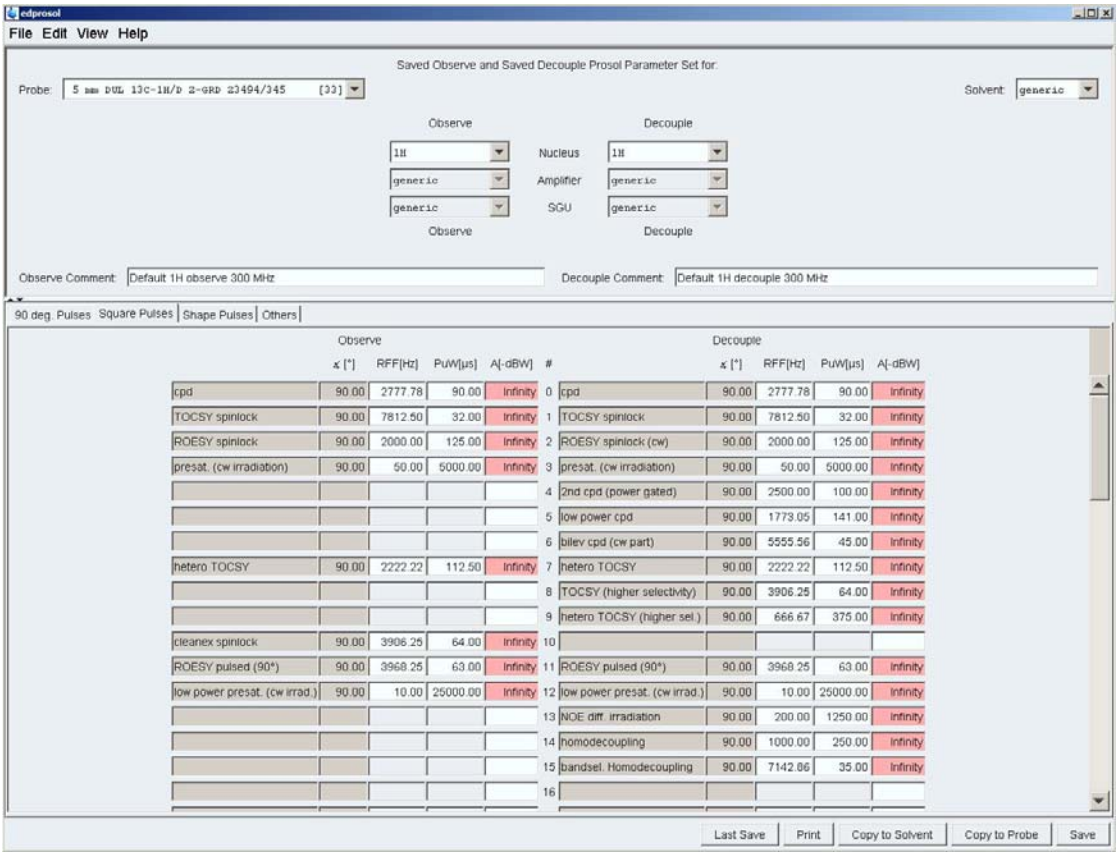

Figure 2.12: Table **Square Pulses** in full view

Figure 2.12 shows that between the pulse description column and the pulse width column two addional colums with flip angles and RF field are diplayed. This is for both, the observe and the decouple side.

Figure 2.13 shows that between the filename column and the pulse width column three addional colums with flip angles, RF field and alignment are diplayed. Again this is for both, the observe and the decouple side.

Instead of basic or full view you may also select only one or two of the additional informations in any combination. The chosen ones are marked in the corresponding popup menu as shown in Figure 2.11.

With the last button of this popup menu you may chose the way of representation for the power level.

By default the power levels will be displayed in units of watt. This is for the first time possible with this new **edprosol** tool. All older versions of **edprosol** handle power levels as attenuation levels in units of dB.

For users who are accustomed to this representation, **edprosol** offers the possibility to switch between the two modi. But you habe to keep in mind that the new presentation of power levels as attenuation levels is not exactly the same. It is shown in units of [-dBW]. Compared to the former description of the power level in dB now all values have a reference point, which is 1 Watt but with opposite algebraic sign to dBW.

