

IMPEACH-MBC

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

In HMBC measurements, signal intensities of long-range correlation peaks depend on magnetization transfer time $1/2 {}^nJ_{CH}$. A basic HMBC pulse sequence, assuming a fixed value of ${}^nJ_{CH}$, cannot give correlation peaks derived from various ${}^nJ_{CH}$ values at once (Fig. 3 top). ACCORD-HMBC, incorporating variable delays, acquires a wider range of ${}^nJ_{CH}$ correlations, but its spectrum may distort along the indirect axis (Fig. 3 middle). IMPEACH-MBC (IMproved PERFORMANCE ACCordion HMBC) solves this problem, by adding cancelling inverse variable delays to ACCORD-HMBC to generate a constant-time sequence. IMPEACH-MBC measurements give spectra where long-range shift correlations can easily be analysed (Fig. 3 bottom).

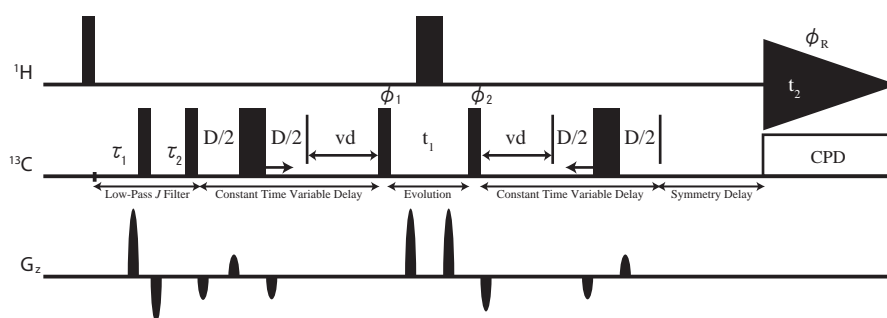


Fig. 1 Pulse diagram of IMPEACH-MBC measurements.

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

$$vd = 1/2({}^nJ_{CH}^{min})^{-1} - y_point\{[1/2({}^nJ_{CH}^{min})^{-1} - 1/2({}^nJ_{CH}^{max})^{-1}]/(y_points - 1)\}$$

$$D = initial_delay + y_point\{[1/2({}^nJ_{CH}^{min})^{-1} - 1/2({}^nJ_{CH}^{max})^{-1}]/(y_points - 1)\}$$

