Acquiring and processing a ^{1}H NMR spectrum on the Bruker ARX-300

Things in **bold** should be typed on the command line
Things underlined are buttons on the left-hand side panel of XwinNMR.
Things *italicized* are buttons on the BSMS keyboard.

1.	Insert sample	If the lock is turned on (LED lit or blinking) , press *Lock On/Off* to turn lock off
		If the spinner is on (LED lit or blinking), press *Spin On/Off* to stop the spinner
		Press *Lift On/Off* to eject the standard
		Put your sample in the spinner, position it with the depth gauge, and place it in the bore
		Press *Lift On/Off* to insert your sample
		Press *Spin On/Off* to turn on the spinner
2.	Set up acquisition parameters	**edc**
		Enter a NAME for the experiment. Don't use special characters (\\$@#""^/ etc.). Use _ or – instead of white space.
		Set the EXPNO (experiment number)
		Click SAVE
		rpar 1h_std all reads standard 1H parameters
3.	Lock	If the lock display window is not open: **lockdisp**
		lopoi and select your solvent from the list
		Press *Lock On/Off* on BSMS
		Press *Lock Gain* and set it at 120 ± 5
		Press *Lock Power* and adjust value to bring the lock level to the upper third of the lock display window
4.	Shim	Press *Lock Phase* and adjust for maximum lock response
		Press *Z* and adjust for maximum lock response
		Press *Z2* and adjust for maximum lock response
		Iterate between *Z* and *Z2* until the signal reaches maximum
		Press *Standby*
5.	Acquire FID	**rga** automatic receiver gain adjustment
		ns to change number of scans, if desired
		zg zero file and go
6.	Window function & Fourier transform	Wait for acquisition to finish
		efp apply standard window function and FT
7.	Phase	Click the |<>| button to display the whole spectrum
		Click the PHASE button to the left of the spectrum window (If you don't see a PHASE button click RETURN first)
		Click the *2 button until details of the baseline are clear
		Click BIGGEST
		Click & Hold PH0
		Drag the mouse up (or down) to adjust the phase of the tallest peak
		Click & Hold PH1

Drag the mouse up (or down) to adjust the phase of all other peaks

Click <u>RETURN</u> → Save and Return

8. Reference

Zoom in on the reference peak (Left click, middle click, middle click, left click)

Click <u>CALIBRATE</u>

Set the cursor on top of the reference peak

Middle click and enter the reference value

9. Peak Pick

Click <u>UTILITIES</u>

Click <u>MI</u> and click <u>OK</u> if you get a pop-up window

Move the mouse up or down to position the blue line. Anything below the line will not be peak picked

Click <u>RETURN</u>

10. Baseline correct

abs   Don't use abs after integration!

11. Integrate

Click the <u>INTEGRATE</u> button to the left of the spectral window

Click inside the spectral display

Middle click to start an integral region

Middle click to close an integral region

Move around the spectrum using the ≤ and ≥ buttons

Zoom in and out using the <> and >< buttons

Repeat until all peaks are integrated

Click <u>RETURN</u> → Save and Return

12. Plot

Click <u>UTILITIES</u>

Click <u>CY</u> and set the blue line slightly above the tallest peak you want plotted.

Left click and enter 10 as the height of the peak.

Click <u>RETURN</u>

Click <u>DP1</u>

Enter values for upper and lower plot limits

plot

To print expansion plots:

    Zoom in on the desired region

    Adjust CY as above, if desired

    Click the <u>PLOT</u> button

13. Eject sample

Press *Lock On/Off* to turn lock off

Press *Spin On/Off* to stop the spinner

Press *Lift On/Off* to eject your sample

Put the standard in the spinner and place it in the bore of the magnet

Press *Lift On/Off* to insert the standard