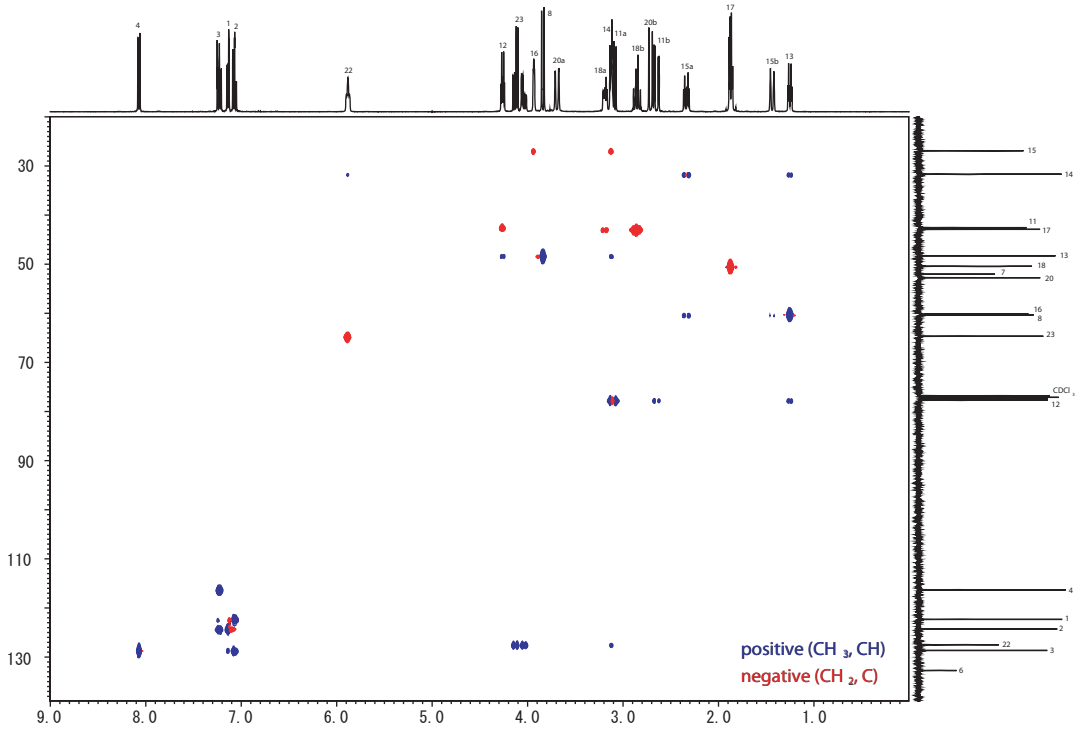
H2BC & Edited H2BC

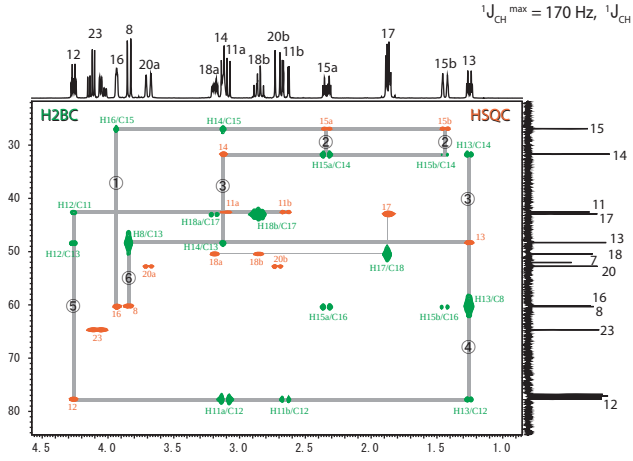
Selective observation of $^{2}J_{CH}$

Long-range correlation peaks in HMBC measurements appear depending on the magnetization transfer time $1/2^{n}J_{CH}$. However, the value of $^{n}J_{CH}$ is not determined by the bond number, and so the correlation peaks give no information on the bond number. In particular, the close values of $^{2}J_{CH}$ and $^{3}J_{CH}$ make it difficult to discriminate the corresponding correlations. H2BC (Heteronuclear 2-Bond Correlation) detects only two-bond away correlations, clarifying the assignments. Furthermore, multiplicity edited H2BC may discriminate attached carbon numbers.

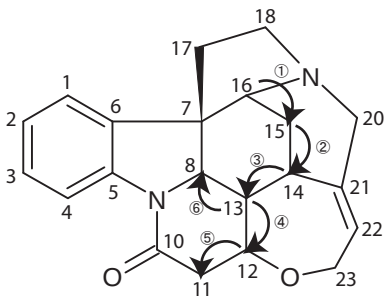


Edited H2BC spectrum of strychnine.

