Let's use a chemical shift prediction tool in JASON!
Confirmation of analysis results by chemical shift prediction (3)

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 a chemical shift prediction tool in JASON

Here is an example of a compound whose molecular formula is $C_6H_6N_2O$. In this compound, an estimated structure was obtained from measurements of ^{13}C, DEPT, ^{1}H–^{13}C HSQC, ^{1}H–^{1}H COSY, ^{1}H–^{13}C HMBC and ^{1}H–^{15}N HMBC (Fig. 1). The ^{13}C chemical shift additivity has been used to confirm the validity of the estimated structure, which can be substituted with a recent chemical shift prediction tool. The chemical shift prediction tool in JASON was applied to the estimated structure. Table. 1 shows the actual and predicted values of the chemical shifts, respectively. Since the predicted values had good agreement with the actual values, we can be more confident that the estimated structure is correct.

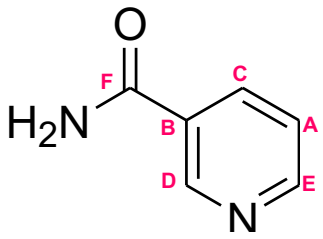

Fig. 1 Estimated structure

	^{13}C CS/ppm	JASON ^{13}C CS Prediction
A	123.9	124.9
B	130.2	129.6
C	135.7	137.0
D	149.2	152.5
E	152.4	148.3
F	167.0	170.6

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

Precaution for using a chemical shift prediction tool

Fig. 2 shows the peak assignment after data analysis and chemical shift prediction. You can find carbons D and E are reversed. In this case, we need to confirm data analysis again. Fig. 3 shows the COSY spectrum showing three correlations of H_D/H_C, H_C/H_A and H_E/H_A. H_C/H_A and H_E/H_A correlations indicates ^{1}H array H_C-H_A-H_E, which means the assignment by the chemical shift prediction tool is wrong. Thus, analysis is necessary even if using a chemical shift prediction tool. When a contradiction arises between an observed data and its chemical shift prediction, it is important to confirm data analysis again.

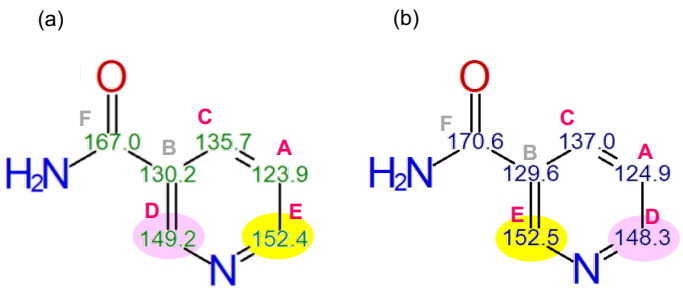

Fig. 2 Chemical shift values after
(a) data analysis (b) chemical shift prediction

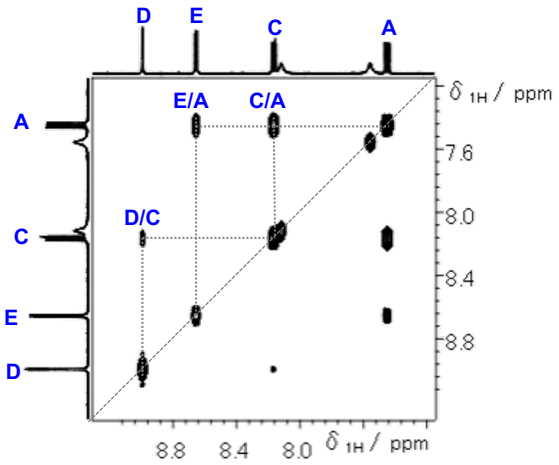

Fig. 3 ^{1}H–^{1}H COSY spectrum

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
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