

2D NMR measurements using hydrogen and carbon nuclei are often used for detailed structural analysis of organic compounds, but when the structure contains heteroatoms, structural information may not be sufficiently obtained. Here, we introduce an example in which 2D NMR measurements using multinuclear are effective for detailed structural analysis of OLED materials.

HMBC: HMBC is one of 2D NMR methods that can provides information on the positional relationships between atoms separated by 2-3 bonds.

A diagram illustrating a correlation peak in a hydrocarbon chain. It shows three carbon atoms (C) in a horizontal line. The first carbon is bonded to a hydrogen atom (H) above it. A green arrow points from the first carbon to the second carbon, and another green arrow points from the second carbon to the third carbon. The text "Correlation peak" is written above the arrows. Below the diagram, the text "A compound composed of hydrogen and carbon" is written.

Correlation peak

X: Hetero atom

A Compound containing heteroatoms

Detailed structural analysis is difficult!

H

C **C** **X**

Correlation peak

X: Hetero atom

Compounds containing heteroatoms

It is an effective tool for detailed structural analysis by combining the results of ^1H - ^{13}C HMBC measurement !

The positional relationship between hydrogen and nitrogen separated by 2-3 bonds is cleared.

The positional relationship between carbon and fluorine separated by 2-3 bonds is cleared.

: Carbons for which correlation peaks with fluorine (peak F1, F2) is observed

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