$$*initial_delay = 2(PFG + recovery\ time)$$

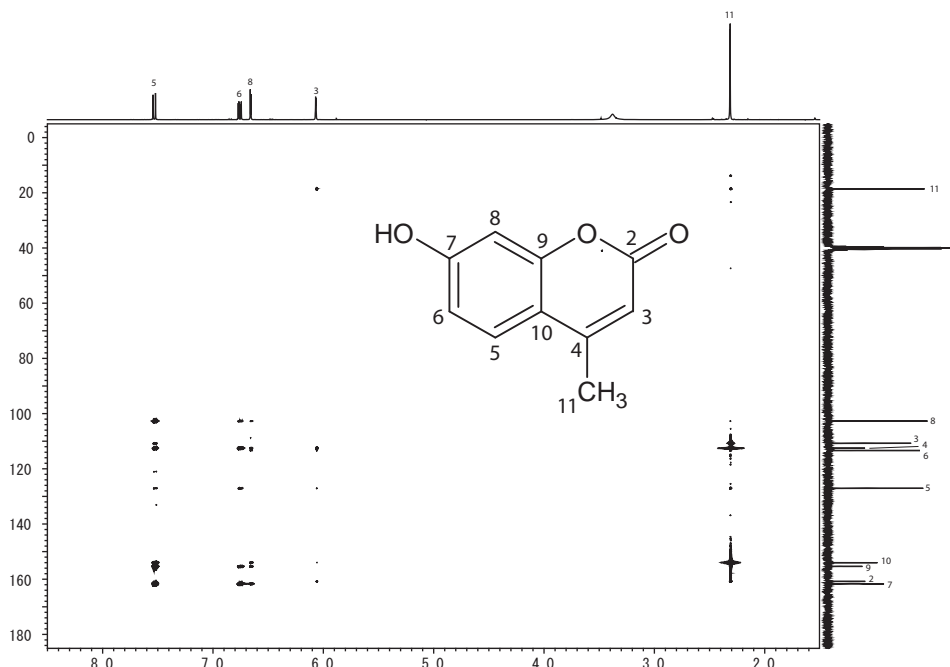


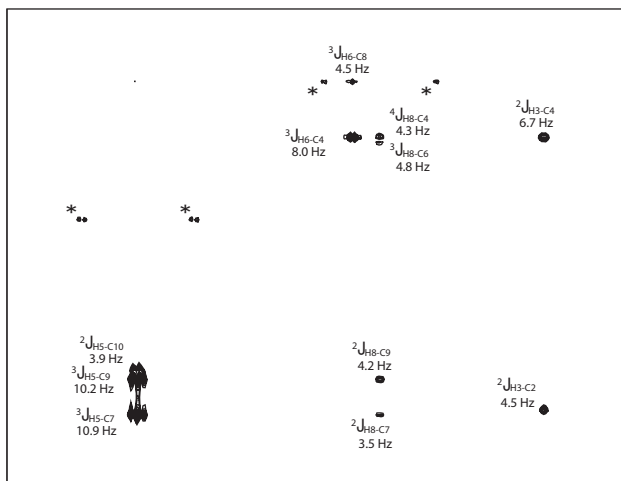
Fig. 2 IMPEACH-MBC spectrum of 4-methyl umbelliferone.

$${}^nJ_{CH}^{max} = 10\ Hz, {}^nJ_{CH}^{min} = 2\ Hz, {}^1J_{CH}^{max} = 170\ Hz, {}^1J_{CH}^{min} = 120\ Hz, y_points = 512$$

Spectrometer: JNM-ECX400

HMBC

```
hmbc_pfg.ex2
long_range_j = 8 Hz
j_constant = 140 Hz
```

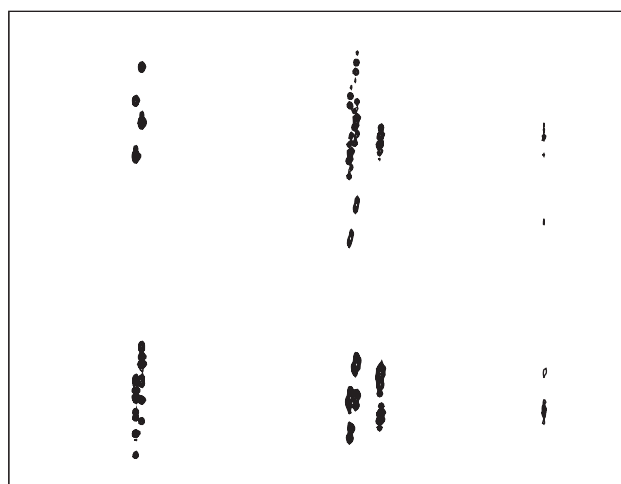


cover a wide range of $^nJ_{CH}$

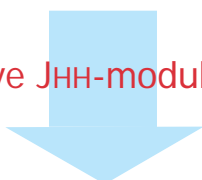


ACCORD-HMBC

```
hmbc_accord_dec_pfg.ex2
y_points = 256
lr_j_min = 1 Hz
lr_j_max = 16 Hz
j_ch_min = 120 Hz
j_ch_max = 160 Hz
```

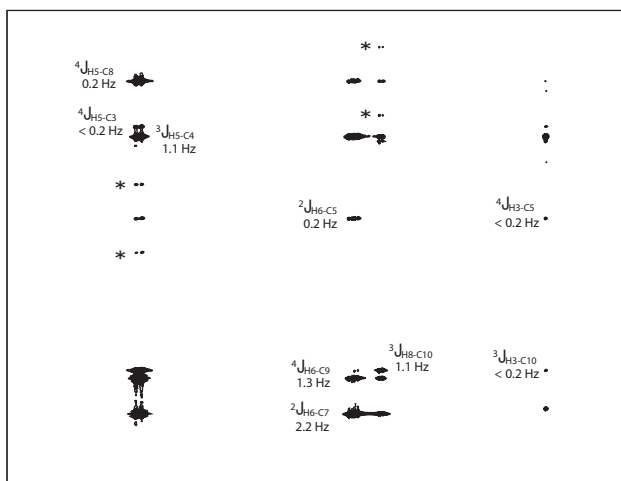


remove J_{HH} -modulation



IMPEACH-MBC

```
impeach_mbc_dec_pfg.ex2
y_points = 512
lr_j_min = 2 Hz
lr_j_max = 10 Hz
j_ch_min = 120 Hz
j_ch_max = 170 Hz
```



Spectrometer: JNM-ECX400

Reference
C.E. Hadden, G.E. Martin and V.V. Krishnamurthy, J. Magn. Reson 140, 274 (1999)