



BRUKER



## NMR

# Chemical Clues from Every Shift

## The Power of Benchtop Nuclear Magnetic Resonance

Innovation with Integrity

### Introduction

- Nuclear Magnetic Resonance (NMR) spectroscopy is a non-destructive analytical technique that reveals how atoms are connected within a molecule. By placing a sample in a magnetic field and detecting how certain nuclei absorb and emit radiofrequency energy, NMR provides detailed insight into molecular structure, functional groups, and atomic interactions. It is an essential tool in chemical education and across research fields, including pharmaceuticals and materials science.
- The molecule 2-(4-(2-methylpropyl)phenyl)propanoic acid, more commonly known as **ibuprofen**, is a widely used over-the-counter anti-inflammatory drug for the treatment of pain, fever, and inflammation. Its molecular complexity makes it an ideal model compound for analysis using benchtop Nuclear Magnetic Resonance (NMR) spectroscopy.
- As an example, the chemical structure of Ibuprofen features eight distinct proton chemical environments (1, 3, 4, 6, 7, 9–11) and ten unique carbon environments (2–11). These features can be clearly observed using the **Fourier 80**, Bruker's benchtop 80MHz NMR spectrometer.



## One-Dimensional (1D) <sup>1</sup>H NMR

- NMR in the simplest form, focuses on a single isotope (e.g., <sup>1</sup>H, <sup>13</sup>C etc.) to understand a molecule's chemical environment
- NMR spectrum shows signal intensity vs. chemical shift (δ) in ppm—helps identify **functional groups** within the molecule
- In <sup>1</sup>H 1D NMR, the **integration** of these 1D NMR peaks allows us to quantify the relative number of nuclei contributing to each signal.
- The **multiplicity** in a <sup>1</sup>H NMR spectrum is the splitting of each signal into peaks that reflect nearby NMR-active nuclei in the molecule

### <sup>1</sup>H 1D NMR

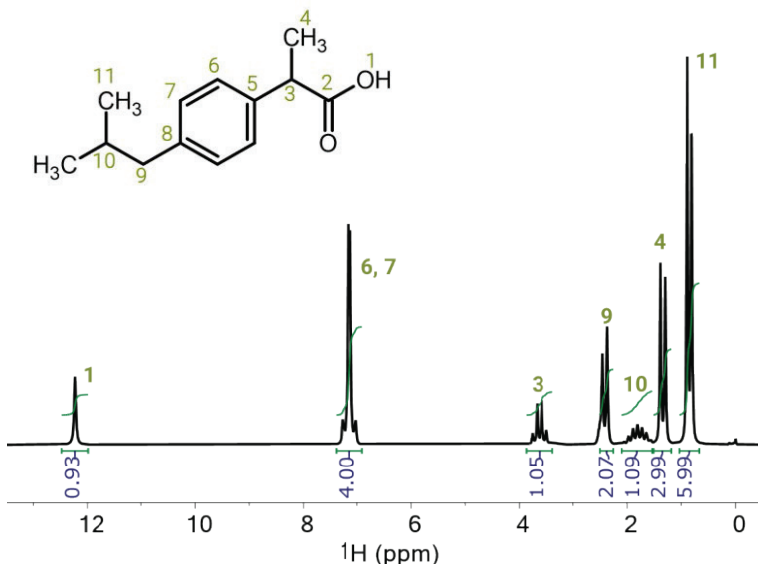


Figure 1: Labeled 1D <sup>1</sup>H NMR Spectrum of Ibuprofen acquired at 80MHz

## One-Dimensional <sup>13</sup>C NMR

- <sup>13</sup>C 1D NMR** is used to identify the carbon atoms in a molecule by detecting the carbon-13 isotope. Each unique carbon environment gives rise to a single peak in the <sup>13</sup>C spectrum due to proton couplings being removed using decoupling
- <sup>13</sup>C DEPT NMR** differentiates carbon types based on the number of attached hydrogens. In DEPT-135, CH<sub>3</sub> and CH groups show positive signals (↑), CH<sub>2</sub> shows a negative signal (↓), and quaternary carbons (C) show no signal. In DEPT 45, all protonated carbons (CH, CH<sub>2</sub>, CH<sub>3</sub>) exhibit positive signals (↑). DEPT-90 only shows CH groups (↑), helping confirm carbon environments

