Quick Guide on BRUKER NMR Systems Princeton University – Chemistry - NMR Laboratory Page 1

 Differences of each spectrometer hardware: Bruker-500, A1: cryo-¹H optimized, Excellent for 1D ¹H experiments, such as acquiring 1D ¹H NMR data; optimum for ¹H detected experiments, such as 2D's ¹H-¹³C(X): HMQC(HSQC), HMBC, etc. Bruker-500, A2: cryo-¹³C optimized, excellent for 1D ¹³C experiments. Bruker-500, A3: cryo-QNP optimized, excellent for 1D ¹H, ¹³C, ³¹P, and ¹⁵N direct detection experiments. 			
1)	Inserting the sample	 Insert the sample in the 5-mm <i>Bruker</i> spinner. Adjust the sample height with the <i>Bruker</i> gauge (prepare your sample always with 45-50 mm length, approx. 500 uL volume). Wipe clean the sample. Find an empty holder in the carousel and insert the sample (<i>BIGGER</i> numbers are OUTSIDE holders and <i>small</i> numbers are INSIDE holders). The carousel has 120 holders. 	
2)	Login using ICON-NMR interface (see right column)	At the workstation, click on the <u>Change User</u> button, and type inside the next 2 input windows: Your NMR username <enter> Your NMR password <enter> Your NMR password <enter> ICON interface will then be available for you to specify the experiment at the holder # where your sample was previous ample was pr</enter></enter></enter>	
3)	Removing sample from the carousel	 Make it sure that you <u>never</u> pick a sample up from below the arm of the autosampler (This procedure leads to various errors, some serious). To remove your sample from the carousel, use the two buttons on the front panel labeled with arrows (forward and backward). Move the carousel <u>only when the autosampler is not in action, handling another</u> 	er
		<u>sample</u> . Remove your sample from its holder, returning the <i>Bruker</i> spinner to the shelf.	<u> </u>