EDPROSOL

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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.

edprosol											
ile Edit View Help											
Probe: 5 mm ONP 1H/13C/31P/19P Z-grad 22245	/0124 [07]	Saved Obse	rve and Save	d Decoup	le Prosol Parar	neter Set for:				Solvent gener	r10
		Obser	ve		D	ecouple					
		18	~	Nucleus	1.8	~					
		generic	4	Amplifier	r generi	2 N					
		generic	Y	SGU	generi	• •					
		Obser	ve		D	ecouple					
Observe Comment. Default 1H obs 600					Decouple Com	ment. Default	1H dec				
0 deg. Pulses Square Pulses Shape Pulses Others						241					
		Observe				Decouple					
	Nucleus	Pulse Width[µs]	Power[W]	Set Pu	lse Width[µs]	Power[W] S	let Nucl	leus			
	1H	0.00	0.0000		6.00	100.00	S 1	н			
	2H	0.00			0.00	0.0000	_	н			
	13C	0.00			0.00	0.0000	_	BC .			
	19F	0.00			0.00	0.0000	_	0F			
	31P	0.00			0.00	0.0000	_				
	Nucleus	Pulse Width(µs)	Power[W]	Set Pu	ise Width(µs)	Power[W] S	et Nuci	leus			

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.

le Edit View Help												
			Saved Obser	ve and Save	d Dec	ouple Prosol Parar	neter Set for	1				
robe: 5 mm CMP 18/13C/31P/19F Z-gra	d 22245/0124	[07] ~								Solvent	generic	Y
	🗹 obs	NUC1										
	🗹 dec	1H 🛩	SGU1	< 🗆	(300 1	w	1111	NA	show RF routing			
	_					_ /	XBB19F					
	dec	NUC2	SGU2	1	H 100	w	XBB19F					
	[_] dec	off 💌	5602		(500 1		XBB19F		-			
	Obs	NUC3				- /	196	_	Ĩ			
	dec	off 🖌	SGU3		(500 1	w_//	1					
	-					_ / /	4					
	obs	NUC4	SGU4	1	H 100							
	Lloet	Un C	3304		(300 1							
	obs	NUC5										
	dec	off 🖌	SGU5			1						
	🗌 obs	NUC6										
	dec 🗌	off 🖌	SGU6	-		_ /						
				2	H 150	w						
				Default	1.	nfo Param						
				Detault								
serve Comment: Default 1H obs 600					_	Decouple Com	ment: Defa	ult 1H	dec			
deg. Pulses Square Pulses Shape Pulses C	Others											
			Observe				Decouple					
		-	Pulse Width[µs]			Pulse Width[µs]		_	Nucleus			
		1H	0.00	0.0000		6.00	100.00		1H			
		tto	0.00	0.0000	-	0.00	0.0000		110			
		off	0.00	0.0000		0.00	0.0000		off			
		off	0.00	0.0000		0.00	0.0000		10			
		017	5.00	0.0000	4	0.00	0.0000	4	off			
				-	-			-				

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:

;	Save	
l	ast Save	
F	Remove	
(Copy to	•
F	Print	,
E	Exit Prosol E	ditor

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.

🙀 Prosol Parameter S	Set Selection 📃 👂	×
Remove the prosol	parameter set fo	r
Dbserve Pulses		
Decouple Pulses	6	
DE and Trim Pul	ses	
Gradient Duratio	ins	
Select <u>a</u> ll rele∨ant	Select <u>n</u> one	
ок	Cancel	

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)

🥌 Prosol Parameter	Set Selection 🔀
Copy the prosol pa	arameter set for
Dbserve Pulses	1
Decouple Pulse	S
DE and Trim Pu	Ilses
🗖 Gradient Durati	ons
Select <u>a</u> ll relevant	Select <u>n</u> one
	Cancel

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).

