Basic 2D NMR Instructions

An efficient way to collect 1D and 2D experiments for a given substance would be to first complete the 1-D experiments, then you can set up the 2D experiments and use 'multizg' to run them all sequentially.

It is generally recommended that all 2D experiments be run without sample spinning. Just don't forget to turn the spinner back on after you're done (for the next person)!

You can set up multiple experiments to run back-to-back by using the 'multizg' command (see last page).

^{1}H - ^{1}H COrrelation SpectroscopY (COSY):

ACQUISITION

"**new file**"	Create a new file
name	Use same name as for your 1D experiment(s), just increment EXPNO
expno	increment sequentially (2, 3...)
procno	1
experiment	COSYGPSW
getprosol	This MUST be selected
dir	C:\data\CHM411
title	Make sure your title indicates what kind of experiment you are running

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"ro off"	If you haven't yet done it, turn the spinner off
"atma"	If you have already tuned ^{1}H and ^{1}C, then you don't need to re-do this
"**rga**"	Determine gain (dependent on experiment and sample concentration)
"**ns**"	Number of scans = 1 x n (recommend 1 scan. Executes 128 experiments for 5 - 8 minute acquisition time)
Select Aquire tab then SetLimits	This will ask you to open the ^{1}H experiment and select the region of your spectrum that contains ^{1}H data, making sure to leave about 0.2 ppm of baseline on either side of the spectrum
"**zg**"	Begin acquisition

PROCESSING

Select 'Process' tab, then select the down-arrow that is inside the 'Proc. Spectrum' button. Select 'Configure Standard Processing' by clicking on it. Disable Auto-Phasing (apk2d), then select 'Execute'.

Use mouse wheel to adjust contour levels

"plot"	Open and apply 'Turk Homonuclear' layout within the 'Turk Layouts' folder

Use mouse wheel to adjust projections and contours

If zooming, select spectrum, then right click and choose 'Expand Tool'. Then click and drag a SQUARE box.

Select the print icon when you are ready to print.

^{1}H - ^{1}H Nuclear Overhauser Effect SpectroscopY (NOESY)

ACQUISITION

"**new file**"	Create a new file
name	Use same name as for your 1D experiment(s), just increment EXPNO
expno	increment sequentially (2, 3...)
procno	1
experiment	NOESYPHSW
getprosol	This MUST be selected
dir	C:\data\CHM411
title	Make sure your title indicates what kind of experiment you are running
"ro off"	If you haven't yet done it, turn the spinner off
"atma"	If you have already tuned ^{1}H and ^{1}C, then you don't need to re-do this
"**rga**"	Determine gain (dependent on experiment and sample concentration)
"d8"	Adjust mixing time to 0.5 sec
"**ns**"	Number of scans = 4 x n (recommend 4 scan. Executes 128 experiments for ~ 50 minute acquisition time)
Select Aquire tab then SetLimits	This will ask you to open the ^{1}H experiment and select the region of your spectrum that contains ^{1}H data, making sure to leave about 0.2 ppm of baseline on either side of the spectrum
"**zg**"	Begin acquisition

PROCESSING

Select 'Process' tab, then select the down-arrow that is inside the 'Proc. Spectrum' button. Select 'Configure Standard Processing' by clicking on it. Make sure that Auto-Phasing (apk2d) is ENABLED - then 'Execute'.

Use mouse wheel to adjust contour levels

"plot" Open and apply 'Turk Homonuclear' layout within the 'Turk Layouts' folder

Use mouse wheel to adjust projections and contours

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Select the print icon when you are ready to print.

^{1}H - ^{13}C Heteronuclear Single Quantum Correlation spectroscopy (HSQC)

ACQUISITION

"**new file**"	Create a new file
name	Use same name as for your 1D experiment(s), just increment EXPNO
expno	increment sequentially (2, 3...)
procno	1
experiment	HSQCEDETGP
getprosol	This MUST be selected
dir	C:\data\CHM411
title	Make sure your title indicates what kind of experiment you are running
"ro off"	If you haven't yet done it, turn the spinner off
"atma"	If you have already tuned ^{1}H and ^{1}C, then you don't need to re-do this
"**rga**"	Determine gain (dependent on experiment and sample concentration)
"**ns**"	Number of scans = 1 x n (recommend 2 scan. Executes 128 experiments for 14 - 18 minute acquisition time)
Select Aquire tab then SetLimits	This will ask you to open the ^{1}H experiment and select the region of your spectrum that contains ^{1}H data, making sure to leave about 0.2 ppm of baseline on either side of the spectrum
Select Aquire tab then SetLimits	This will ask you to open the ^{13}C experiment and select the region of your spectrum that contains ^{13}C data, making sure to leave about 0.2 ppm of baseline on either side of the spectrum.
"**zg**"	Begin acquisition

PROCESSING

Select 'Process' tab, then select the down-arrow that is inside the 'Proc. Spectrum' button. Select 'Configure Standard Processing' by clicking on it. Make sure that Auto-Phasing (apk2d) is ENABLED - then 'Execute'.

Use mouse wheel to adjust contour levels

"plot" Open and apply 'Turk Homonuclear' layout within the 'Turk Layouts' folder

Use mouse wheel to adjust projections and contours

If zooming, select spectrum, then right click and choose 'Expand Tool'. Then click and drag a SQUARE box.

Select the print icon when you are ready to print.

^{1}H - ^{13}C Heteronuclear Multiple Bond Correlation spectroscopy (HMBC)

ACQUISITION

"**new file**"	Create a new file
name	Use same name as for your 1D experiment(s), just increment EXPNO
expno	increment sequentially (2, 3...)
procno	1
experiment	HMBCGP
getprosol	This MUST be selected
dir	C:\data\CHM411
title	Make sure your title indicates what kind of experiment you are running
"ro off"	If you haven't yet done it, turn the spinner off
"atma"	If you have already tuned ^{1}H and ^{1}C, then you don't need to re-do this
"**rga**"	Determine gain (dependent on experiment and sample concentration)
"**ns**"	Number of scans = 4 x n (recommend 4 scan. Executes 128 experiments for 14 - 18 minute acquisition time)
Select Aquire tab then SetLimits	This will ask you to open the ^{1}H experiment and select the region of your spectrum that contains ^{1}H data, making sure to leave about 0.2 ppm of baseline on either side of the spectrum
Select Aquire tab then SetLimits	This will ask you to open the ^{13}C experiment and select the region of your spectrum that contains ^{13}C data, making sure to leave about 0.2 ppm of baseline on either side of the spectrum.
"**zg**"	Begin acquisition

PROCESSING

Select 'Process' tab, then select the down-arrow that is inside the 'Proc. Spectrum' button. Select 'Configure Standard Processing' by clicking on it. Disable Auto-Phasing (apk2d), then select 'Execute'.

Use mouse wheel to adjust contour levels

"plot"	Open and apply 'Turk Homonuclear' layout within the 'Turk Layouts' folder

Use mouse wheel to adjust projections and contours

If zooming, select spectrum, then right click and choose 'Expand Tool'. Then click and drag a SQUARE box.

Select the print icon when you are ready to print.