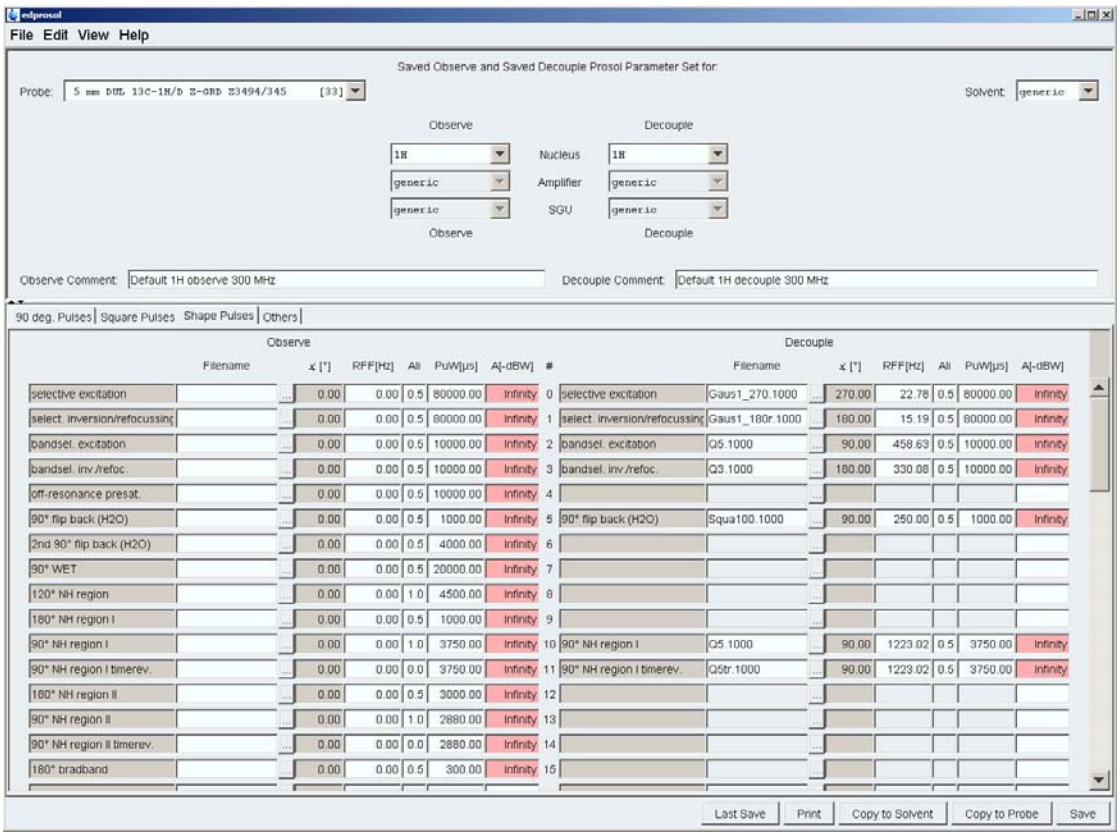

Figure 2.13: Table **Shape Pulses** in full view

The last button of the menu bar is the **Help** button. Again a popup menu will be opened when clicking this button (Figure 2.14)

Figure 2.14: Popup menu after clicking the **Help** button

From here you may open the present **Edprosol Manual** and at a future date a **Setprosol Manual** and a **Getprosol Manual**, too.

Clicking **About Prosol** informs you about the current **edprosol** version.

2.2 The toolbar of the edprosol window

The toolbar at the bottom of the **edprosol** window gives you a quick access to the most important commands available by clicking the **File** button from the menu bar and then selecting from the popup menu (Figure 2.1).

The buttons are named like the ones of the popup menu. Using the buttons **Copy to Solvent**, **Copy to Probe** or **Save**, it is necessary to know the administrator password. You will be prompted to enter this when the command is the first diskwrite command of the session.

2.3 The upper area of the edprosol window

Prosol parameters must be defined for each probe separately, so initially you have to select the probe (as defined with **edhead**) to be prepared for the prosol parameter set. In the upper area of the **edprosol** window, the 'Probe' field in the upper left part (see Figure 1.1) contains a list of all probes announced to your system.

A solvent, for which the parameter set should be valid, must be chosen in the 'Solvent' field in the upper right part. You can choose a specific solvent (acetone, methanol etc.) or generic, means all solvents for which no specific parameter set is defined. If you select a specific solvent, the prosol parameters will be stored for this solvent only.

As prosol parameters must also be set for each nucleus separately, now you have to select an observe and decouple nucleus corresponding to the chosen probe in the 'Observe' and 'Decouple' fields in the center of this window section.

With suitable probe and preamplifier equipment, a selection of inner and outer coil might appear for a given nucleus, labelled X@i or X@o. An example would be a TBI probe allowing ^{13}C on the inner and/or outer coil. If corresponding preamplifiers are availablefor both, this selection will be activated.

Optional, you have the possibility to add a comment (for example the conditions under which the pulses or power levels have been determined) for both observe and decouple part in the 'Observe/Decouple comment' field.

If you have decided to work in the individual mode, this part of the **edprosol** window looks like shown in Figure 2.15.

Here a number of nuclei, SGU, amplifiers and preamplifiers are shown explicitly.

In the beginning the default routing for your system is chosen and displayed. Right clicking on the combined nucleus, SGU and amplifiers will delete the routing and you can choose your individual signal path, if technical possible. **Edprosol** will detect illegal routings and suggest others. You then have to check, if this is suitable for your system configuration.

If there are several SGUs, amplifiers and preamplifiers available for the system, this mode allows you to prepare prosol parameters for different signal paths.

This method should only be applied by experienced users.

For more information about the routing see also EDASP description.