Edit	Se	arch							
			5	8	15	- 20		h	-65
	1		I	I		1		I	1
	1		Solvent +		2000 C 2000			Amplifier	-
	I		generic	1H	obs	1	generic	generic	1
	I			I I	dec	I	generic		1
	1		l I	+ 13C	obs	1	generic		1
	1		l I		dec	, I	generic		1
	+	33	+ generic	+ 1н			generic	+ generic	+ I
			1	1	 +		2	2 +	l +
			1	1	diec 	- 13	generic 2		1
			l	+ 2н	•		qeneric	+ qeneric	.+ 1
	Í		I	Î.	+	-+		+	+
	I		I	1	dec	1	generic	generic	1
	1		I	+	+	-+		+	+
	I		l	130			generic		1
	I		I	I				+	+
	I		l	1			generic	-	1
	+		•		••••••			+	+
	1		generic				generic		1
	+		+	+	+	-+		+	+

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:

Enable the Individual Mode
Enable the Solid State Mode
Set Default Pulse Widths
Set Default Descriptions
Save Pulse Descriptions
Edit Tunefile
Import Old 90° Pulses

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° Pulses**.

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

Select tunefile		×		
Select one of the available	e tune file:	5:		
example				
quickall				
tuneall				
tunezz2				
l r				
New tune file:				
				1
Edit probe tunefile	Edit	Execute	Delete	Cancel

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.

1	90 degree pulse import for	
2	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/2H_obs failed	
3	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/2H_dec failed	
4	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/15N_obs failed	
5	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/15N_dec failed	
5	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/19F_obs failed	
7	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/19F_dec failed	
3	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/31P_obs failed	
9	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/31P_dec failed	
0	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/CH3CN+D20/13C_obs failed	
1	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/1H_obs_succeeded	
2	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/1H_dec succeeded	
3	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/13C_obs succeeded	
4	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/generic/13C_dec succeeded	
5	C:/Bruker/TopSpin3.0.b.8/conf/instr/spect/prosol/33/CH3CN+D20/13C_dec succeeded	
6		
7	Get more information about failed imports by typing "hist"!	
3	Please check the succeeded imports experimentally!	
9	The customized import from within edprosol provides more chances.	

Figure 2.8: Import protocol

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

You may impo from old Prose Select the file	ol files to n	ew on	es.
Solvent	Nucleus	o/d	Old Filename
🗖 generic			
CH3CN+D2O			
Solvent	Nucleus	o/d	Old Filename

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)

You may imp from old Pro Select the fil	sol files to	new one	es.
Solvent	Nucleus	o/d	Old Filename
🗹 generic	☑ 1H	🔽 obs	• 1H.F1.A2
		🗖 dec	
	₽ 2H	🔽 obs	• 2H.F1.A9
		🗹 dec	• 2H.F2.A9
	🗹 13C	🗖 obs	
		🗹 dec	• 13C.F2.A1
CH3CN+D2O	☑ 13C	🗹 dec	• 13C.F2.A1
Solvent	Nucleus	o/d	Old Filename

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:

Base View	
Full View	
 Show Flip Angles 	
Show RF Fields	
 Show Alignments 	
View Mode for Powe	er ∙

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.

