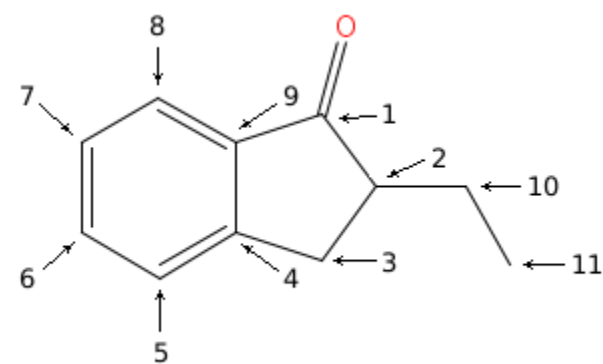


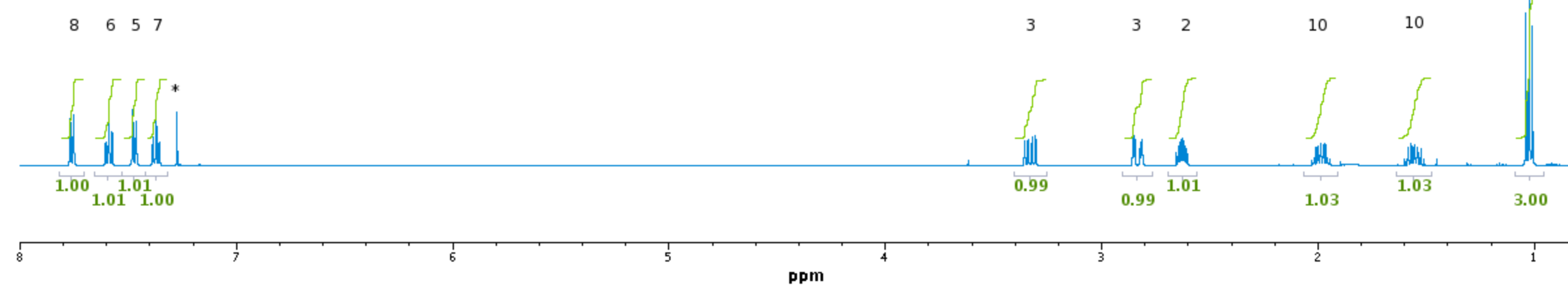
## 2-ethyl-1-indanone



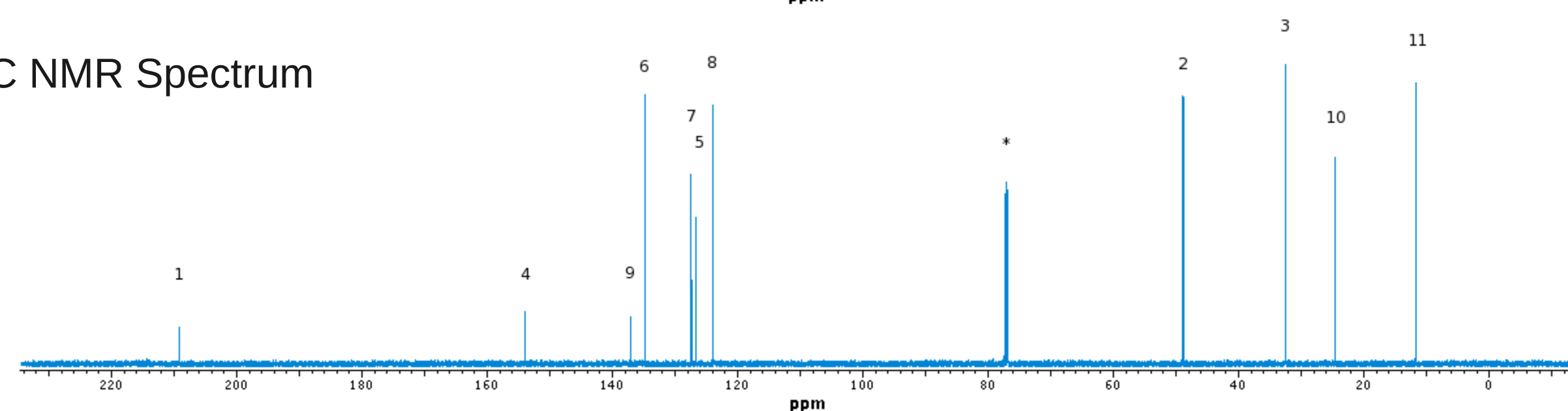
A sample of 2% 2-ethyl-1-indanone in  $\text{CDCl}_3$  was used to acquire all these examples. These data were acquired on an Agilent ProPulse 500 with a OneProbe by Agilent.

