Let's use a chemical shift prediction tool in JASON!
Confirmation of analysis results by chemical shift prediction (1)

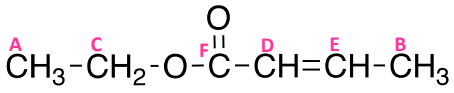
Product used：Nuclear Magnetic Resonance (NMR)

The results of structural analysis by NMR should be judged based on consistency with various measurement data. In recent years, there has been remarkable development in software-based chemical shift prediction. By comparison of actual chemical shift values with chemical shift prediction, it's possible to improve the accuracy of analysis. Here, we report an example to use a chemical shift prediction tool in JASON*. (JASON: JEOL Analytical Software Network)

Confirmation of an estimated structure by HMBC

Here is an example of analysis of a compound whose molecular formula is $C_6H_{10}O_2$. In this compound, two estimated structures I and II were derived by measurements of ^{13}C, DEPT, HMQC and COSY (Fig. 1). The difference is the position of the oxygen bonding to the carbonyl carbon **F**. Therefore we measured HMBC, which could detect long range ^{1}H-^{13}C correlations, usually 2 or 3 bonds apart. The result showed carbonyl carbon **F** had three correlations with $\mathbf{H_C}$, $\mathbf{H_D}$, and $\mathbf{H_E}$. In estimated structure I, all these protons exist within 3 bonds, while in structure II, correlation between **F** and $\mathbf{H_E}$ is apart 4 bonds. Thus, we can consider structure I is correct.

Estimated structure I



Estimated structure II

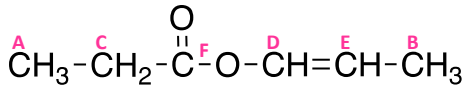
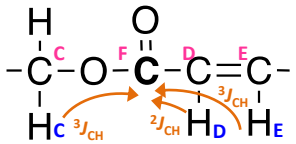


Fig. 1 Two estimated structures I and II

Estimated structure I



Estimated structure II

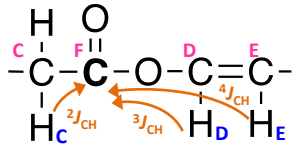
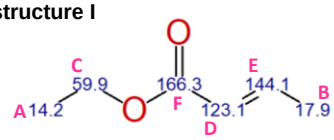


Fig. 2 Long range ^{1}H-^{13}C correlations detected by HMBC measurement

Confirmation of an estimated structure by a chemical shift prediction tool in JASON

The accuracy of the analysis can be further improved by using HMBC in combination with a chemical shift prediction tool in JASON. The chemical shift prediction tool was applied to both estimated structures I and II (Fig. 3). Table. 1 shows the actual and predicted values of the chemical shifts. The predicted values of estimated structure I had good agreement with the actual values. Thus, we can be more confident that structure I is the correct structure.

Estimated structure I



Estimated structure II

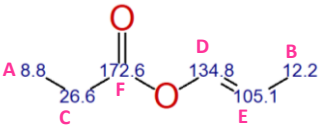


Fig. 3 Chemical shift prediction values

	^{13}C CS/ppm	^{13}C CS/ppm prediction	
		I	II
A	14.2	14.2	8.8
B	17.9	17.9	12.2
C	60.0	59.9	26.6
D	122.8	123.1	134.8
E	144.4	144.1	105.1
F	166.5	166.3	172.6

Table. 1 Comparison of actual chemical shift values with prediction values

JEOL Ltd.
3-1-2 Musashino Akishima Tokyo 196-8558 Japan Sales Division Tel. +81-3-6262-3560 Fax. +81-3-6262-3577
www.jeol.com ISO 9001 • ISO 14001 Certified
▼ Local office
• AUSTRALIA & NEW ZEALAND • BELGIUM • BRAZIL • CANADA • CHINA • EGYPT • FRANCE • GERMANY • GREAT BRITAIN & IRELAND • ITALY • KOREA • MALAYSIA • MEXICO • RUSSIA • SCANDINAVIA • SINGAPORE • TAIWAN • THE NETHERLANDS • USA