

Measuring methods available and examples of their applications

^{13}C NMR APT (Attached Proton Test)

The Attached Proton Test (APT) experiment is a simple method to assign C-H multiplicities in ^{13}C NMR spectra. It provides information on all carbon multiplicities within a single experiment.

The APT (or J-resolved) experiment yields methine (CH) and methyl (CH₃) signals negative and quaternary (C) and methylene (CH₂) signals positive (In North America, opposite phasing is usually used). It is slightly less sensitive than DEPT but a single experiment shows all carbon signals at once unlike DEPT which needs three different spectra.

Even though this technique does not distinguish fully between CH_n groups, it is so easy and reliable that it is frequently employed as a first attempt to assign peaks in the spectrum and elucidate the structure. It is sometimes possible that a CH and CH₂ signal have coincidentally equivalent chemical shifts resulting in signal cancelation in the APT spectrum due to the opposite phases. For this reason the conventional $^{13}\text{C}\{^1\text{H}\}$ spectrum or HSQC are usually also acquired.

Examples of APT spectra

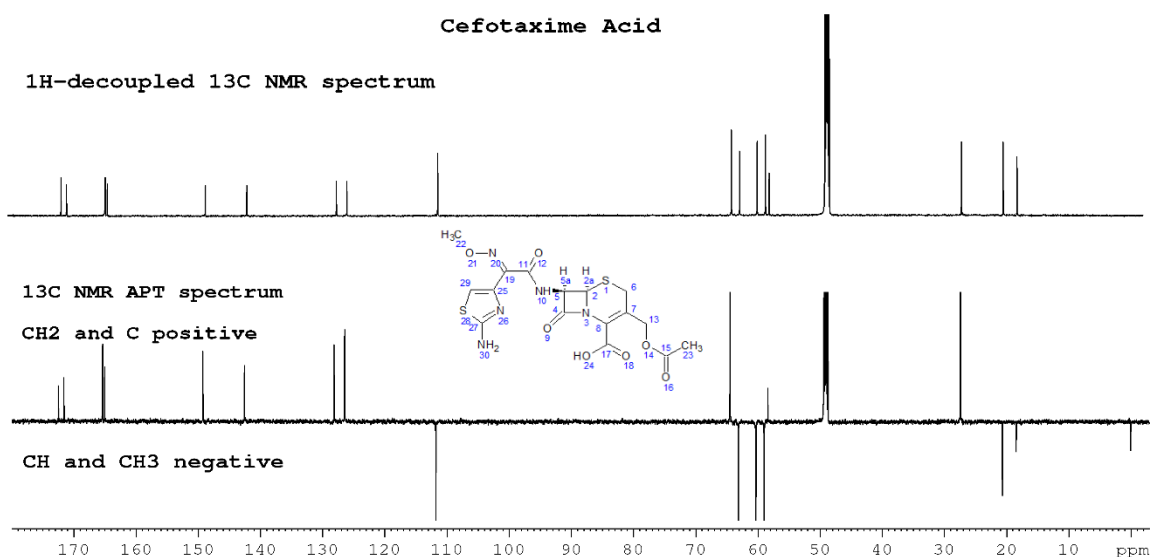


Fig. 1. Cefotaxime Acid (cephalosporin antibiotic of third-generation). **APT spectrum of Cefotaxime showing CH and CH₃ negative while CH₂ and C are positive.** Spectrometer: AVANCE III HD 700, Probehead: 5 mm CPTXO $^{13}\text{C}/^{15}\text{N}$ - $^1\text{H}/\text{D}$ with z gradients, Experiment time: 12 min

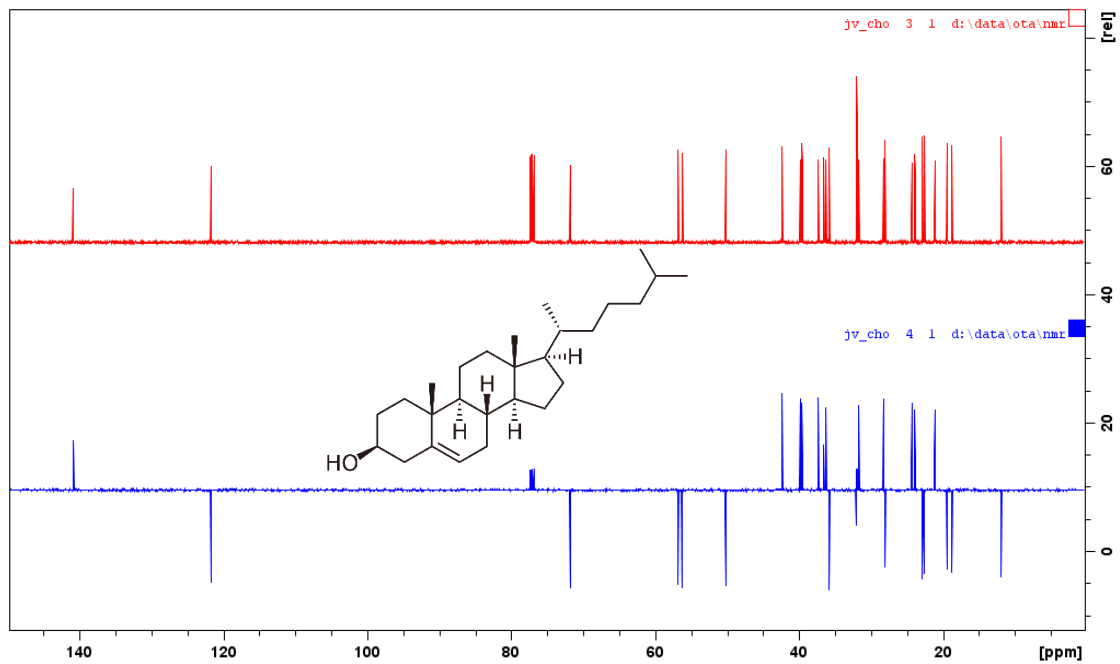


Fig. 2. Comparison of the ¹³C NMR spectra with proton decoupling (red) and APT experiment for the molecule of cholesterol. APT spectrum shows CH and CH₃ negative while CH₂ and C are positive.