The 1D spectra on this sample were easily acquired, as the sample is quite concentrated (~128mM). The  $^1\text{H}$  spectrum was acquired with a single scan, and the  $^{13}\text{C}$  spectrum was acquired with 256 scans in 8min 44sec.

### $^1\text{H}$ NMR Spectrum

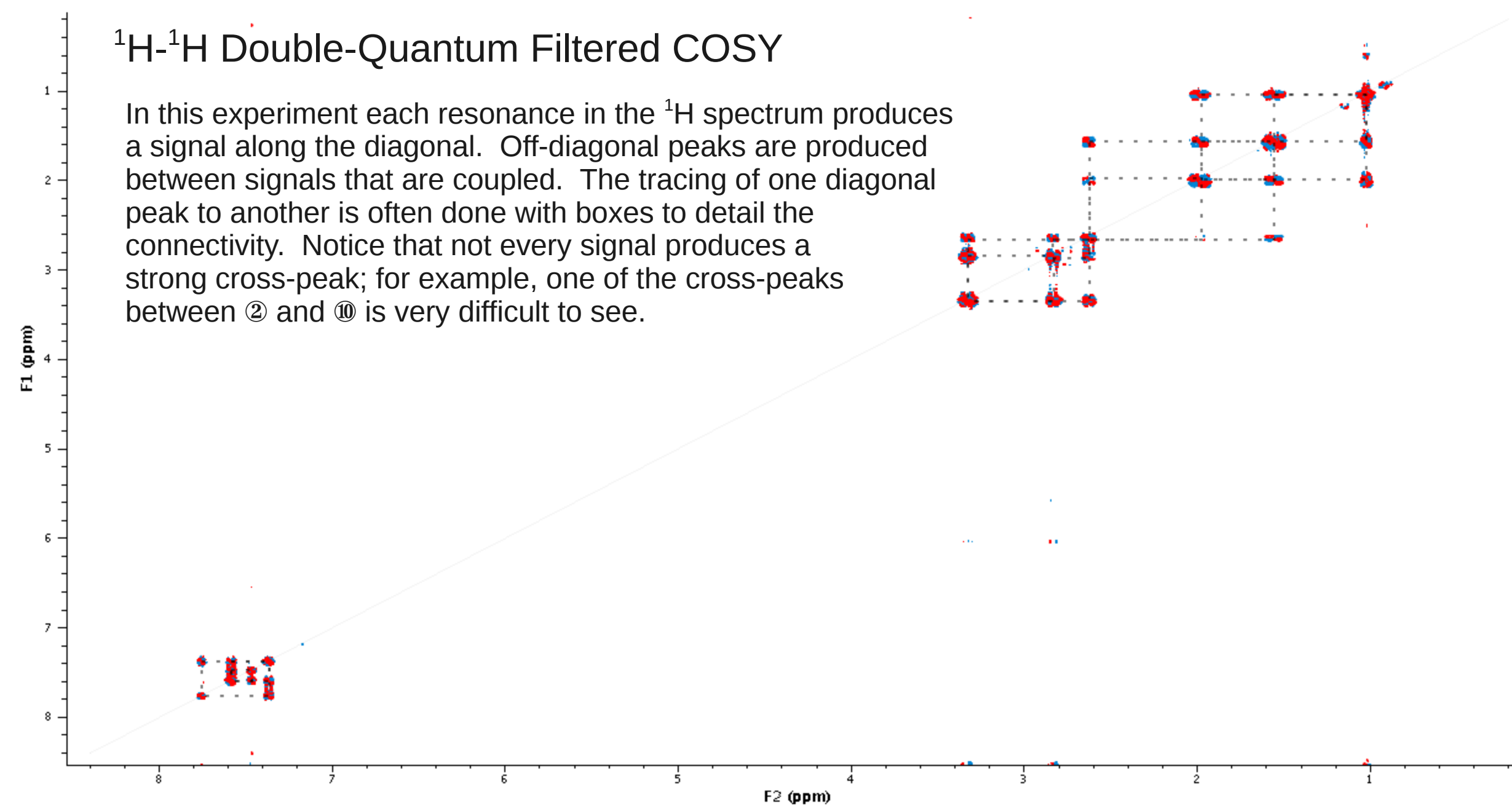


### $^{13}\text{C}$ NMR Spectrum



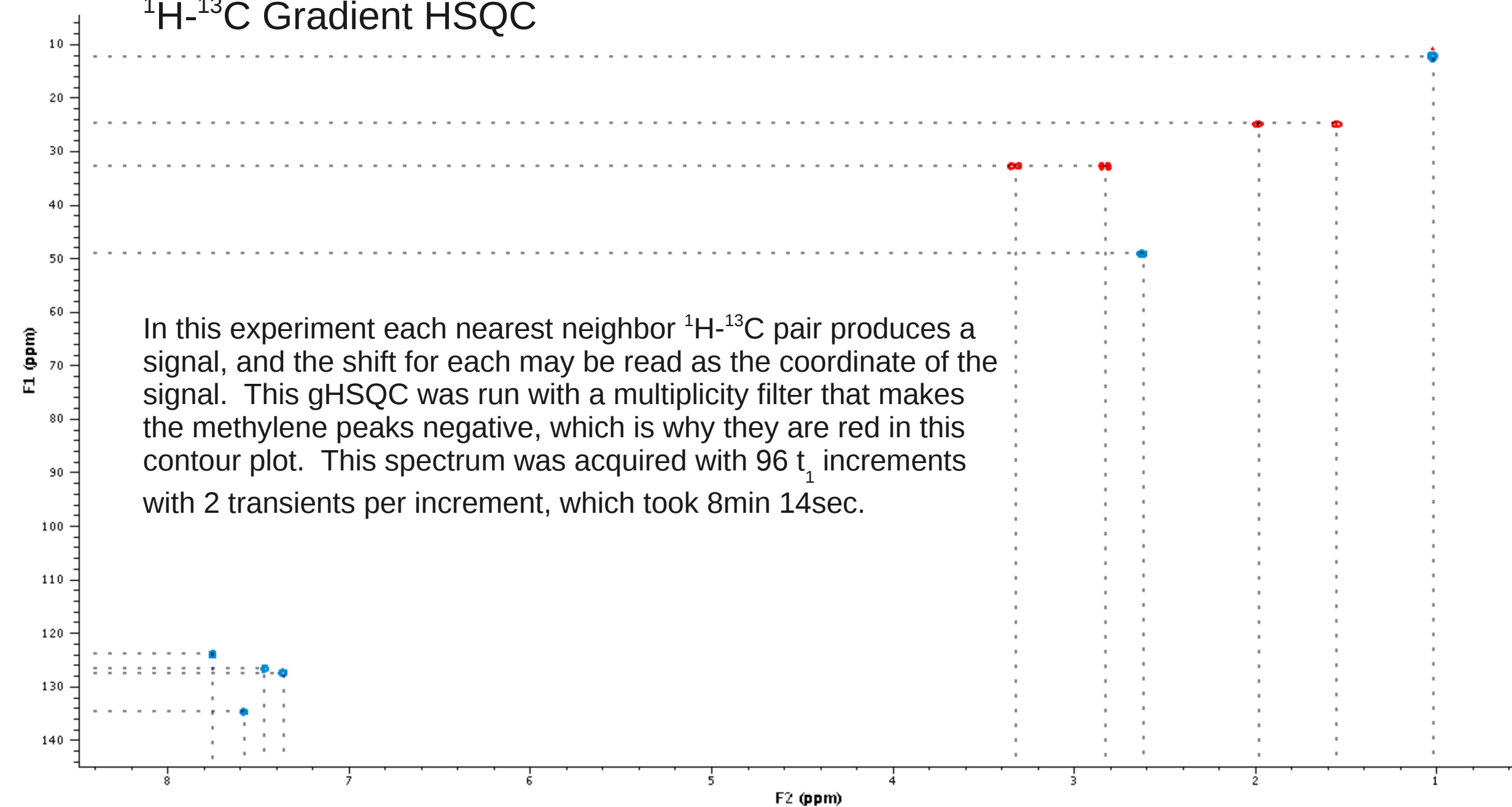
### $^1\text{H}$ - $^1\text{H}$ Double-Quantum Filtered COSY

In this experiment each resonance in the  $^1\text{H}$  spectrum produces a signal along the diagonal. Off-diagonal peaks are produced between signals that are coupled. The tracing of one diagonal peak to another is often done with boxes to detail the connectivity. Notice that not every signal produces a strong cross-peak; for example, one of the cross-peaks between ② and ⑩ is very difficult to see.



