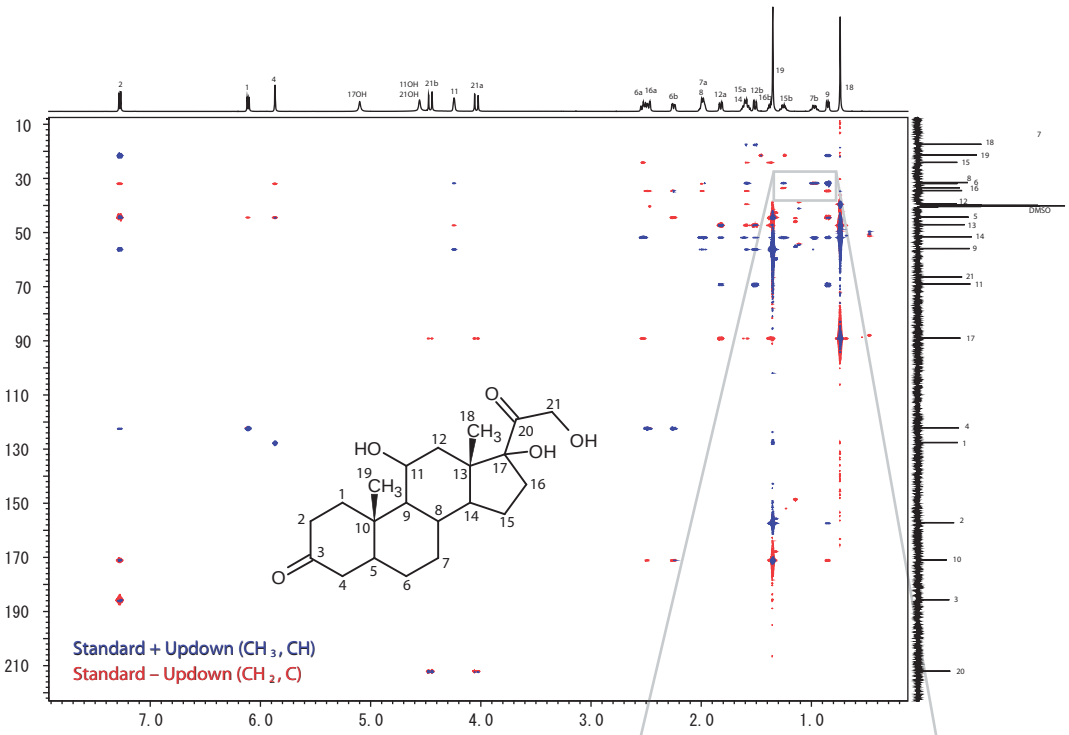
Multiplicity Edited HMBC

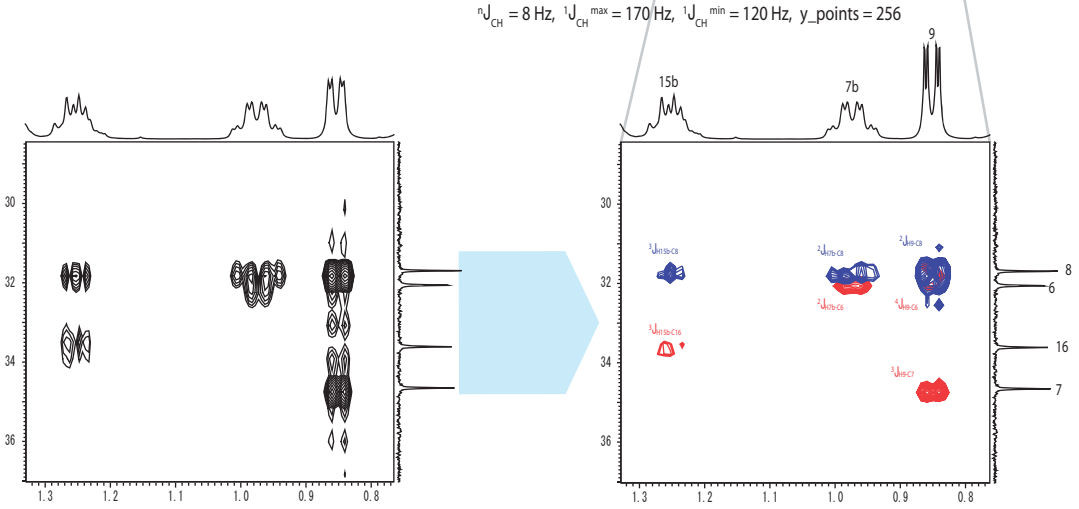
Discrimination of correlation peaks depending on attached carbon numbers

In general, overlapping of correlation peaks often makes their assignment ambiguous. Also, inverse measurements such as HMBC may suffer from lack in resolution along the indirect axis which has a wide frequency range and less sampling points. Multiplicity Edited HMBC may solve these problems: The pulse sequence inverts some correlation peaks depending on their attached carbon numbers, and so the overlapped peaks may be discriminated and assigned when their attached carbon numbers are different with each other.