			Saved	Observe a	nd Saved	Dece	ouple Prosol Parameter Set fo	or:					
robe: 5 mm DUL	13c-1H/D 2-GRD 23494/345 [33] 👻										Solvent gen	eric 💌
				Observe			Decouple						
			18		*	Nucl	eus 1H	*					
			gener	ic	-	Amp	after generic	+					
			gener	ic	-	so	U generic	-					
				Observe	_		Decouple						
bserve Comment	Default 1H observe 300 MHz						Decouple Comment: Defau	it 1H deco	uple 300 M	Hz			
deg. Pulses Squa	ere Pulses Shape Pulses Others												
		Obser	ve					Decoupt	1				
		x [*]	RFF[Hz]	PuW[µ5]	A[-dBW]	#		x [*]	RFF[Hz]	PuW[µs]	A[-dBW]		
	cpd	90.00	2777.78	90.00	Infinity	0	cpd	90.00	2777.78	90.00	Infinity		
	TOCSY spinlock	90.00	7812.50	32.00	Infinity	1	TOCSY spinlock	90.00	7812.50	32.00	infinity		
	ROESY spinlock	90.00	2000.00	125.00	Infinity		ROESY spinlock (cw)	90.00	2000.00	125.00	Infinity		
	presat. (cw irradiation)	90.00	50.00	5000.00	Infinity		presat. (cw irradiation)	90.00	50.00	5000.00	Infinity		
							2nd cpd (power gated)	90.00		100.00			
							low power cpd	90.00	1773.05	141.00			
							bilev cpd (cw part)	90.00	5555.56	45.00			
	hetero TOCSY	90.00	2222.22	112.50	Infinity		hetero TOCSY	90.00	2222.22	112.50			
							TOCSY (higher selectivity)	90.00	3906.25	64.00			
					-		hetero TOCSY (higher sel.)	90.00	666.67	375.00	infinity		
	cleanex spinlock	90.00	3906.26	64.00	Infinity								
	ROESY pulsed (90*)	90.00	1000000	1			ROESY pulsed (90*)	90,00	100000000	63.00			
	low power presat. (cw irrad.)	90.00	10.00	25000.00	Infinity		low power presat. (cw irrad.)	90.00		25000.00			
							NOE diff. irradiation	90.00	200.00	1250.00			
		1				14		90.00			Infinity		
						1.0	bandsel. Homodecoupling	90.00	7142.86	35.00	Infinity		

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.

