CIGAR-HMBC

Improvement of wide $^{n}J_{CH}$ range ^{1}H-detected long-range shift correlation measurements

CIGAR-HMBC (Constant-time Inverse-detected Gradient Accordion Re-scaled long-range HMBC) is a further improved method of IMPEACH-MBC. In CIGAR-HMBC, J_{HH}-modulation, or spectral distortion along the indirect axis, is completely removed by making the sequence constant-time not only for the magnetization transfrer time but also for the evolution time t_1 through a parameter J_{scale}: When J_{scale}=0, J_{HH}-modulation is removed; when J_{scale}=1, J_{HH}-modulation is equivalent to that in IMPEACH-MBC; when J_{scale} is set to be much larger, J_{HH}-modulation can purposely be introduced, which may be utilized to confirm the correlation peaks.

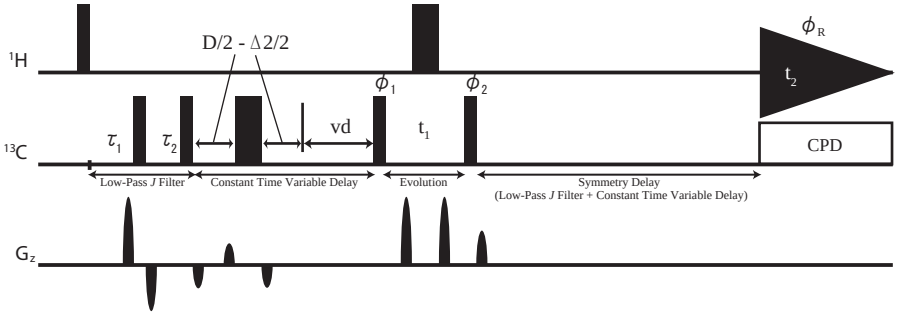

Fig. 1 Pulse diagram of CIGAR-HMBC measurements.

$\tau_1 = 1/2\{^{1}J_{CH}{}^{max} + 0.146(^{1}J_{CH}{}^{max} - {}^{1}J_{CH}{}^{min})\}^{-1}$, $\tau_2 = 1/2\{^{1}J_{CH}{}^{max} - 0.146(^{1}J_{CH}{}^{max} - {}^{1}J_{CH}{}^{min})\}^{-1}$

$vd = 1/2(^{n}J_{CH}{}^{min})^{-1} - y\_point[\{1/2(^{n}J_{CH}{}^{min})^{-1} - 1/2(^{n}J_{CH}{}^{max})^{-1}\}/(y\_points - 1)]$

$D = initial\_delay^{*} + y\_point[\{1/2(^{n}J_{CH}{}^{min})^{-1} - 1/2(^{n}J_{CH}{}^{max})^{-1}\}/(y\_points - 1)]$

$\Delta 2 = (J_{scale} - 1)\,t_1/2$ *initial_delay = 2(PFG + recovery time)

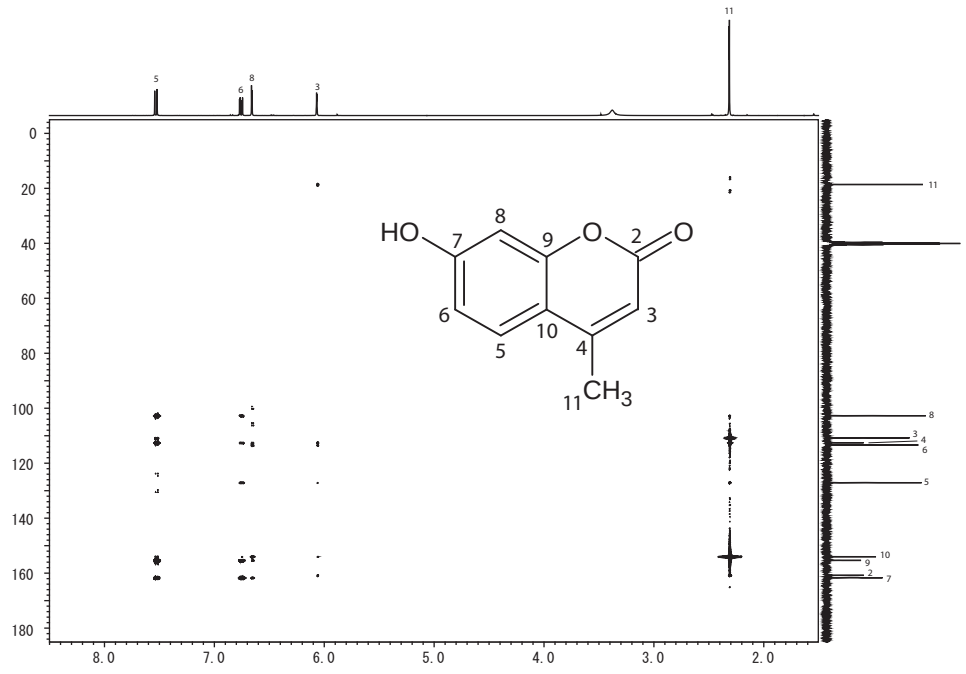

Fig. 2 CIGAR-HMBC spectrum of 4-methyl umbelliferone.

