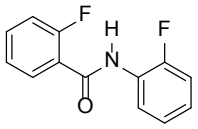
^{14}N decoupled ^{1}H–^{19}F HOESY with ROYALPROBE™ HFX

Product used : Nuclear Magnetic Resonance (NMR)

Fluorine and nitrogen containing organic compounds are often found in a variety of fields such as pharmaceutical and material sciences. Such compounds show unique properties based on their conformations and orientations, which are often induced by hydrogen bonds between N-H and F atoms. Therefore, analysis of molecular conformations and inter-molecular interactions are important. Here, we report ^{14}N decoupled ^{1}H–^{19}F HOESY (hetero nuclear NOE) for fluorinated benzanilide (**1**) as a demonstration.



fluorinated benzanilide (**1**)

Measurements of ^{14}N decoupling ^{1}H–^{19}F HOESY

It often happens that ^{1}H NMR analysis is prevented with the severe line broadening of ^{1}H signal that is bound to ^{14}N atom. In such a case, the ^{14}N decoupling technique is useful. ^{1}H–^{19}F 1D-HOESY spectra *with* and *without* ^{14}N decoupling are shown in Fig.1. Selective excitation was done at F5 (Fig.1: upper) and F6 (Fig.1: bottom), respectively. The amide ^{1}H signal intensity in 1D-HOESY is increased by twice, compared to that measured without ^{14}N decoupling. Since NOE measurements have generally difficulty in low sensitivity, the ^{14}N decoupling technique is useful for observation of cross peaks with ^{1}H–^{14}N signals. 2D-HOESY with ^{14}N decoupling measurement is also available(Fig.2).

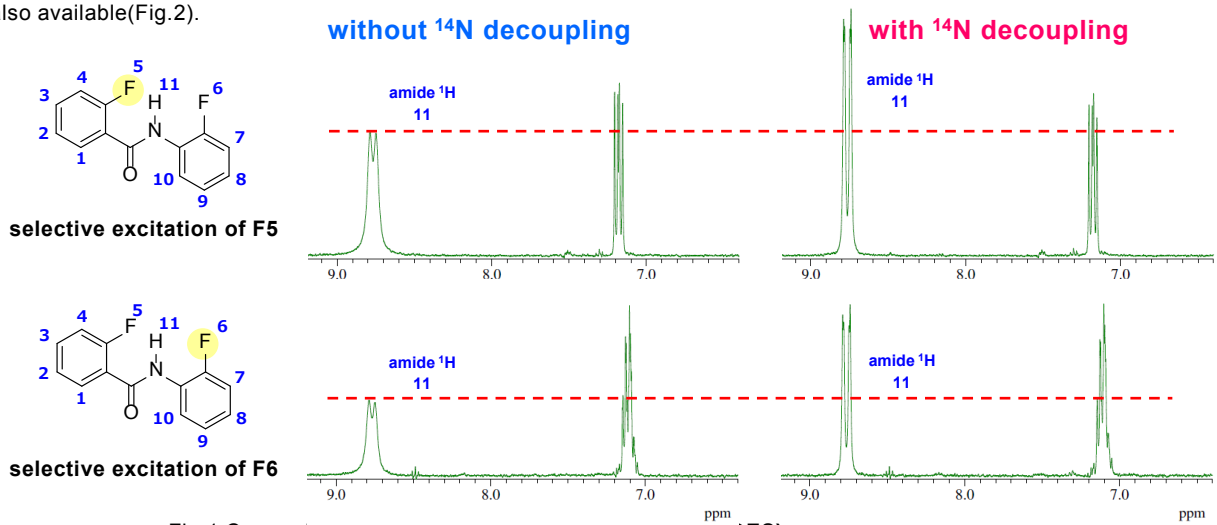


Fig.1 Comparison of amide ^{1}H signal intensities in 1D-HOESY spectra *with* or *without* ^{14}N decoupling (upper: selective excitation at F5; bottom: F6).

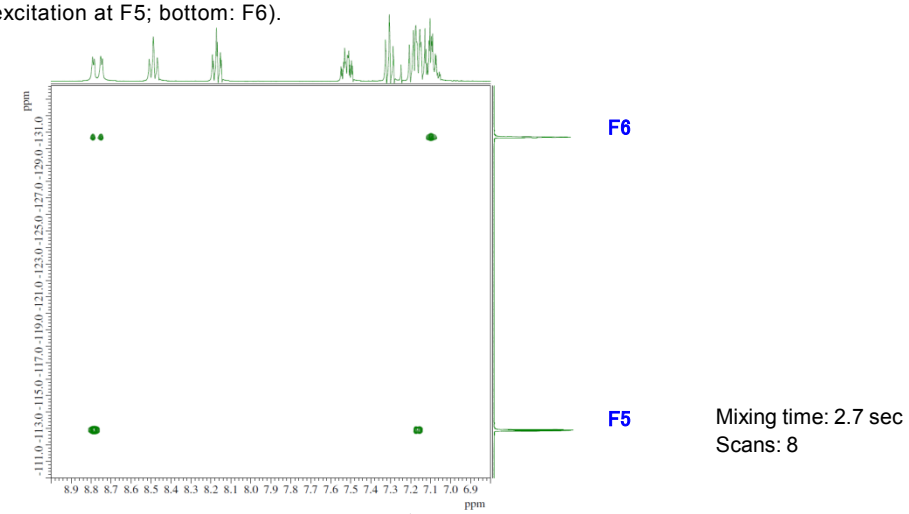


Fig.2 2D-HOESY spectrum of **1** under the ^{14}N decoupling condition.

Sample: 36 mg fluorinated benzanilide in chloroform-*d*

Equipment: JNM-ECZ400S with ROYALPROBE™ HFX※

※Special modification for ^{14}N nuclei required.

References

G. N. Manjunatha Reddy, M. V. Vasantha Kumar, T. N. Guru Row, N. Suryaprakash, *Phys. Chem. Chem. Phys.*, **12**, 13232–13237 (2010).

L. E. Combettes, P. Clausen-Thue, M. A. King, B. Odell, A. L. Thompson, V. Gouverneur, T. D. W. Claridge, *Chem. Eur. J.*, **18**, 13133–13141 (2012).

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