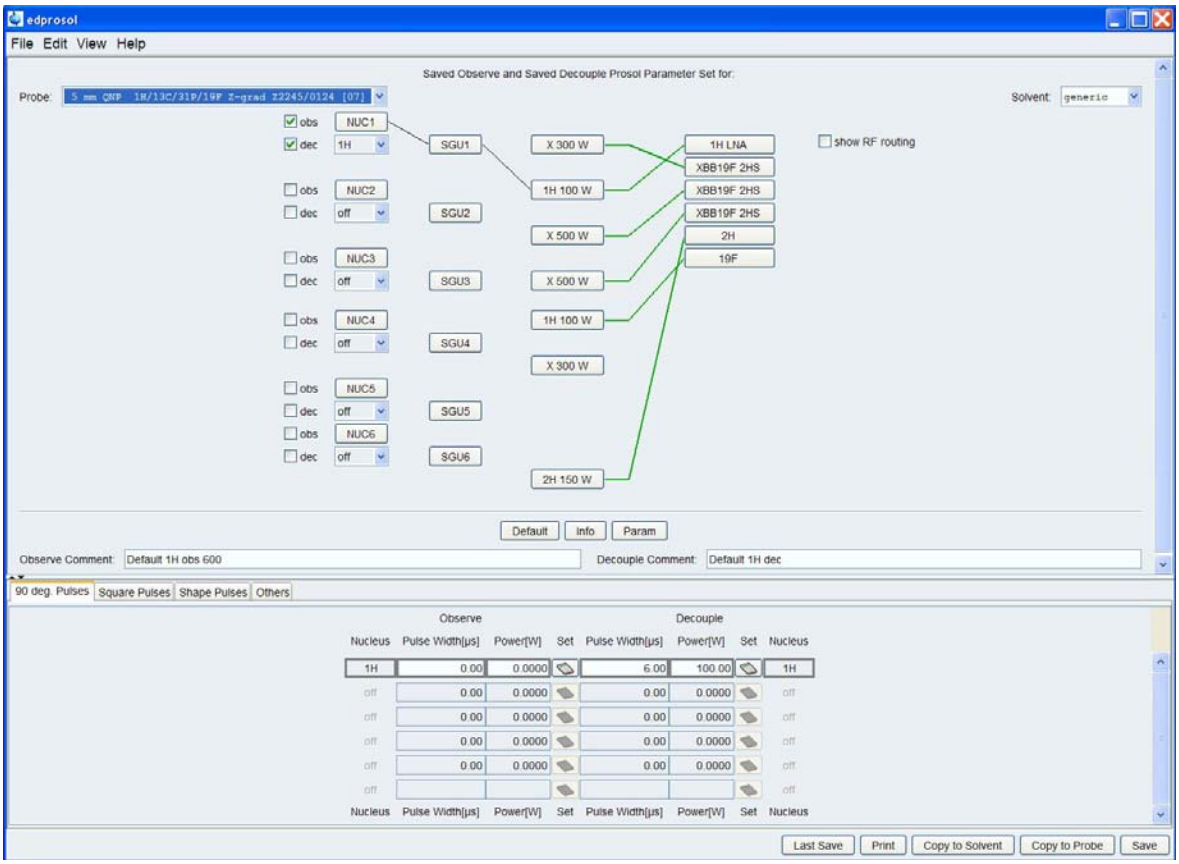

Figure 2.15: Edprosol window in individal mode

2.4 The lower area of the edprosol window

In this part of the **edprosol** window all pulse lengths and power levels for the selected frequency channel(s) of the current probe and solvent (see capter 2.3) will be defined.

Due to this purpose there are four tables for your settings which can be chosen by clicking the corresponding tab.

2.4.1 The ‘90 deg. Pulses’ table

The first table (see figure 2.16) contains the 90° hard pulses for both observe and decouple channel. You should have determined these pulses before starting **edprosol**.

After selecting the desired probe, solvent and nuclei as described before (see chapter 2.3), you will notice the highlighted frames for the parameter fields of the chosen nuclei in the ‘90° pulses’ table.

As an example in Figure 2.16 a $^{1}H/^{13}C/^{31}P/^{19}F$ quadrupol probe was chosen with ^{13}C observe and ^{1}H decouple nucleus.

The choise of the nucleus is always sychronized in the upper and lower part of the **edprosol** window. So the nucleus is chosen for all tables.

In the '90° pulses' table now nucleus, pulse width and power level fields for ^{13}C as observe nucleus and the corresponding fields for 1H as decouple nucleus are marked with a high lighted grey frame.