Edit View Help							_			_			_
		Saved Observe and	d Saved D	ecouple Pr	osol Parameter Sel	for							
DDC: 5 mm DUL 13C-1H/D Z-GRD Z	23494/345 [33] 💌										Solvent	generic	-
		Observe			Decouple								
		18	• N	lucleus	1H	*							
		generic	- A	mplifier	generic	Y							
		generic	v	SGU	generic	*							
		Observe			Decouple								
serve Comment: Default 1H observe 3	300 MHz		11	Decoup	le Comment. Def	ault 1H decouple 300	MHZ						
leg. Pulses Square Pulses Shape Pu	ilses Others						-						
reg. reises equale reises singles a	Observe					Dec	ouni						-
Filena		F[Hz] All PuW[µs] A	J-dBMI			Filename	oup	- - ∡ [*]	RFF[Hz]	All	PutMust	AL-dRWI	
elective excitation	0.00	0.00 0.5 80000.00			e excitation	Gaus1_270.1000		270.00			80000.00	Infinity	1
elect. inversion/refocussing	0.00			Construction of	2007000100000	Gaus1_180r.1000	-	180.00			80000.00		1
		0.00 0.0 00000.00	o on may	a langer	interator interocourse		1.000	100.00		0.0	00000.00	nummy	
	0.00	0.00.0.5 10000.00	Infinity	2 handse	excitation	05 1000	1	90.00	458.63	0.5	10000.00	Intinity	1
andsel. excitation	0.00	0.00 0.5 10000.00			I. excitation	Q5.1000		90.00			10000.00		1
andsel, excitation andsel, inv./refoc.	0.00	0.00 0.5 10000.00	Infinity	3 bandse	I. excitation I. inv./refoc.	Q5.1000 Q3.1000		90.00 180.00			10000.00		1
andsel, excitation andsel, inv /refoc. ff-resonance presat.		0.00 0.5 10000.00	Infinity	3 bandse	l. inv./refoc.			Longer/	330.08	0.5			
andsel. excitation andsel. inv./refoc. ff-resonance presat. ff' flip back (H2O)	0.00	0.00 0.5 10000.00	Infinity	3 bandse 4 5 90* flip		Q3.1000		180.00	330.08	0.5	10000.00	Infinity	
andsel, excitation andsel, inv /refoc. ff-resonance presat. 10° flip back (H2O) Ind 90° flip back (H2O)	0.00 0.00	0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 10000.00	Infinity Infinity Infinity	3 bandse 4 5 90* flip 6	l. inv./refoc.	Q3.1000		180.00	330.08	0.5	10000.00	Infinity	
andsel, excitation andsel, inv /refoc. ff-resonance presat. ff lip back (H2O) ff lip back (H2O) ff lip back (H2O) ff WET	0.00 0.00 0.00	0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 1000.00 0.00 0.5 1000.00 0.00 0.5 4000.00	Infinity Infinity Infinity Infinity	3 bandse 4 5 90* flip 6 7	l. inv./refoc.	Q3.1000		180.00	330.08	0.5	10000.00	Infinity	
andset, excitation andset, inv /refoc. ff-resonance presat, 0* flip back (H2O) nd 90* flip back (H2O) 0* WET 20* NH region	0.00	0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 1000.00 0.00 0.5 1000.00 0.00 0.5 4000.00 0.00 0.5 20000.00	Infinity Infinity Infinity Infinity Infinity	3 bandse 4 5 90* flip 6 7 8	l. inv./refoc.	Q3.1000		180.00	330.08	0.5	10000.00	Infinity	
vandset, excitation sandset, inv /refoc. /ff-resonance presat. 10° flip back (H2O) Ind 90° flip back (H2O) 10° WET 20° NH region 100° NH region 1	000	0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 20000.00 0.00 0.5 20000.00 0.00 0.5 20000.00 0.00 1.0 4500.00 0.00 0.5 1000.00	Infinity Infinity Infinity Infinity Infinity Infinity	3 bandse 4 5 90* flip 6 7 8	I. inv /refoc. back (H2O)	Q3.1000		180.00	330.08	0.5	10000.00	Infinity	
andset, excitation andset, inv /refoc. ff-resonance presat. 0* flip back (H2O) 0* WET 20* NH region 80* NH region 1 0* NH region 1	000	0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 1000.00 0.00 0.5 1000.00 0.00 0.5 20000.00 0.00 0.5 20000.00 0.00 1.0 4500.00 0.00 0.5 1000.00 0.00 1.0 3750.00	Infinity Infinity Infinity Infinity Infinity Infinity Infinity	3 bandse 4 5 90* flip 6 7 8 9 9 9	I. inv /refoc. back (H2O)	Q3.1000 Squa100.1000		180.00	330.08 250.00 (() () () () () () () () ()	0.5	10000.00	Infinity	
andsel, excitation andsel, inv /refoc. ff-resonance presat. ff-fresonance presat. ff-fre		0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 1000.00 0.00 0.5 1000.00 0.00 0.5 20000.00 0.00 0.5 20000.00 0.00 1.0 4500.00 0.00 0.5 1000.00 0.00 1.0 3750.00 0.00 0.0 3750.00	Infinity Infinity Infinity Infinity Infinity Infinity Infinity	3 bandse 4 5 90* flip 6 7 7 8 9 9 10 90* NH 11 90* NH	I. inv /refoc. back (H2O) region I	Q3.1000 Squa100.1000		180.00 90.00	330.08 250.00 (() () () () () () () () ()	0.5	10000.00	Infinity	
vandset, excitation vandset, inv /refoc. vandset, inv /refoc. vandset, inv /refoc. vandset, inv /refoc. vandset, inv /refor va		0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 1000.00 0.00 0.5 1000.00 0.00 0.5 20000.00 0.00 0.5 20000.00 0.00 1.0 4500.00 0.00 0.5 1000.00 0.00 1.0 3750.00 0.00 0.0 3750.00	Infinity Infinity Infinity Infinity Infinity Infinity Infinity	3 bandse 4 5 90* flip 6 7 7 8 9 9 10 90* NH 11 90* NH 12	I. inv /refoc. back (H2O) region I	Q3.1000 Squa100.1000		180.00 90.00	330.08 250.00 (() () () () () () () () ()	0.5	10000.00	Infinity	
sandset. excitation sandset. inv./refoc. infi-resonance presat. infi		0.00 0.5 10000.00 0.00 0.5 10000.00 0.00 0.5 1000.00 0.00 0.5 1000.00 0.00 0.5 1000.00 0.00 0.5 2000.00 0.00 0.5 2000.00 0.00 1.0 4500.00 0.00 0.5 1000.00 0.00 1.0 3750.00 0.00 0.5 3000.00 0.00 0.5 3000.00	Infinity Infinity Infinity Infinity Infinity Infinity Infinity Infinity	3 bandse 4 5 5 90* flip 6 7 7 8 9 9 10 90* NH 11 90* NH 12 13	I. inv /refoc. back (H2O) region I	Q3.1000 Squa100.1000		180.00 90.00	330.08 250.00 (() () () () () () () () ()	0.5	10000.00	Infinity	

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)

Edprosol Manual
Setprosol Manual
Getprosol Manual
About Prosol

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 ¹³C on the inner and/or outer coil. If corresponding preamplifiers are available for 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.