$^{1}J_{CH}{}^{max}$ = 170 Hz, $^{1}J_{CH}{}^{min}$ = 125 Hz, y_points = 128, T = 22 msec



H2BC and HSQC spectra of strychnine.

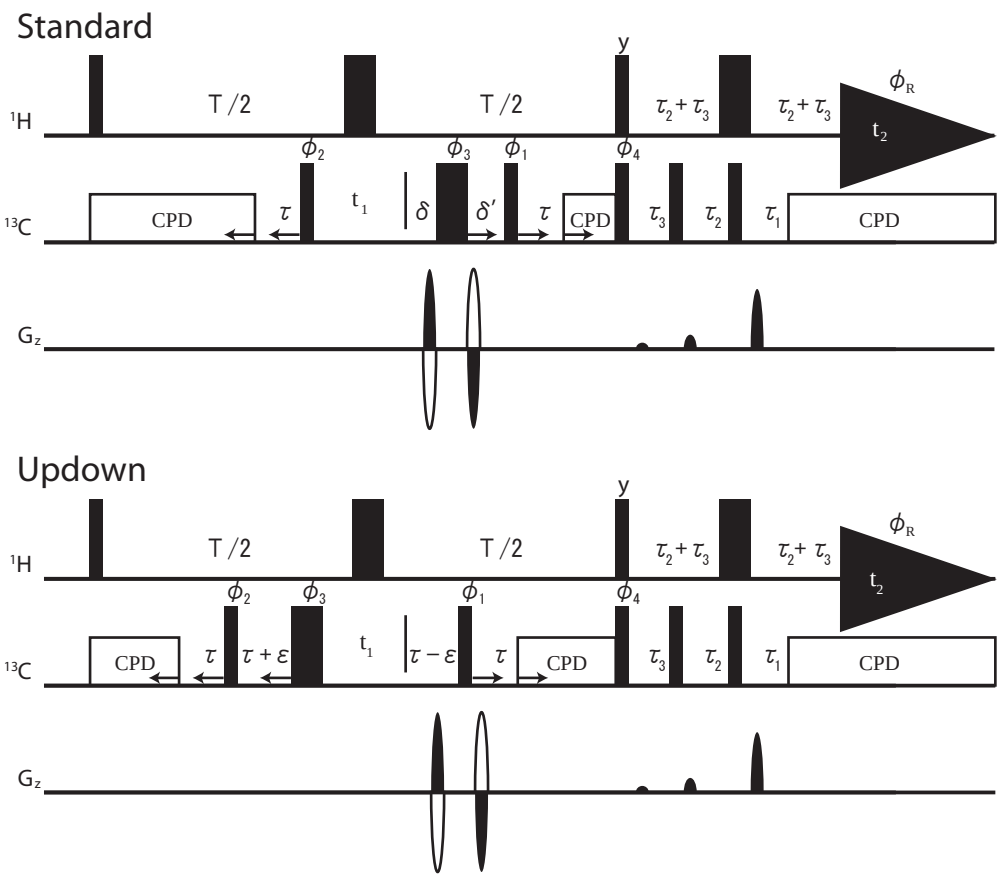


strychnine

Spectrometer: JNM-ECX400

By linking correlation peaks in H2BC and HSQC spectra, ^{13}C connectivities can be revealed. Thus, the combination of H2BC and HSQC gives a method for determining sequences of ^{13}C bonding with ^{1}H.

JEOL RESONANCE



Pulse diagram of H2BC and Edited H2BC measurements.

$\tau_1 = 1/2\{^1J_{CH}{}^{max} + 0.07(^1J_{CH}{}^{max} - {}^1J_{CH}{}^{min})\}^{-1}$, $\tau = \tau_2 = 1/(^1J_{CH}{}^{max} + {}^1J_{CH}{}^{min})$,
$\tau_3 = 1/2\{^1J_{CH}{}^{max} - 0.07(^1J_{CH}{}^{max} - {}^1J_{CH}{}^{min})\}^{-1}$, $\varepsilon = t(\pi^H)$,
δ= PFG delay, $\delta' = \delta + t(\pi^H)$, 14 < T < 22 msec

Reference
N.T. Nyberg, J.Ø. Duus and O.W. Sørensen, J. Am. Chem. Soc. 127, 6154 (2005)
N.T. Nyberg, J.Ø. Duus and O.W. Sørensen, Magn. Reson. Chem. 43, 971 (2005)