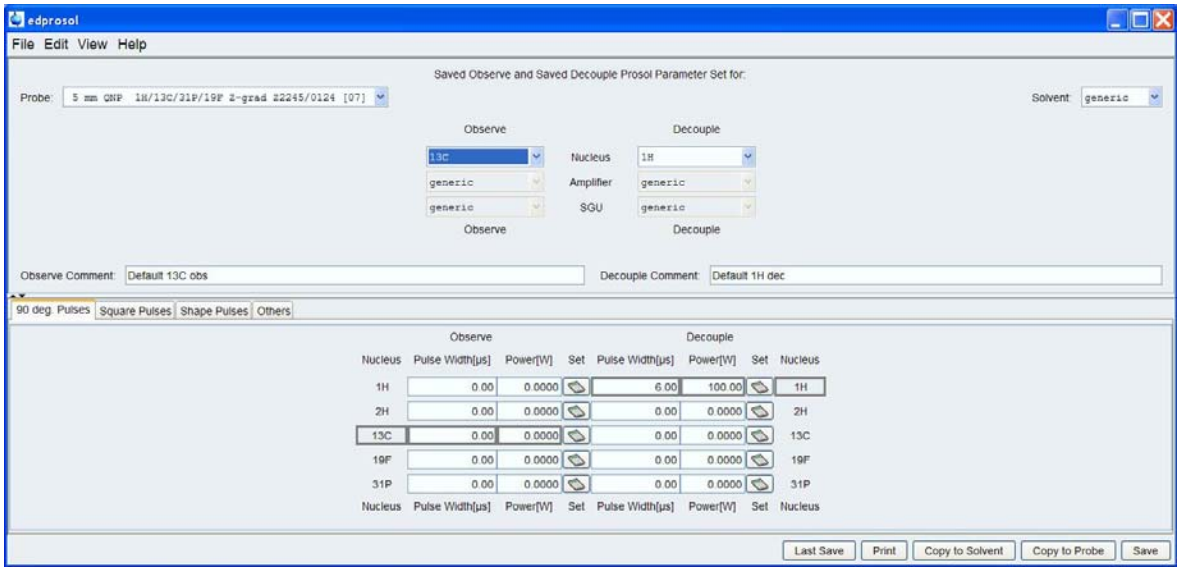

Figure 2.16: **Edprosol** window with 90° Pulses table in lower part

The determined pulse width and power level are entered in these fields.

Although only two parameters for each chosen nucleus of a probe in combination with a solvent will be set in this table, they are the most important ones in the **edprosol** tool. All values in the 'Square Pulses' and 'Shape Pulses' table will be calculated with these entries.

Therefore it is important to know, that Amplifier linearity is mandantory to use this routines. To ensure this linearity, the 'cortab' table for the given nucleus must be available.

For more information you might look up in the 'Cortab' description.

To calculate the pulse widths for all available experiments, you have to click the 'Set' button right beneath the power level field of each possible nucleus (for both observe and decouple channel). The following popup dialog window will be opened:

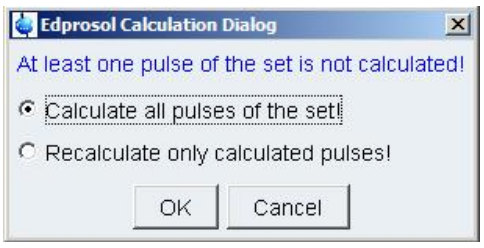

Figure 2.17: Edprosol Calculation Dialog window

You have the possibility to calculate all pulses of a set or to recalculate only the calculated pulses. The last option allows to set one or more pulses as you may have deter-

mined them. The Edprosol tool can distinguish between manually entered values and calculated ones.

2.4.2 The ‘Square Pulses’ table

Calculation of a parameter set with your determined 90° transmitter pulse at a certain power level will directly affect ‘Square Pulses’ and ‘Shape Pulses’ tables. The figures 2.18 to 2.20 show these tables.

