

Dependence of the average experiment duration of 1D and 2D NMR experiments  
on the substance concentration and the spectrometer used

<i>Experiment</i>	<i>DRX250 (QNP probe)</i>				<i>AV600 (BBO probe)</i>					
	Resolution FIDRES (Hz)	<i>molarity</i>								
		0.1 M	0.05 M	0.01 M	0.05 M	0.025 M	0.01 M	0.005M	10 <sup>-5</sup> M	
<b>1D</b>										
<sup>1</sup> H	0.13	1'	2' (16)	9' (128)	1' (16)	1' (16)	1' (16)	2' (32)		0.29
<sup>13</sup> C { <sup>1</sup> H}	0.45	9' (256)	37' (1024)	10h (16k)	6' (128)	35' (1024)	1h 9' (2048)	2h 17' (4k)		0.55
<b>DEPT</b> 135(90)	0.45	4' (96)	15' (256)	3h 36' (4k)	3' (48)	17' (400)	34' (800)	1h 7' (1600)		0.55
<i>sel.NOE</i>	0.15	10' (64)	26' (200)	3h 19' (1600)	4' (32)	18' (128)	36' (256)			0.29
<sup>31</sup> P { <sup>1</sup> H}	0.62		2' (32)							
<sup>31</sup> P	0.62		6' (128)							
<sup>19</sup> F { <sup>1</sup> H}	0.57		3' (32)							
<sup>19</sup> F	0.57		4' (128)							

- 5 to 10 minutes for shimming the field homogeneity of a homogeneous sample (after filtration) in high quality tube and 2 extra minutes for tuning and matching of the frequency of every nuclei are needed.
- The experiment duration is measured in minutes (') or hours, in brackets the recommended number of scans are shown. Data were tested for pure substances with the known concentration (molarity). These values could be recommended for 80% of the analyzed samples. The experiments can be recorded faster or slower depending on the individual characteristics of the particular molecule, solvent, etc.
- As a rule of thumb, the concentration for high-quality proton spectra should not exceed 0.05M (0.01M is recommended).

Experiment	DRX250 (QNP probe)				AV600 (BBO probe)					
		molarity								
	Resolution FIDRES (Hz)	0.1 M	0.05 M	0.01 M	0.05 M	0.025M	0.01 M	0.005M	10 <sup>-5</sup> M	Resolution FIDRES (Hz)
<b>2D</b>	F2/F1									F2/F1
<i>cosy qf</i> 2k/128	1.2/20	5' (1)	9' (2)	24' (4)	7'34" (1)	7'34" (1)	7'34" (1)	15" (2)		3.5/28
<i>noesy ph</i> 1k/256	2.5/10	28' (2)	1h (4)	4h (16)	42' (2)	1h 22' (4)	1h 22' (4)	2h 43' (8)		3.8/30
<i>tocsy ph</i> 2k/256	1.2/10	1h 27' (8)	2h 52' (16)	8h 33' (48)	1h 18' (8)	1h 18' (8)	1h 18' (8)	1h 18' (8)		3.5/28
<i>hmqc qf</i> 1k/128	3/94	16' (4)	30'/1h (8/16)	4h (64)	29' (4)	58' (8)	58' (8)	2h 58' (>32)		3.5/112
<i>hmqc ph</i> 2k/200	3/60	25' (4)	50'/100' (8/16)	6h 40' (64)	23' (4)	45' (8)	45' (8)	-		3.5/112
<i>hsqcedsi ph</i> 2k/200	3/60	12' (2)	48' (8)	3h 5' (32)	15' (2)	15' (2)	30' (4)	2h (16)		3.5/112
<i>hmhc qf</i> 2k/128	1.2/120	20' (4)	2h 44' (32)	5h 28' (64)	17'/33' (2/4)	33'/1h 4' (4/8)	2h 8' (16)	4h 38' (>48)		1.5/141

- The sample solutions for good quality NOESY spectra (or for the selective equivalents) of “small molecules” must be oxygen-free. Recommended is to bubble dry argon or nitrogen gas through it for about 10 minutes. The quantity of the dissolved substance should not exceed 30 mg. Determination of the optimum mixing time takes about 5 extra minutes.
- In HSQC-type heteronuclear correlation experiments distortion of the signal phase could be observed, which is an indication of the presence of  $^1J_{CH}$  coupling constants outside of the standard range 125-160 Hz.
- The above indicated times do not include processing of the spectra. Our recommendation is to reprocess the downloaded spectra on the local computer to ensure complete correspondence with the last acquired FID. Final calibration and phase correction should be made after that.
- The phase-sensitive versions of the experiments are marked with *ph* and magnitude spectra with *qf*.
- If sample concentration is lower than 0.005M the usage of solvents with higher deuterium enrichment and sample tubes with higher quality than Norell 507-HP is advised.