🖉 edprosol												
File Edit View Help												
			Saved Obse	rve and Save	d Dec	ouple Prosol Parar	neter Set for					
Probe: 5 mm CNP 18/13C/31P/19F Z-g	rad 22245/012	4 [07] 👻									Solvent generic	• •
	🗹 obs	NUC1										
	dec 🖉	1H 💌	SGU1	< =	K 300	w	1H L	_	show RF rou	ting		
	obs	NUC2		1	H 100	w	XBB19		า			
	dec	off 🛩	SGU2			_ /	XBB19F	2HS	5			
					(500	w /	21	i.				
	🗌 obs	NUC3				_ /	19	F				
	dec 🗌	off 👻	SGU3		K 500	w /	1					
	obs	NUC4			H 100	\sim						
	dec	off 🛩	SGU4			/						
		harring and the second s			(300	w /						
	🗌 obs	NUC5										
	dec	off 🖌	SGU5									
	🗌 obs	NUC6										
	🗌 dec	off 👻	SGU6			_ /						
				2	H 150							
				Default	10	nfo Param						
Observe Comment: Default 1H obs 600						Decouple Com	ment Defa	111	dec			-
•					_	j becoupie com	Incin. [Deite		460			
90 deg. Pulses Square Pulses Shape Pulses	Others											
			Observe				Decouple	200				
			Pulse Width[µs]	Power[W]		Pulse Width[µs]	Power[W]					
		1H	0.00	0.0000		6.00	100.00		1H			
		off	0.00		-	0.00	0.0000		TIO			
		off	0.00	1		0.00	0.0000		off			
		off	0.00		-	0.00	0.0000	1000	off			
		off	0.00	0.0000		0.00	0.0000		off			
		off			1	-		1	off			
		Bluesterie				Pulse Width[µs]	DamarDid	Cat	Alusiana			

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 **ed-prosol** window. So the nucleus is chosen for all tables.

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

edprosol											
File Edit View Help											
Probe: 5 mm CNP 18/13c/31P/19F 2-grad 22245/0124 [07]	Saved Obser	ve and Saved	d Deco	ouple Prosol Parar	meter Set for				Solvent gen	eric 💌	
- · · · · · · · · · · · · · · · · · · ·	Observ	e		D	ecouple						
	13C	~	Nucl	leus 1H		Y					
	generic		Ampi	difier generic	-	3					
	generic	-	so	GU generic	c						
	Observ	e		D	ecouple						
Observe Comment: Default 13C obs				Decouple Comm	ent: Defau	t 1H d	ec				
			_			_					
90 deg. Pulses Square Pulses Shape Pulses Others											
	Observe				Decouple						
Nucleus	Pulse Width[µs]	100000000000	and.	Pulse Width[µs]	Power[W]	11144	Nucleus				
1H	0.00	0.0000	0	6.00	100.00	0	1H				
2H	0.00	0.0000	0	0.00	0.0000	0	2H				
13C	0.00	0.0000	0	0.00	0.0000	0	13C				
19F	0.00	0.0000	0	0.00	0.0000	0	19F				
31P	0.00	0.0000	0	0.00	0.0000	0	31P				
Nucleus	Pulse Width[µs]			Pulse Width[µs]	Power[W]		Nucleus				
							Last Save	Print	Copy to Solvent	Copy to Probe	Save

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:

🝓 Edprosol	Calculation	Dialog	×
At least on	e pulse of	the set is not ca	Iculated!
• Calcula	te all pulse	es of the set!	
C Recalcu	late only (calculated pulses	il.
	ОК	Cancel	

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.