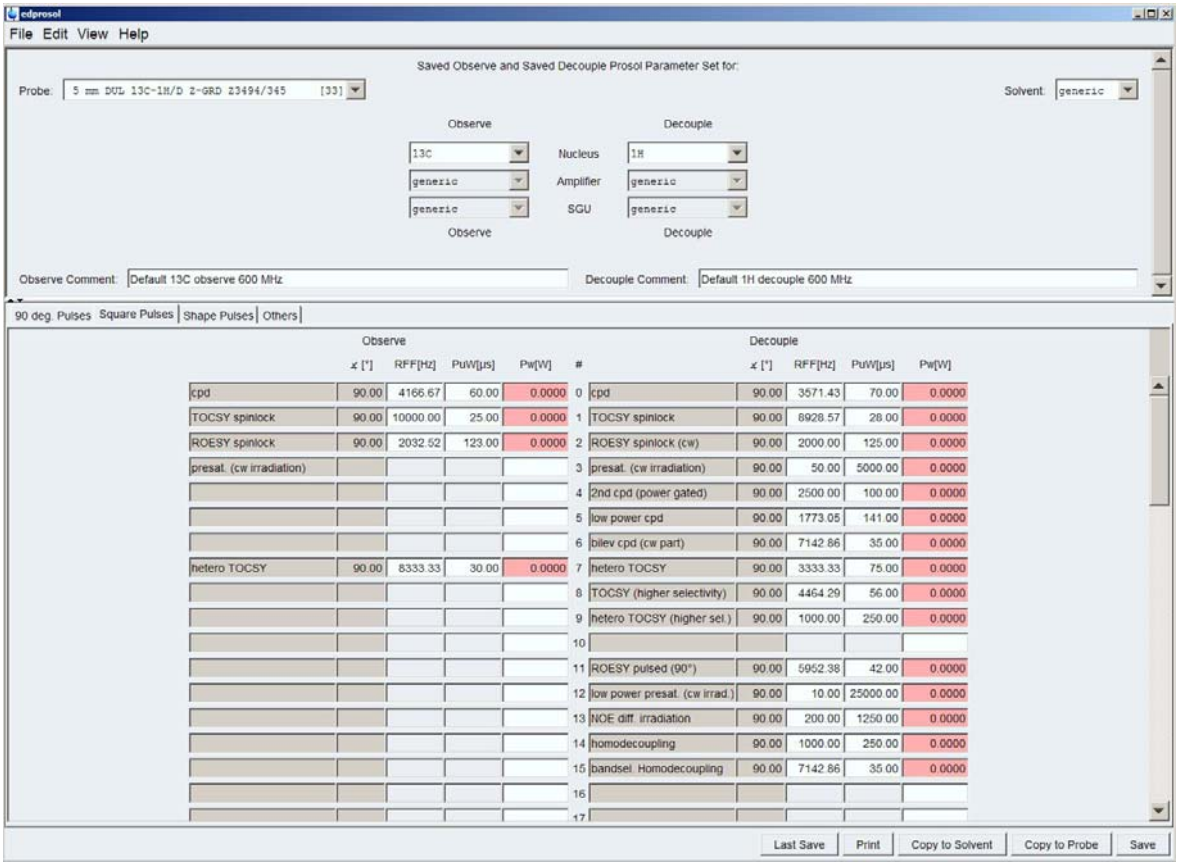

Figure 2.18: **Edprosol** window with ‘Square Pulses’ table in lower part, Power level [W]

The table contains a set of certain square pulses. The required flip angle, the RF field, pulse width (corresponding to the flip angle) and the power level for both, the observe and the decouple channel are listed. In contrary to this full view of the table in the basic view only pulse width and power level are shown.

The first three parameters (flip angle, RF field and pulse width) are fixed parameters of your data set. The power level is the one to be calculated with your determined 90° pulse at a certain power level. In Figure 2.18 for all possible experiments, the power level is 0[W] which is the default value. No calculation has been done yet.

A double click on the description field opens a window where the descption and the flip angle can be edited. An angle of 0° is only accepted, if the description is empty, which deactivates the pulse. An empty description is only accepted, if the angle is 0°. Deactiva-

tion of a pulse might be interesting if you do not want to transfer this special pulse to your aquisition parameter later

RF field and Pulse width are always editable by directly writing in the corresponding field. Changing one of them will adept the other and additionally the power level will be adapted.

The power level is always editable by writing into the corresponding field. A red coloured field informs about a not calculated value,

If you recalculate the parameter set by clicking the ‘calculate’ button (see Fig. 2.16) and then choose ‘Recalculate only calculated pulses’ in the popup window (see Fig. 2.17), this manually set value won’t be affected.

In figure 2.18 the power level is displayed according to the **edprosol** handling using Watt units.

The view mode (see capter 2.1 and Fig. 2.11) can be changed for users accustomed to the old description in attenuation A [-dBW]. But the powel level handling has changed significantly for **TopSpin 3.0**.

You habe to keep in mind that the new presentation of power levels as attenuation levels is not exactly the same as in former **TopSpin** versions. It is shown in units of [-dBW]. Compared to the former description of the power level in dB now all values have a reference point, which is 1 Watt but with opposite algebraic sign to dBW.

Now the ‘Square Pulses’ table is displayed like in Figure 2.19.

