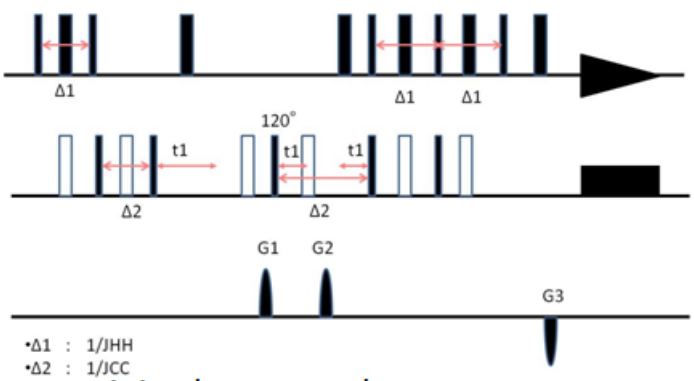
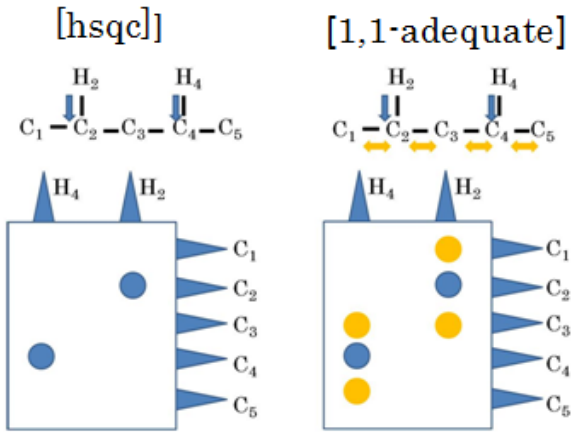
Applications of 1,1-adequate

NM160002E

1,1-adequate is a technique to obtain heteronuclear correlation similarly to hmbc. While correlation signals from hmbc do not separate $^{2}J_{CH}$ from $^{3}J_{CH}$, 1,1-adequate, which exclusively observes $^{1}J_{CH}$ amd $^{2}J_{CH}$, can be combined with hsqc to identify $^{2}J_{CH}$. 1,1-adequate uses $^{1}J_{CH}$ and $^{1}J_{CC}$ coupling for signal observation. This technique is effective for compounds rich in quaternary carbon and for aromatic ring identification.



1,1-adequate pulse sequence

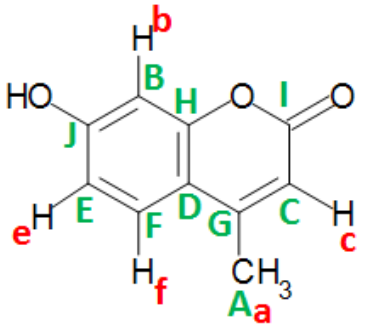


1,1-adequate signal emergence

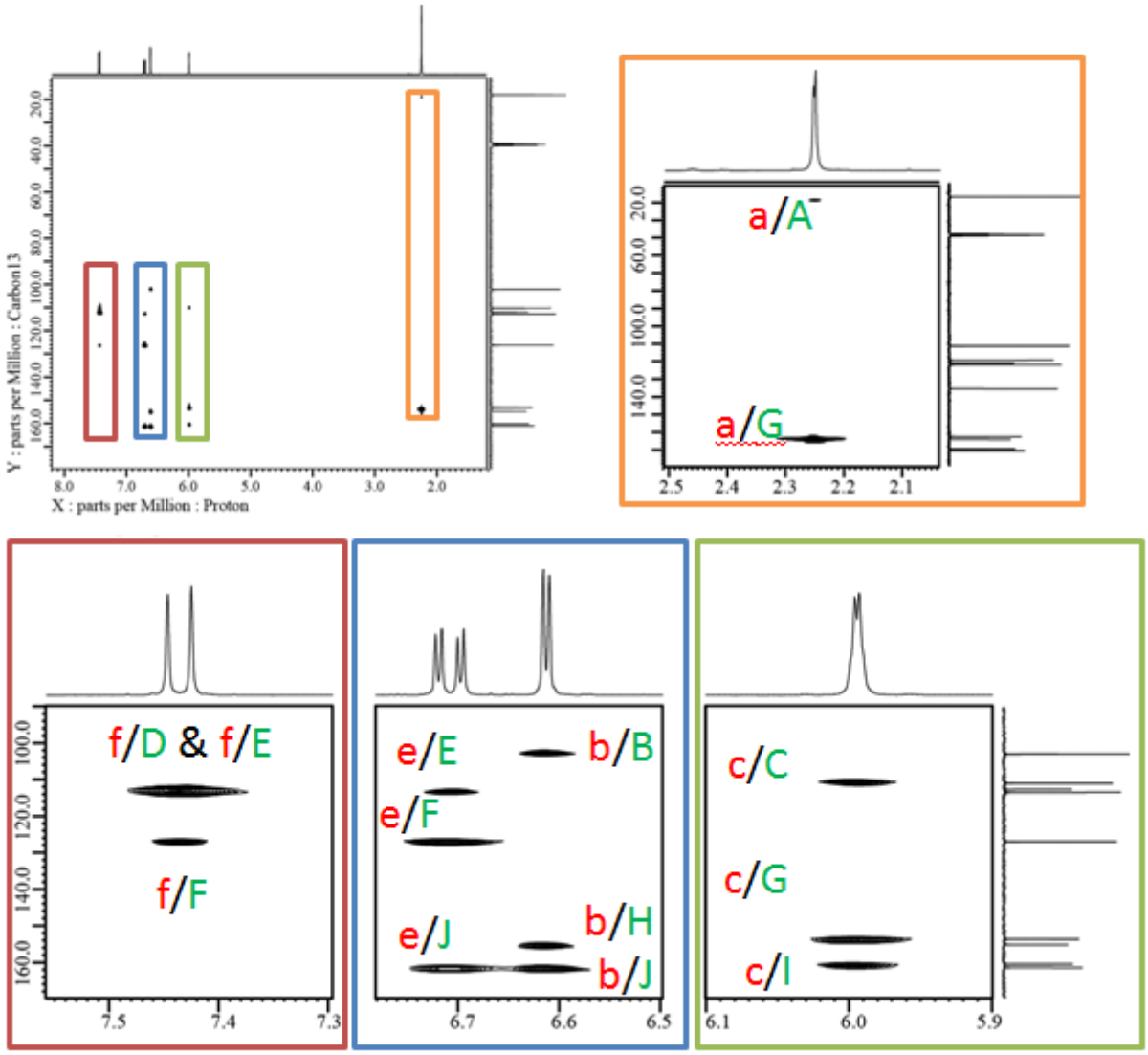
1,1-adequate is not high in sensitivity because it uses $^{1}J_{CC}$ for signal observation. However, being an inverse analysis on the ^{1}H side, 1,1-adequate is capable of higher sensitivity analysis than inadequate. For measurement conditions, parameters for $^{1}J_{CH}$ and $^{1}J_{CC}$ are defined.

100 mg 4-methylumbelliferone/DMSO-d_6

Shown below are total and magnified views of 1,1-adequate.



4-methylumbelliferone



Instruments used: JNM-ECZ400S+ROYAL probe

Measuring conditions: 48 scans (7h), J_constant=140 Hz, JCC=60 Hz

Reference

B. Reif, M. Kock, R. Kerssebaum, H. Kang, W. Fenical, C. Griesinger, JMR ser-A 1996, 118, 282-285 M. Kock, R. Kerssebaum, W. Bermel, MRC 2003, 41, p65-69