Preparation for 2D

- 1. Run and process a normal ¹H experiment running any 2D experiment.
- 2. Expand the region of interest in the ¹H NMR spectrum. Then click 4
- 3. The window pictured below will open. Write down the values for "SW" and
 - "O1".

			Search] 🗆 Match Ca
SW	=	5.8947 ppm		
SWH	=	2948.113 Hz		
01	=	1658.40 Hz		
SF01	=	500.1316744 M	Hz	

- 4. After referencing the 1H spectrum, type "<u>sr</u>" and note down the value.
- 5. Type "ro off" to stop sample spinning.
- 6. Type "**topshim gui**" to open the TOPSHIM menu. From the "Before" drop-down list, choose "Z-X-Y-XZ-YZ-Z". Click "Start" to start TOPSHIM.

<u>1H-1H COSY</u>

Set-Up:

1. Type "new" on the TOPSPIN command line to create a new data set.

NAME	Ethylbenzene			
EXPNO	1			
PROCNO	1			
DIR	C:\Documents and S	Settings\Advi	sonDesktop	
USER	yourname			
Solvent			CDCI3	~
Experiment TITLE		co	SY	~
COSY at 500	MHz for Ethylbenzene			-

2. Type "<u>sw</u>" and enter the value that you had noted down from the ¹H NMR spectrum into both F1 and F2 dimension

Construction (CC		
Spectral width (F2	(,+1)	
SW [ppm] =	9.2500	9.2500

3. Type "**o1**" and enter the value that you had noted down from the ¹H NMR spectrum.

Of the	Ency Unset (12,11)	0110	0.65	
01 [HZ] =	2119.55	2119.3	55	
		OK	Cancel	

- 4. Set the required number of scans by typing "ns"
- 5. You can check the time required for finishing the experiment by typing "expt".
- 6. Type "**rga**" to set receiver gain.
- 7. Type "**zg**" to start the acquisition.

1. Type "**sr**" and enter the value noted down from the 1H spectrum.

	100000	
Spectrum reference freque	incy (F2, F1)	
SR [Hz] =	0.00	ļ

- 2. Type " \underline{xfb} " Fourier Transform in both the dimensions.
- 3. Type "<u>abs2</u>" automatic baseline correction in the f2 dimension.
- 4. Type "<u>abs1</u>" for automatic baseline correction in the f1 dimension.
- 5. Type "<u>sym</u>" makes the 2D spectrum symmetric.

<u>1H-13C HMBC</u>

<u>Set-Up:</u>

8. Type "new" on the TOPSPIN command line to create a new data set.

NAME	Ethylbenzene		
EXPNO	1		
PROCNO	1		
DIR	C:\Documents and S	Settings\Advisor\E)esktop
USER	yourname		
Solvent		CD	CI3 🗸
Experiment TITLE		COSY	~
COSY at 500	MHz for Ethylbenzene		^

9. Type "<u>sw</u>" and enter the value that you had noted down from the ¹H NMR spectrum into the F2 dimension only.

😋 sw			×
Spectral width (F2	(,F1)		
SW (ppm) =	9.2500	9.250	00
		OK	Cancel

10. Type "**o1**" and enter the value that you had noted down from the ¹H NMR spectrum.

Transmitter frequ	ency offset (F2, F1)	<u> </u>	
O1 [Hz] =	2119.55	2119.	55
		OK	Cancel

- 11. Set the required number of scans by typing "ns"
- 12. You can check the time required for finishing the experiment by typing "expt".
- 13. Type "**rga**" to set receiver gain.
- 14. Type "**zg**" to start the acquisition.

2. Type "**sr**" and enter the value noted down from the 1H spectrum for the F2 dimension only.

			🔄 SR
	1)	ce frequency (F2, F	Spectrum referen
	0.00	0.00	SR [Hz] =
	0.00	000	SR [Hz] =

- 2. Type "<u>**xfb**</u>" Fourier Transform in both the dimensions.
- 3. Type "<u>abs2</u>" automatic baseline correction in the f2 dimension.
- 4. Type "<u>abs1</u>" for automatic baseline correction in the f1 dimension.