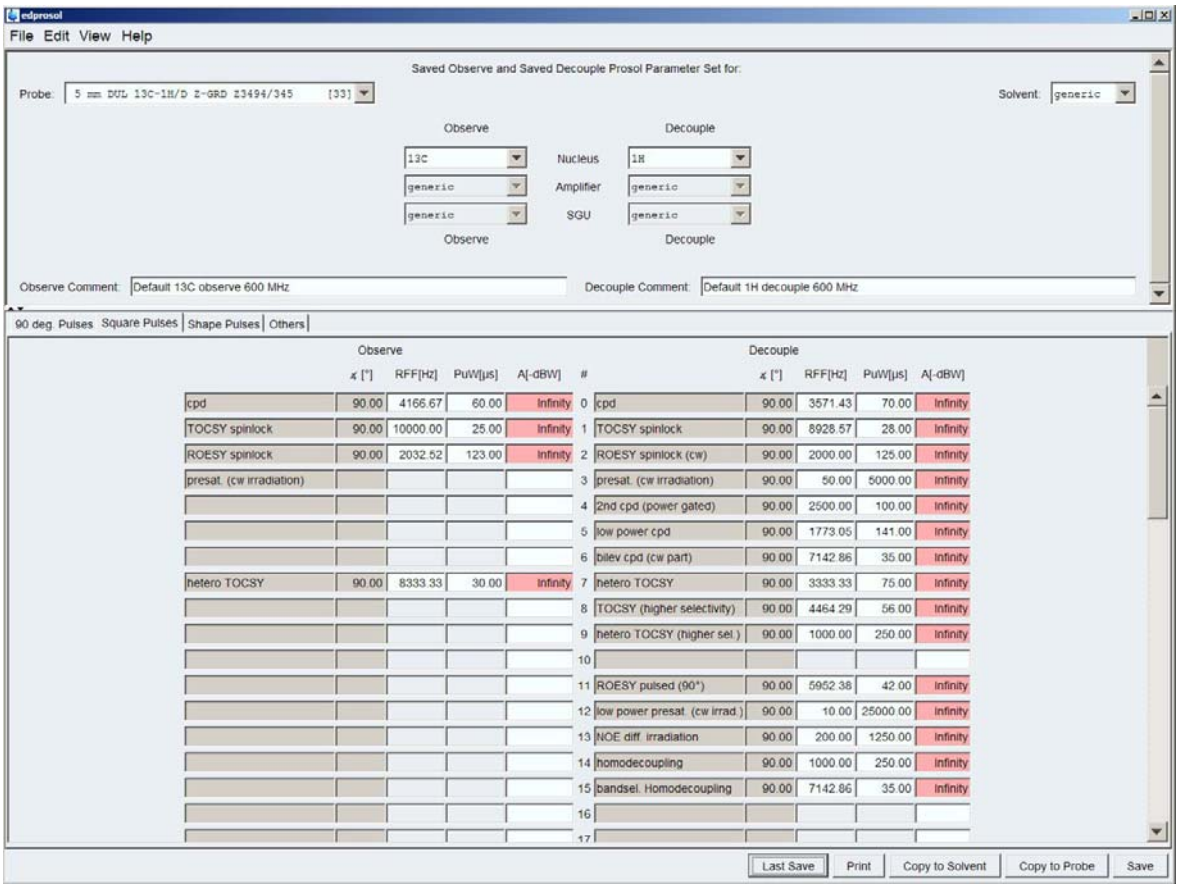

Figure 2.19: **Edprosol** window with ‘Square Pulses’ table in lower part, Attenuation level [dBW]

2.4.3 The ‘Shape Pulses’ table

In the ‘Shape Pulses’ table (see Figure 2.20) you can find shape pulses for the chosen dependencies (which are probe, solvent, nuclues and furthermore amplifier and SGU when working in the individaual mode). Again the required flip angle, the RF field, pulse width and the power level for both, the observe and the decouple channel are listed. Additionally the filename for each pulse descrition and the alignment is shown.

As discussed for the square pulses, again the flip angle, the RF field and the pulse width are fixed parameters and the power level respective the attenuation will be calculated from your 90° transmitter pulse if you use the calculate button or do other calculations.

Similar to the ‘Square Pulses’ table, here most of the parameter fields may also be edited.

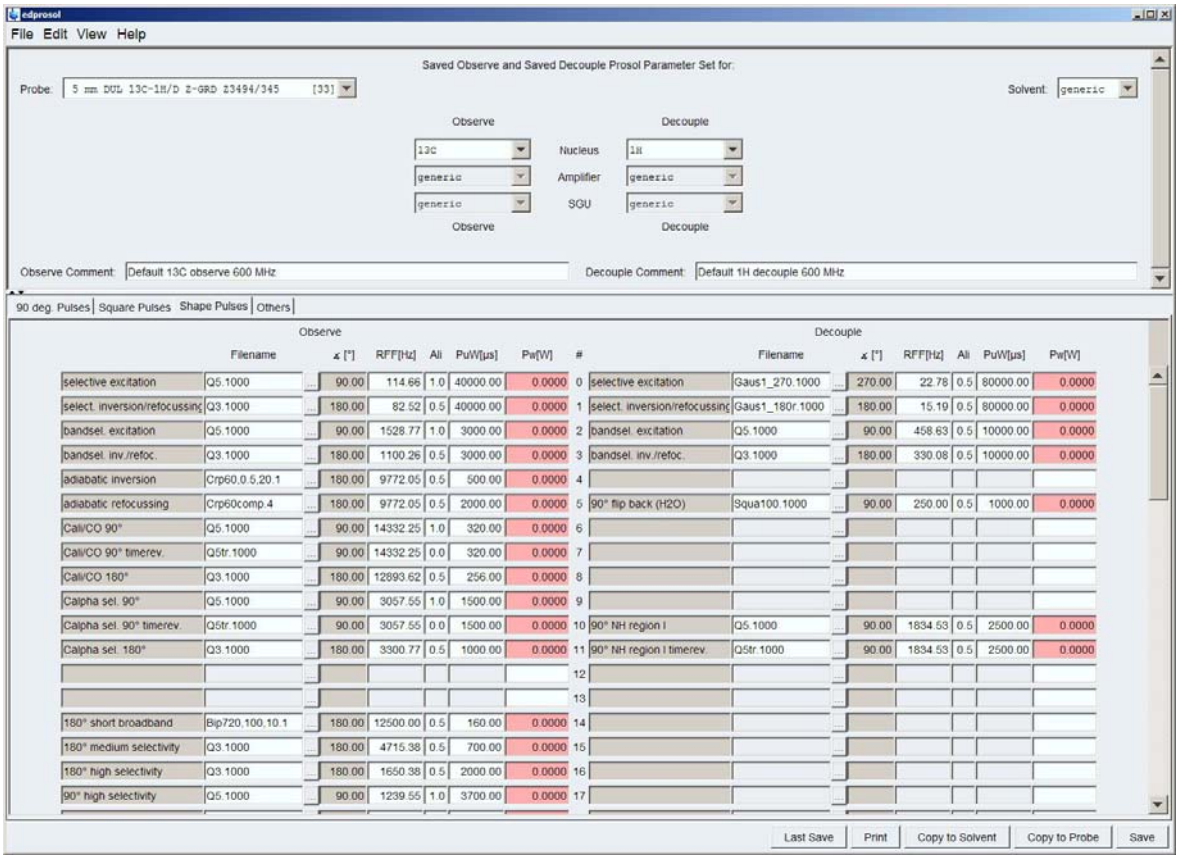

Figure 2.20: **Edprosol** window with ‘Shape Pulses’ table in lower part, Power level [W]