Probe: 5 mm DUL 13C-	1H/D Z-GRD 23494/345 []		Saved	Observe a	nd Saved D	ecoupl	e Prosol Parameter Set for:						
Probe: 5 mm bob 130-	18/D 2-GKD 23494/345 [.	13] 💌		Observe			Decouple					Solvent generic	
			130	Ouser ve	* N	icleus	18	a					
			genera		=	nplifier		-					
			-		=			-					
			generi	Observe		SGU	generic Decouple						
				0030140			Decoupie						
Observe Comment: Defa	ult 13C observe 600 MHz					De	ouple Comment Default	1H decou	ple 600 MH	tz			-
	1 1 1					100042							
0 deg. Pulses Square Pul	ses Shape Pulses Others		1.50						2.0				-
		Obse ∡ [*]	RFF[Hz]	DutAfree1	Pw[W]	#		Decoup	RFF[Hz]	DutAffred)	Pw[W]		
	Billion C					_	-						
	cpd TOCSY spinlock	90.00	4166.67	60.00 25.00	0.0000	-	CSY spinlock	90.00	3571.43 8928.57	and the state of t	0.0000		
	ROESY spinlock		2032.52	123.00		_	DESY spinlock (cw)	90.00		1	0.0000		
	presat. (cw irradiation)	90.00	2032.52	123.00	0.0000	-	esat. (cw irradiation)	90.00	50.00		0.0000		
	preser (en inseision)						id cpd (power gated)	90.00	2500 00		0.0000		
	17					_	w power cpd	90.00	1773.05		0.0000		
						1	ev cpd (cw part)	90.00	7142.86		0.0000		
	hetero TOCSY	90.00	8333.33	30.00	0.0000	-	tero TOCSY	90.00	3333.33		0.0000		
					100001000	8 1	DCSY (higher selectivity)	90.00	4464.29	56.00	0.0000		
						9 10	tero TOCSY (higher sel.)	90.00	1000.00	250.00	0.0000		
		-	1	i		10							
						11 R	DESY pulsed (90°)	90.00	5952.38	42.00	0.0000		
				2				90.00	10.00	25000.00	0.0000		
						12 10	w power presat. (cw irrad.)	20.00					
							w power presat. (cw irrad.) DE diff irradiation	90.00	200.00	1250.00	0.0000		
						13 N			200.00	and the state of the	0.0000		
						13 N	DE diff. irradiation	90.00		and the state of the			

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 description 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.

			Saved	Observe an	d Saved De	cou	ple Prosol Parameter Set for:							-
Probe: 5 mm DUL	13C-1H/D 2-GRD 23494/345	[33] 🔻	c	Observe			Decouple					Solvent: g	eneric	
			13C		▼ Nu	icleu	IS 18 💌							
			generi		=	plifi								
			generi		=	SGU								
			1.	bserve	<u> </u>	300	Decouple							
bserve Comment	Default 13C observe 600 MHz					C	ecouple Comment: Default 1	H decoup	le 600 MHz	62				
dea Pulses Squar	e Puises Shape Puises Others					-								
	1	Obser	ve			-	la la	Decouple						
		≭ [°]	RFF[Hz]	PuW[µs]	A[-dBW]	#		x [°]	RFF[Hz]	PuW[µs]	A[-dBW]			
	cpd	90.00	4166.67	60.00	Infinity	0	cpd	90.00	3571.43	70.00	Infinity			
	TOCSY spinlock	90.00	10000.00	25.00	Infinity	1	TOCSY spinlock	90.00	8928.57	28.00	Infinity			
	ROESY spinlock	90.00	2032.52	123.00	Infinity	2	ROESY spinlock (cw)	90.00	2000.00	125.00	Infinity			
	presat. (cw irradiation)					3	presat. (cw irradiation)	90.00	50.00	5000.00	Infinity			
						4	2nd cpd (power gated)	90.00	2500.00	100.00	Infinity			
						5	low power cpd	90.00	1773.05	141.00	Infinity			
						6	bilev cpd (cw part)	90 00	7142.86	35.00	Infinity			
	hetero TOCSY	90.00	8333.33	30.00	Infinity	7	netero TOCSY	90.00	3333.33	75.00	Infinity			
						1.1	TOCSY (higher selectivity)	90 00	4464 29	56.00	Infinity			
						9	hetero TOCSY (higher sel.)	90.00	1000.00	250.00	Infinity			
						10					<u> </u>			
							ROESY pulsed (90*)	90.00	5952.38	42.00	Infinity			
						100	low power presat. (cw irrad.)	90.00		25000 00	Infinity			
							NOE diff irradiation	90.00	200.00		Infinity			
							homodecoupling	90.00	1000.00	250.00	Infinity			
							bandsel. Homodecoupling	90.00	7142.86	35.00	Infinity			
						16								