$^{n}J_{CH}{}^{max}$ = 10 Hz, $^{n}J_{CH}{}^{min}$ = 2 Hz, $^{1}J_{CH}{}^{max}$ = 170 Hz, $^{1}J_{CH}{}^{min}$ = 120 Hz, J_{scale} = 0, y_points = 512

Spectrometer: JNM-ECX400

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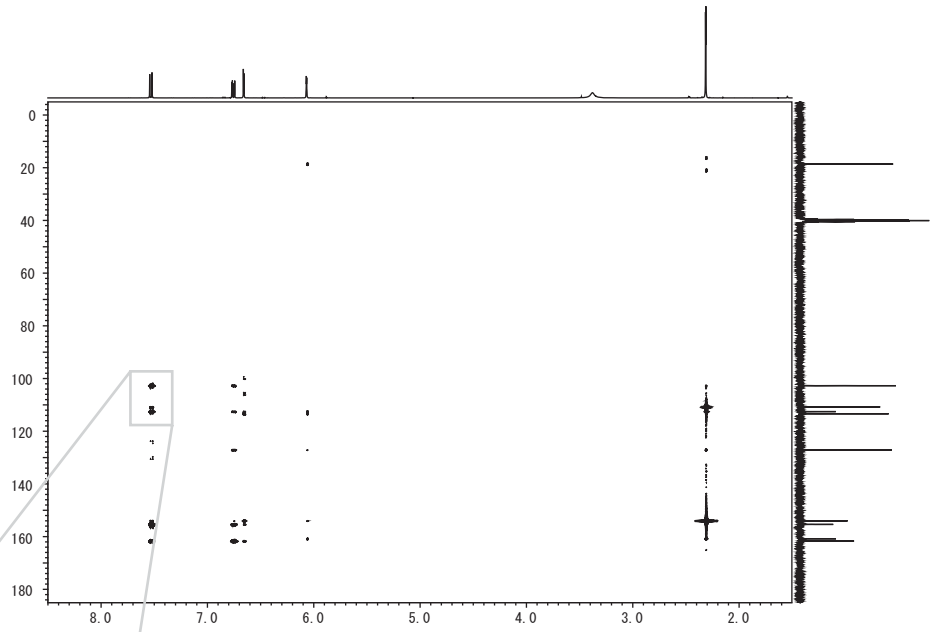
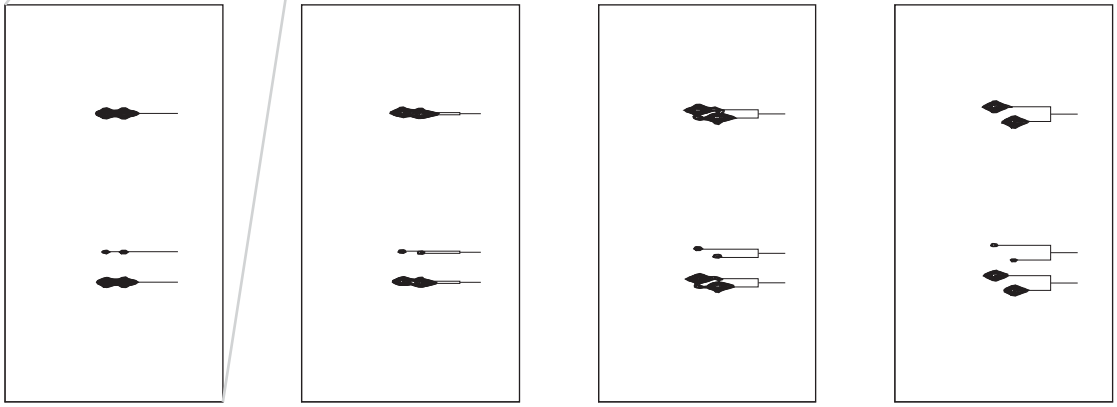
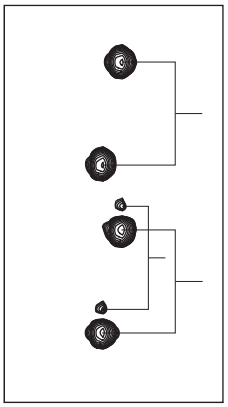


CIGAR-HMBC spectrum of 4-methyl umbelliferone.



J_{scale} = 0 J_{scale} = 1 J_{scale} = 5 J_{scale} = 10

Spectrometer: JNM-ECX400



ACCORD-HMBC

Reference
C.E. Hadden, G.E. Martin and V.V. Krishnamurthy, Magn. Reson. Chem.38, 143(2000)

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