

Useful Experiments — What Do I Use to ...

Here is a list of common NMR experiments, arranged by the kind of information that they provide.

Connectivity

H-H	Selective Decoupling	1D	difference spectra useful if peak is buried
	COSY	2D	workhorse technique
	SPT / SPI	1D	
	TOCSY	1- or 2D	shows spin groups
X-H	HMQC, HSQC	2D	fast. HSQC has better X-resolution (F1)
	HETCOR	2D	slow but good resolution in X-dimension
X-X	INADEQUATE	2D	slow!! F1 is <i>not</i> J_{XX} ; instead, J_{XX} is seen in F2
	ADEQUATE	2D	less slow: INEPT/INADEQUATE hybrid, so has polarzn transfer.

Coupling Constants

H-H	Direct Observation	1D	sufficient if simple, non-overlapping peaks
	Selective Decoupling	1D	simplifies multiplets to allow extraction of J values
	J -Resolved Spectr.	2D	chem shift <i>vs</i> coupling const.
X-H	Gated Decoupling		slow but simple; interlaced (2nd order?) multiplets if peaks overlap
	^1H Satellite peaks		need good S/N; difficult to find with certainty — spinning sidebands?
	INEPT	1D	
	J -Resolved Spectr.	2D	chem shift <i>vs</i> coupling const.
X-X	INADEQUATE	1D	Slow: filters out central peak leaving sidebands. No polarzn xfr.
	ADEQUATE	1D	INEPT/INADEQUATE hybrid. Polarization transfer, so less slow.

Carbon Assignment

	APT	1D	CH_2 and quats go one way; CH and CH_3 the other
	DEPT	1D	full spectral editing possible. DEPT-135 similar to APT.

(see also “Connectivity” above)

Distance

	NOE Difference Spectra	1D	Allows quantitative NOE values
	NOESY	2D	

Kinetics/Exchange

Qualitative Evidence

	NOE Difference Spectra	1D	Has polarized proton moved to another peak?
	EXSY (NOESY)	2D	ditto

Quantitative (rates, ΔG^\ddagger , etc)

	Lineshape Analysis	1D	fitting lineshapes to calculated ones at several temps
	Coalescence Temp.	1D	single-point version of Lineshape Analysis

*Other handy techniques***Water Suppression**

	presaturation		
	WATERGATE		easy to do; excellent results
	WATR		

etc

	RIDE	1D	suppresses baseline distortion with quadrupolar nuclei
	ACOUSTIC	1D	phase-cycled version of RIDE