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 individual 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.

				S	aved	Observe a	nd Saved I	Deco	uple Prosol Parameter Set for								
e: 5 mm DUL 13C-1H/D Z-0	GRD 23494/345	[3	3] 🔻												Solver	nt generic	-
						Observe			Decouple								
				13	c		-	Nucle	eus IH	-							
				ge	neri	c	5,	Ampi	fler generic	-							
				ae	neri	ie.	*	SG	U generic P	-							
				14-		Observe	_	~~	Decouple	-							
erve Comment: Default 13C ob	oserve 600 MHz							18	Decouple Comment Defaul	t 1H decouple 600 MH	łz			_			
eg. Pulses Square Pulses Sha	ne Pulses Other	-						_			-			-			
eg. Puises oquare Puises ona	pe ruises Others	Obse	0.010		_			-		Dec		ola		_			_
	Filename	003	¥["]	RFF(Hz)	Ali	PuW[µs]	Pw[W]			Filename	ou	¥ ["]	RFF[Hz]	Ali	PuW[µs]	Pw[W]	
selective excitation	Q5.1000	- J.	90.00	114.66	1.0	40000.00	0.000	0 0	selective excitation	Gaus1_270.1000]	270.00	22.78	0.5	80000.00	0.0000	
select. inversion/refocussing	Q3.1000	-	180.00	82.52	0.5	40000.00	0.000	0 1	select. inversion/refocussing	Gaus1_180r.1000	J	180.00	15.19	0.5	80000.00	0.0000	
bandsel, excitation	Q5.1000		90.00	1528.77	1.0	3000.00	0.000	0 2	bandsel, excitation	Q5.1000	J	90.00	458.63	0.5	10000.00	0.0000	
bandset. inv./refoc.	Q3.1000		180.00	1100.26	0.5	3000.00	0.000	0 3	bandsel, inv./refoc.	Q3.1000	_	180.00	330.08	0.5	10000.00	0.0000	
adiabatic inversion	Crp60.0.5,20.1		180.00	9772.05	0.5	500.00	0.000	0 4]						
adiabatic refocussing	Crp60comp.4		180.00	9772.05	0.5	2000.00	0.000	0 5	90° flip back (H2O)	Squa100.1000	J	90.00	250.00	0.5	1000.00	0.0000	
CalvCO 90°	Q5.1000		90.00	14332.25	1.0	320.00	0.000	0 6	8		J		3				
Call/CO 90° timerev.	Q5tr.1000		90.00	14332.25	0.0	320.00	0.000	0 7]						
Call/CO 180*	Q3.1000		180.00	12893.62	0.5	256.00	0.000	0 8			J						
Calpha sel. 90*	Q5.1000		90.00	3057.55	1.0	1500.00	0.000	0 9]						
Calpha sel. 90° timerev.	Q5tr.1000		90.00	3057.55	0.0	1500.00	0.000	0 10	90° NH region I	Q5.1000	J	90.00	1834.53	0.5	2500.00	0.0000	
Calpha sel. 180°	Q3.1000		180.00	3300.77	0.5	1000.00	0.000	0 11	90° NH region I timerev.	Q5tr 1000	J	90.00	1834.53	0.5	2500.00	0.0000	
								12			J						
								18			J						
180° short broadband	Bip720,100,10.1		180.00	12500.00	0.5	160.00	0.000	0 14		6	J		3				
180° medium selectivity	Q3.1000		180.00	4715.38	0.5	700.00	0.000	0 18			J			Γ			
180° high selectivity	Q3.1000		180.00	1650.38	0.5	2000.00	0.000	0 16			J	5	-	Г			
	Q5.1000		90.00	1239.55		3700.00	0.000		10 m		- 1		2	_			