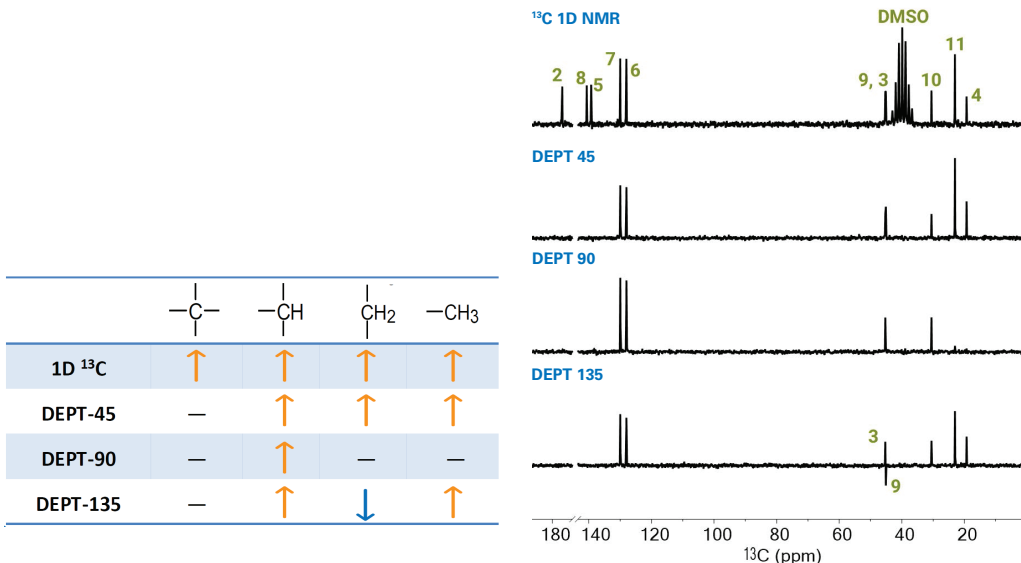
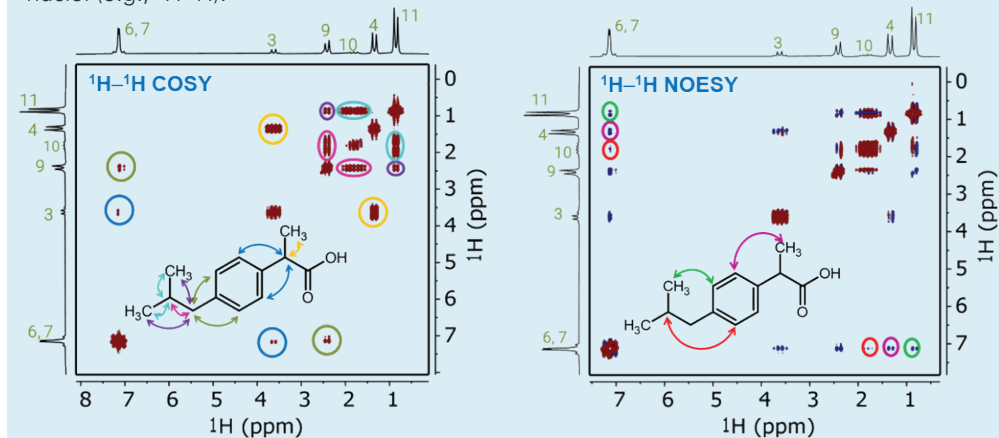


Figure 2: LEFT <sup>13</sup>C DEPT NMR graphical illustration showing CH, CH<sub>2</sub>, and CH<sub>3</sub> carbons differentiated by their characteristic NMR signals. RIGHT Stacked <sup>13</sup>C and DEPT NMR Spectra of Ibuprofen. The chemical shift scale is segmented to include the carbonyl position in ibuprofen at 176 ppm. DEPT-135 NMR spectrum can distinguish the overlapping <sup>13</sup>C signals for carbons at positions 9 and 3.

## Two-Dimensional (2D) NMR

- Unlike 1D NMR, which shows signals based on a single frequency axis, 2D NMR spreads data across **two frequency dimensions** - revealing interactions between nuclei and uncovering complex connectivity patterns that are invisible in 1D spectra. These interactions can be observed using the Fourier 80, Bruker's benchtop 80 MHz NMR spectrometer

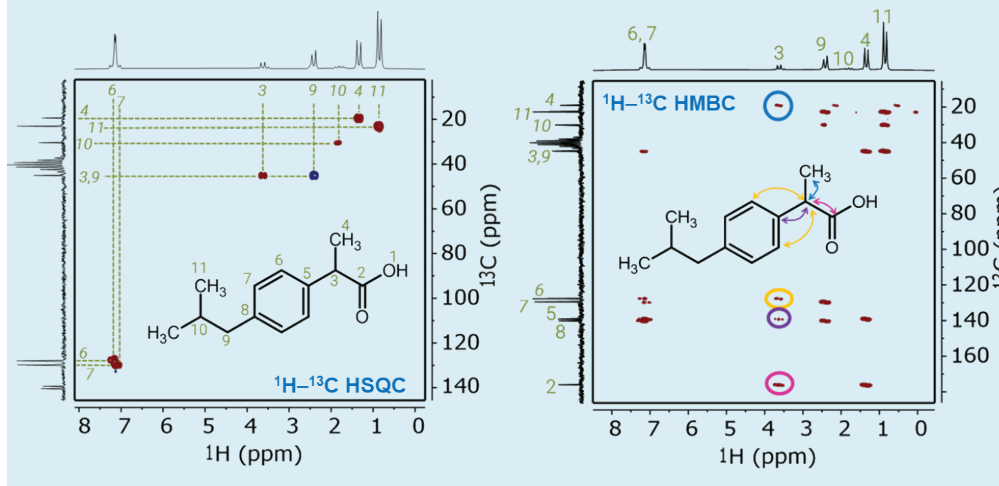
### Homonuclear Two-Dimensional NMR - Focuses on the coupling between the same nuclei (e.g., $^1\text{H}$ - $^1\text{H}$ ).



**$^1\text{H}$ - $^1\text{H}$  COSY** (left) – identifies proton couplings through 2–3 bonds. Off-diagonal cross-peaks show which protons are near each other in the structure

**$^1\text{H}$ - $^1\text{H}$  NOESY** (right) – Shows off-diagonal cross-peaks between protons that are not necessarily bonded but are spatially near each other

### Heteronuclear 2D NMR - Explores interactions between different nuclei (e.g., $^1\text{H}$ - $^{13}\text{C}$ )



**$^1\text{H}$ - $^{13}\text{C}$  HSQC** (left) – Shows direct connectivity between  $^1\text{H}$  and  $^{13}\text{C}$  atoms

- Cross peaks identify only protons that are **DIRECTLY** attached to which carbons

**$^1\text{H}$ - $^{13}\text{C}$  HMBC** (right) – Shows long-range correlations between  $^1\text{H}$  and  $^{13}\text{C}$  atoms over 2 to 3 bonds

- Cross peaks identify only protons that are **NOT DIRECTLY** attached to which carbons

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