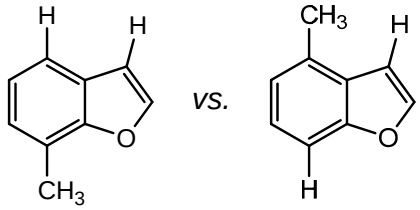
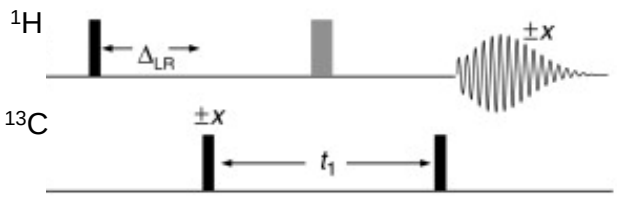
Heteronuclear Multiple-Bond Correlation (HMBC) Spectroscopy

Used to study ^{2}J and ^{3}J correlations between ^{13}C and ^{1}H, multiple bonds away.

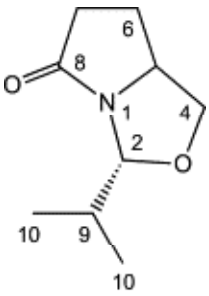
Main advantage: Can observe connectivity with/through nuclei without attached protons.



Pulse sequence incorporates long-range delay Δ_{LR} to suppress ^{1}J correlations.

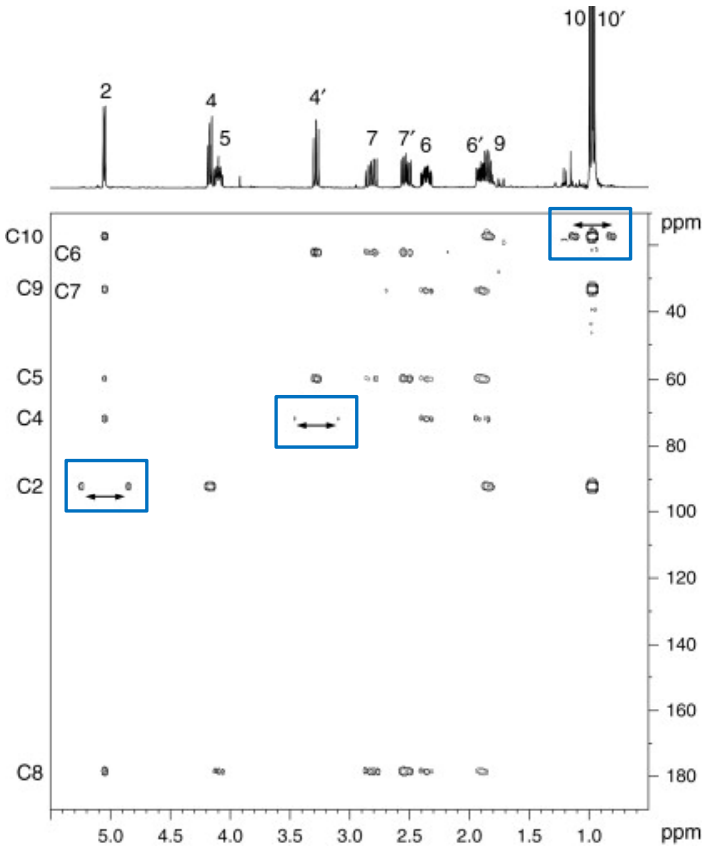


HMBC

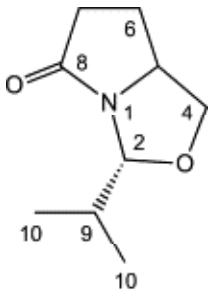


Each peak corresponds to a ^{2}J(CH) or ^{3}J(CH) correlation.

^{1}J correlations sometimes break through filter; show up as multiplet crosspeaks.



HMBC

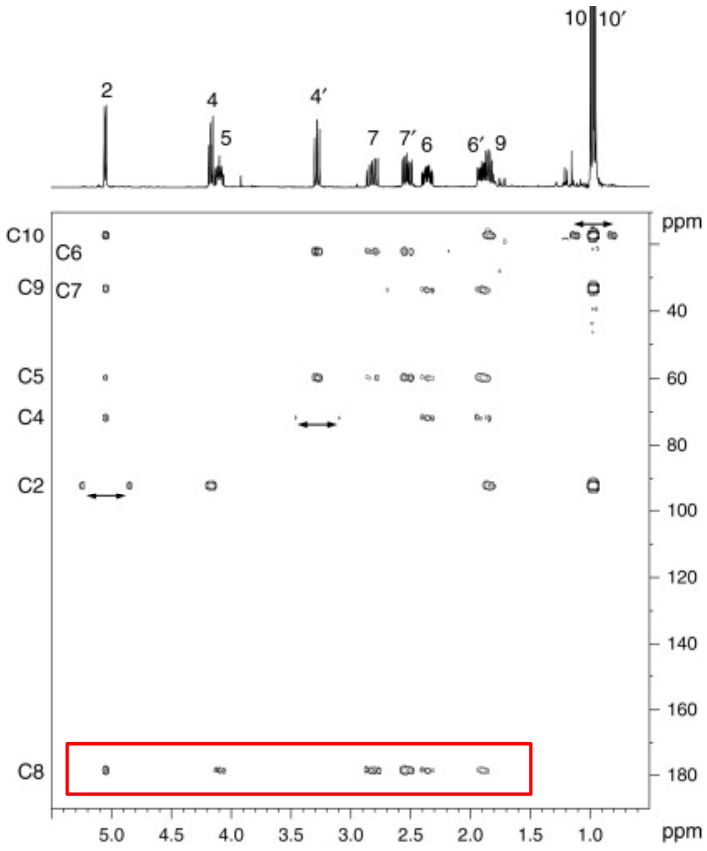


C8 exhibits:

^{2}J with H7, H7'

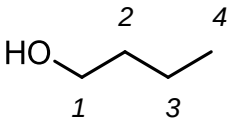
^{3}J with H2, H5, H6, H6'

So, C8 & C2 must be on the same side of the molecule.



^{13}C-^{13}C Homonuclear Correlation (INADEQUATE)

Low probability of ^{13}C-^{13}C pairs makes this correlation spectroscopy extremely insensitive. DQF method improves resolutions somewhat.



Horizontal pairs correspond to ^{1}J(CC) correlations.