A left double click on any parameter field will open a window to edit the description field. You can deactivate this pulse by clicking the ‘Deactivate the Pulse’ button and then the OK button. The Pulse Description can be changed or deleted too.

For activating a pulse, left double click on an empty parameter field. The following window will be displayed:

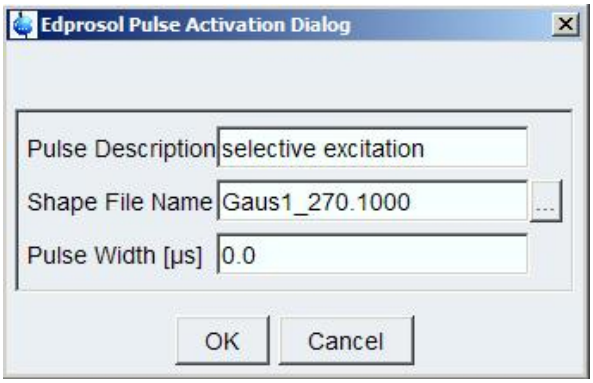

Figure 2.21: Edprosol Pulse Activation Dialog

Now you can enter a pulse description and choose a shape file by clicking the button beneath the corresponding field and selecting it from the upcoming ‘Shape files’ window (see Figure 2.22). Then enter a pulse width >0, otherwise the pulse will remain deactivated.

Clicking the button right beneath the Filename field, will open the ‘Shape Files’ window as shown in figure 2.22. It contains a list of all shape pulse files. In the source field on the top right site of this window you will find the location of these files:

\[Home]\TopSpin\exp\stan\nmr\lists\wave

Bruker also provides a directory for you own shape pulse files, with can be chosen as source directory by clicking the arrow beneaqth the source field:

\[Home]\TopSpin\exp\stan\nmr\lists\wave\user

For more information about creating our own pulse shapes click the ‘Help’ button of this window and use the Shapetool manual and the Pulse Programming manual.

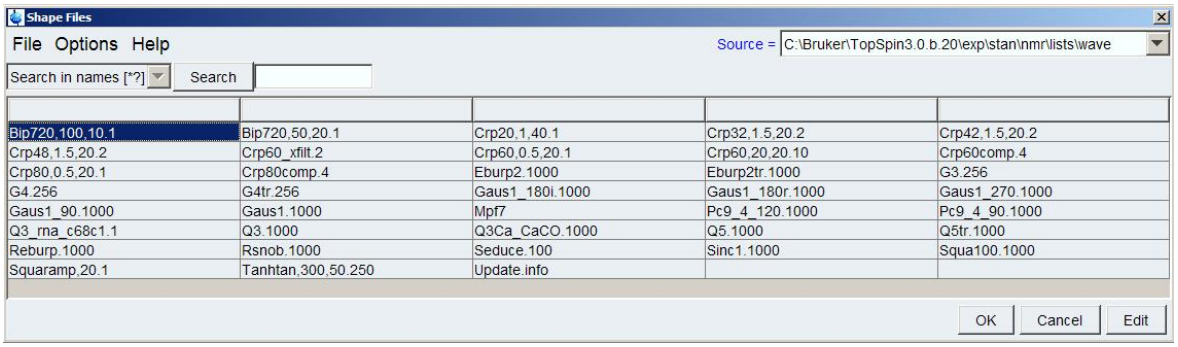

Figure 2.22: ‘Shape Files’ window with provided pulse shapes by Bruker

If you don’t want to overwrite certain shape pulse parameters in your acquisition parameters you can deactivate these shape pulse values in the **edprosol** tool. Otherwise using the ‘getprosol’ command will transfer all prosol parameters to the aquisition parameters which are specified in the corresponding pulseassign file.

The flip angle field is not editable, this parameter will always be taken from the shape file.

Similar to the ‘Square Pulse’ table, both RF field (if visible) and Pulse width are always editable by directly writing in the corresponding field. If changing one of them, the other and additionally the power level will be adapted.

Again the power level is always editable by writing into the corresponding field. Then a red coloured field informs about a not calculated value.

Additionally you can find an **Alignment** button in the 'Shape Pulses' table.This parameter defines where the phase of the shape pulse is correct. 0 is for flipback pulses, 0.5 means 180° selective/refocusing pulses and 1 defines excitation pulses.

2.4.4 The ‘Others’ table

The last table of the lower part of the **edprosol** window, accessible by clicking the ‘Others’ tab, is independent from the 90° transmitter pulse and therefore from the other tables. It is shown in Figure 2.23 .