# Interpretation of 2D NMR Spectra

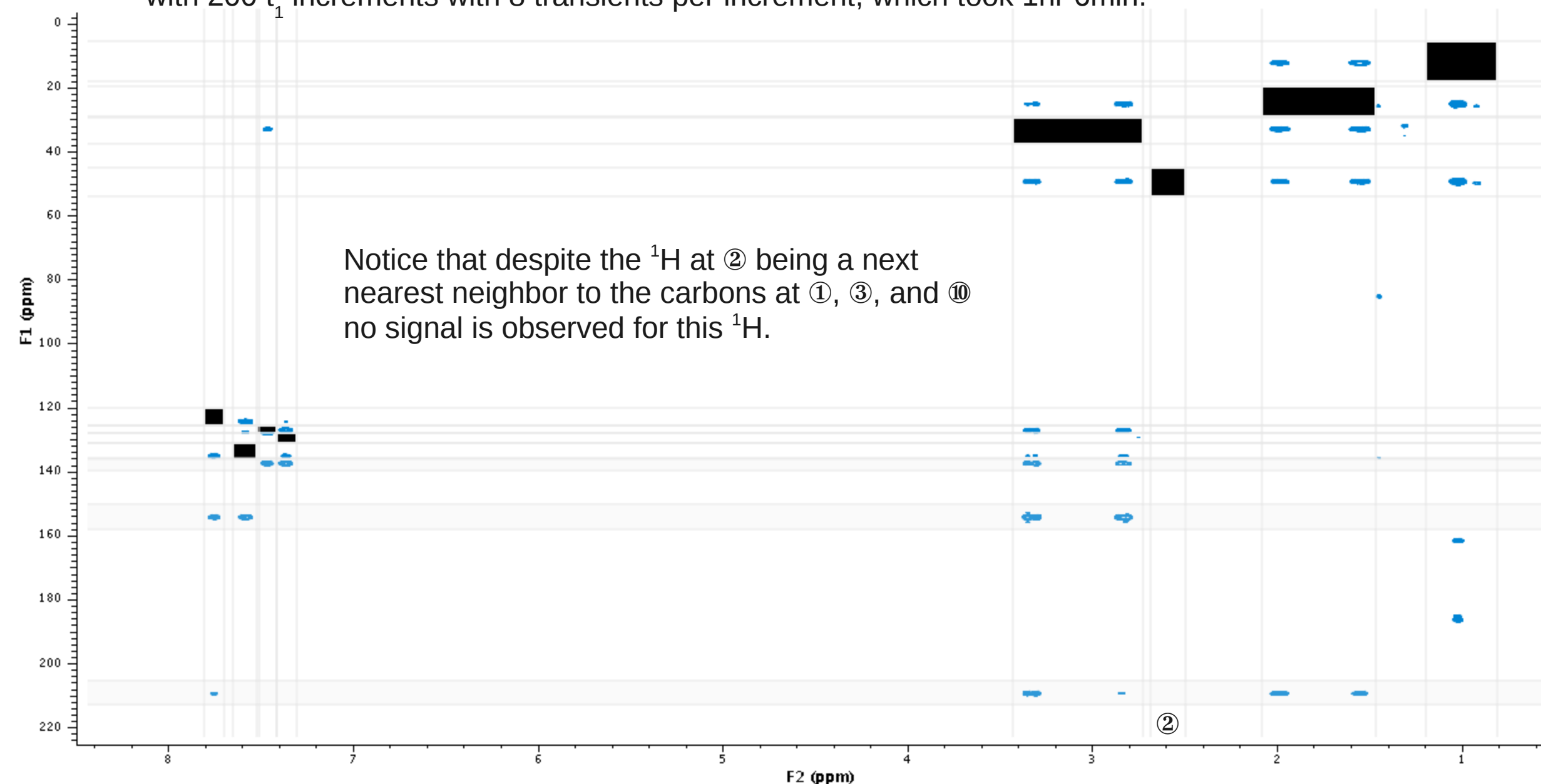
### $^1\text{H}$ - $^{13}\text{C}$ Gradient HSQC



In this experiment each nearest neighbor  $^1\text{H}$ - $^{13}\text{C}$  pair produces a signal, and the shift for each may be read as the coordinate of the signal. This gHSQC was run with a multiplicity filter that makes the methylene peaks negative, which is why they are red in this contour plot. This spectrum was acquired with 96  $t_1$  increments with 2 transients per increment, which took 8min 14sec.

### $^1\text{H}$ - $^{13}\text{C}$ Gradient HMBC

In this experiment signals are produced by  $^{13}\text{C}$  atoms coupled to  $^1\text{H}$  that are not directly attached. Typically, the experiment is set up to show couplings between next nearest neighbors ( $^2\text{J}$  couplings). The spectrum is deciphered below with intersecting boxes, the black fields have no signal as they would be where a nearest neighbor ( $^1\text{J}$ ) coupling would exist. Notice that the quaternary carbons, which produced no signal in the HSQC above, do show up here and are highlighted in gray. This spectrum was acquired with 200  $t_1$  increments with 8 transients per increment, which took 1hr 6min.



Notice that despite the  $^1\text{H}$  at ② being a next nearest neighbor to the carbons at ①, ③, and ⑩ no signal is observed for this  $^1\text{H}$ .