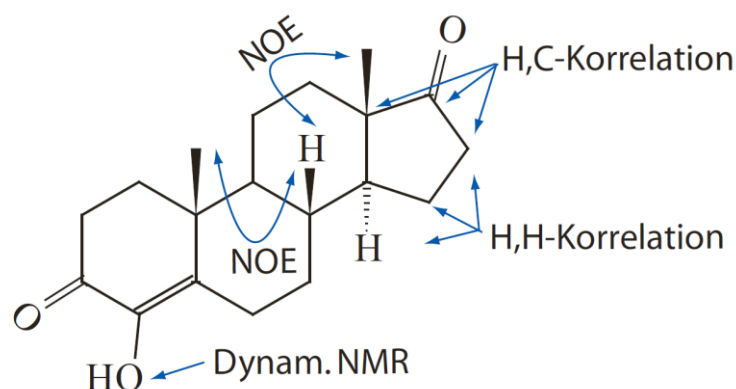


NMR puls sequences: Scope of application



General remarks:

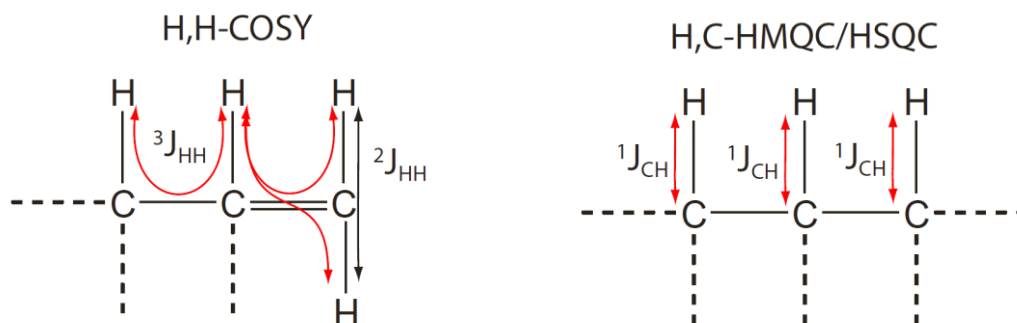
(1) If the structure is already known or **the structure is most likely as expected** it is sufficient to only run a **^1H NMR spectrum** (if molecule contains an adequate number of protons)!

(2) If additionally **isomers or configurations** need to be assigned (e.g. *E/Z* or *eq/ax*), as a first step $^3J_{\text{HH}}$ couplings should be evaluated from the 1D spectrum (if sufficiently resolved) and/or **1D NOE spectra** can be recorded (AV400 – AV600).

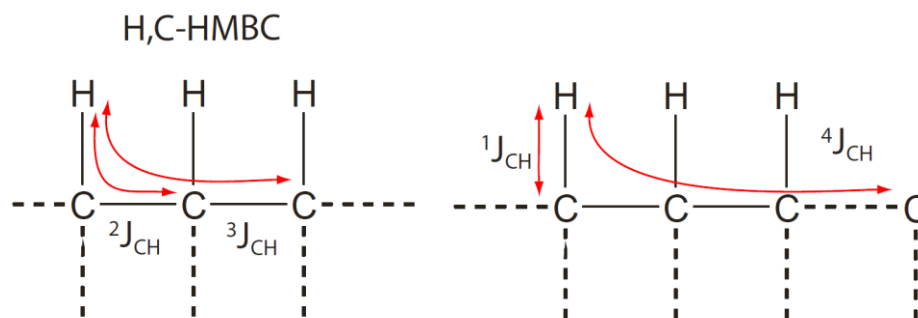
(3) For **new**, so far unknown **compounds**, a **complete characterisation** should be performed, i.e. recording ^1H NMR spectrum, H,H COSY, H,C correlations through $^1J_{\text{CH}}$ (HMQC or HSQC) and H,C correlations through $^nJ_{\text{CH}}$ (HMBC). If necessary, also an APT **or (!)** $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum can be recorded.

(4) In case of flexible compounds or molecules which participate in chemical exchange, additionally “dynamic” NMR spectra should be recorded at several temperatures (AV400 – AV600).

Informations, that different kinds of spectra contain



HMQC can be processed w/o phase correction, HSQC/HSQCed is a phase-sensitive variant



For sp^2 carbons (aromatic/olefinic molecules), mainly $^3J_{CH}$ couplings can be observed, from sp^3 carbons also $^2J_{CH}$ couplings. Extreme „long range“ coupling (4J and more) may also be present. If $^1J_{CH}$ coupling is not suppressed, it always can be recognized by its doublet splitting in the 1H dimension (distance between peaks corresponds to coupling constant, ca. 110-240 Hz).

1D sel. NOE (dpgseNOE) oder H,H-NOESY