Multiplicity Edited HMBC spectrum of prednisolone

$^{n}J_{CH}$ = 8 Hz, $^{1}J_{CH}^{max}$ = 170 Hz, $^{1}J_{CH}^{min}$ = 120 Hz, y_points = 256

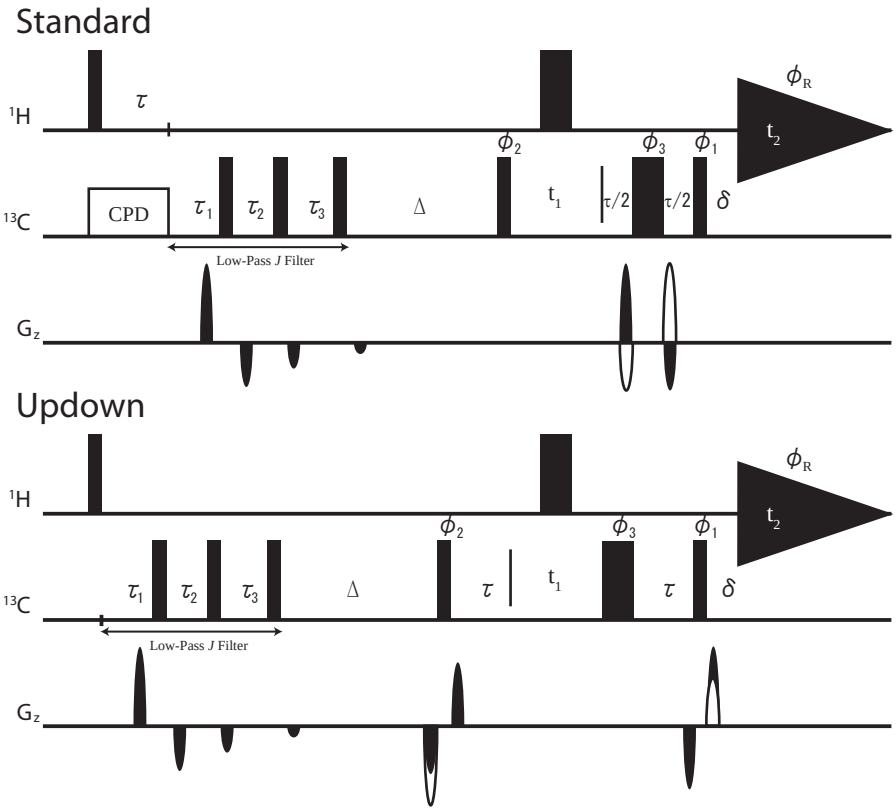


Mixed phase HMBC spectrum

$^{n}J_{CH}$ = 8 Hz, $^{1}J_{CH}^{max}$ = 170 Hz, $^{1}J_{CH}^{min}$ = 120 Hz, y_points = 256

Spectrometer: JNM-ECA600
Probe: H5XAT/FG2

JEOL RESONANCE



Pulse diagram of Multiplicity Edited HMBC measurements.

$\tau_1 = 1/2\{^1J_{CH}{}^{max} + 0.07(^1J_{CH}{}^{max} - {}^1J_{CH}{}^{min})\}^{-1}$, $\tau = \tau_2 = 1/(^1J_{CH}{}^{max} + {}^1J_{CH}{}^{min})$,
$\tau_3 = 1/2\{^1J_{CH}{}^{max} - 0.07(^1J_{CH}{}^{max} - {}^1J_{CH}{}^{min})\}^{-1}$, δ= PFG delay

Reference

N.T. Nyberg and O.W. Sørensen, Magn. Reson. Chem.44, 451 (2006)
A.J. Benie and O.W. Sørensen, Magn. Reson. Chem.44, 739 (2006)

JEOL RESONANCE