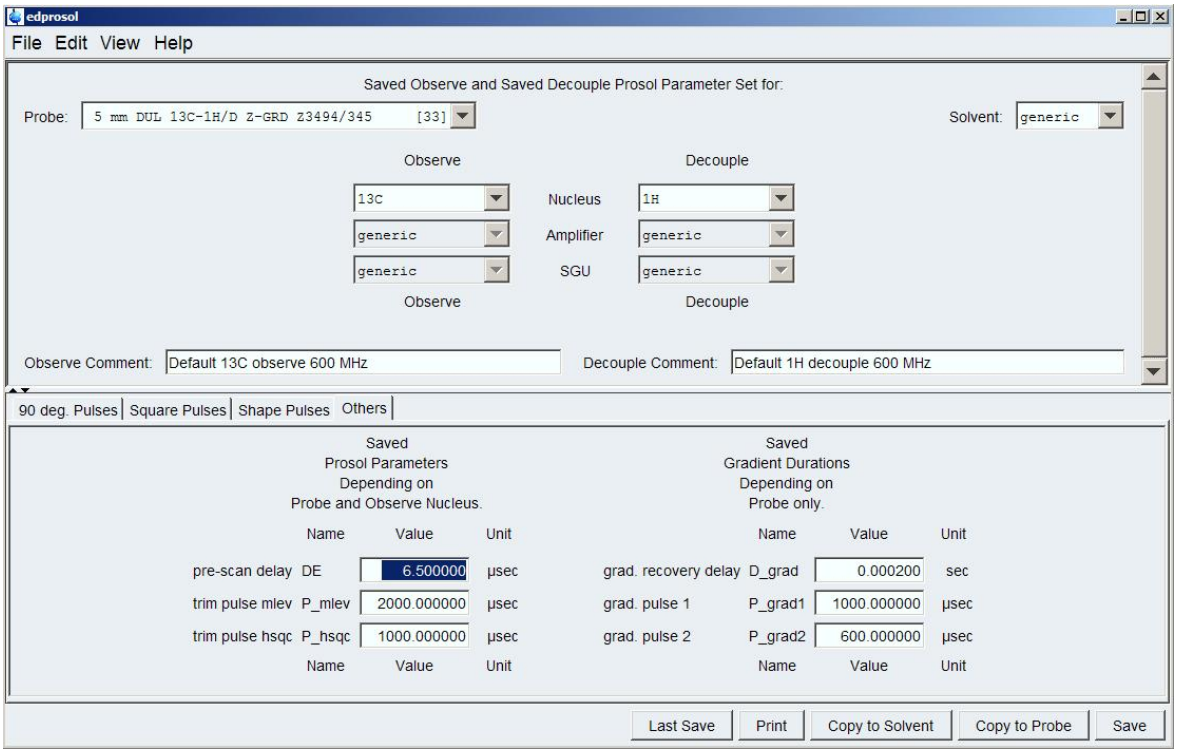

Figure 2.23: **Edprosol** window with ‘Others’ table in lower part

The parameters in this table are general parameters. On the left side of the window, they depend on the probe and the nucleus selected for observe. The gradient parameters on the left side only depend on the probe.

Bruker provided a pre-scan delay and two trim pulses (mlev and hsqc) as well as gradient recovery delay and two gradient pulses (P_grad1 and P_grad2). It is not recommended to change these values, but you may edit them to suit our needs.

3 Prosol Parameter Directories

All prosol parmeters can be found in the following data path:

<tshome>/conf/instr/<instument>/prosol

The directory prosol itself contains some subdirectories.

For each installed probe a further subdirectory, which is named by the probe ID, is created. These subdirectories contain the optional solvent directories with their individual prosol parameters. Additionally the `bsmspar` file as created by **edlock** is stored here.

In the `generic` directory the prosol parameters for solvents without an own parameter set are located. New within the probe directories are the files containing the parameters corresponding to the 'Others' table. These files are the file *grad*, containing the gradient parameters, and the files named by nuclei, containing the others.

In the prosol directory you will also find the file version and the subdirectories description and pulseassign.

The pulse assignment files substitute the relation files. They are delivered within ***<tshome>/exp/stan/nmr/lists/prosol/pulsassign*** and will be copied to the subdirectory pulseassign of the working directory, during the installation of a new **edprosol** version.

3.1 The Version Control

Parameter files, description files and pulseassign files must be mutually compatible and compatible with the program, so they are substituted to the following version control when upgrading TopSpin:

The **edprosol** file version of a TopSpin distribution is connected with the file *version* in the prosol parameter directory. Each concerned file contains its own version. The *version* file itself contains the parameter ProgramVersion and FileVersion. The file of a user directory may contain the further parameter IgnoreVersion.

This last parameter allows you to ignore the inconsitency that may occure by updating, on your own risk when using **eduserprosol**.

Eduserprosol is a 'user specific' **prosol** and will have the same user interface (only the window titles will be different) as **edprosol**. Whereas **edprosol** works on the global tree of TopSpin, **eduserprosol** will do this on the personal tree of a current user.

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