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:

1	e <mark>excita</mark> ti	UII	
e Gaus1_	270.100	0	
	ne Gaus1 s] 0.0		ne Gaus1_270.1000

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 beneagth 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.

File Options Help			Source = C:\Bruker\TopS	Spin3.0.b.20\exp\stan\nmr\lists\wave
Search in names [*?]	Search			
Bip720,100,10.1	Bip720,50,20.1	Crp20,1,40.1	Crp32,1.5,20.2	Crp42,1.5,20.2
Crp48,1.5,20.2	Crp60 xfilt.2	Crp60,0.5,20.1	Crp60,20,20.10	Crp60comp.4
Crp80,0.5,20.1	Crp80comp.4	Eburp2.1000	Eburp2tr.1000	G3.256
G4.256	G4tr.256	Gaus1_180i.1000	Gaus1_180r.1000	Gaus1_270.1000
Gaus1 90.1000	Gaus1.1000	Mpf7	Pc9 4 120.1000	Pc9 4 90.1000
Q3 ma c68c1.1	Q3.1000	Q3Ca CaCO.1000	Q5.1000	Q5tr.1000
Reburp.1000	Rsnob.1000	Seduce.100	Sinc1.1000	Squa100.1000
Squaramp,20.1	Tanhtan, 300, 50. 250	Update.info		

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.

	Sa	aved Observe a	and Saved	Decouple Pr	osol Paramete	r Set for:			
robe: 5 mm DUL 13C-1H/D Z-GRD	Z3494/345	[33] 🔻						Solvent:	generic 💌
		Observe			Deco	iple			
	13C	2	•	Nucleus	1H	•			
	gen	neric	-	Amplifier	generic	-			
	gen	neric	-	SGU	generic	-			
bserve Comment: Default 13C observ	ve 600 MHz	Observe		Decou	Decou ole Comment:		decouple 600 MHz	:]
oserve Comment: Default 13C observ deg. Pulses Square Pulses Shape P				Decou			decouple 600 MHz	<u>!</u>	
	Pulses Others	's aved		Decou	ole Comment:	Default 1H		!	
	Pulses Others Sa Prosol P	s		Decou	ole Comment:	Default 1H official Saved	ations	:	
deg. Pulses Square Pulses Shape P	Pulses Others Sa Prosol P Depen	's aved		Decou	ole Comment:	Default 1H	ations	:	
deg. Pulses Square Pulses Shape P	Pulses Others Sa Prosol P Depen	s	s. Unit	Decou	ole Comment:	Saved Gradient Dur Depending	ations	Unit	
' deg. Pulses Square Pulses Shape P	Pulses Others Sa Prosol P Depen Probe and Ob Name	rs aved Parameters nding on bserve Nucleus			ole Comment:	Saved Saved Gradient Dur Depending Probe on Name	ations on y.		
deg. Pulses Square Pulses Shape P	Pulses Others Sa Prosol P Depen Probe and Ot Name DE	s aved arameters nding on bserve Nucleus Value	Unit	gra	ole Comment:	Saved Saved Gradient Dur Depending Probe on Name	ations on y. Value	Unit	
' deg. Pulses Square Pulses Shape P I pre-scan delay	Pulses Others Sa Prosol Pr Depen Probe and Ob Name DE P_mlev	s aved 'arameters ding on bserve Nucleus Value 6.500000	Unit µsec	gra	ole Comment:	Saved Saved Gradient Dur Depending Probe on Name ay D_grad	ations on y. Value 0.000200	Unit sec	

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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