

7.7: 2-D NMR Problems

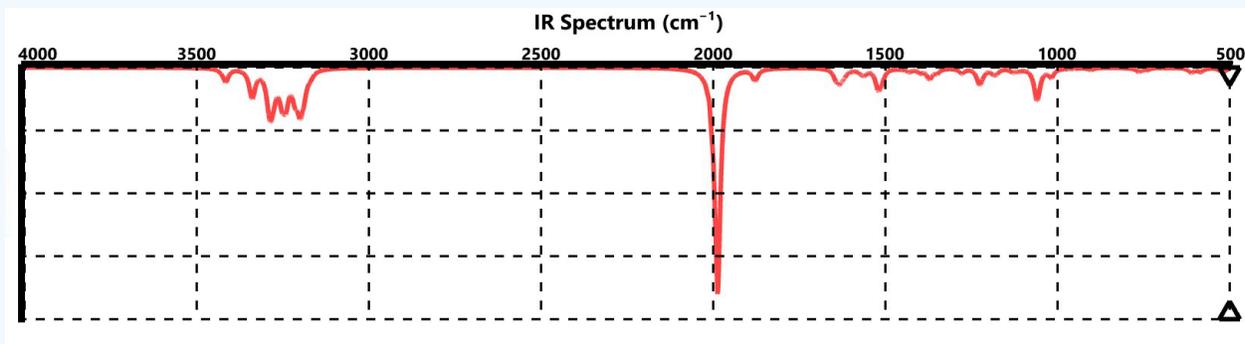
Learning Objectives

- Solve unknown problems using a variety of spectra and the molecular formula.

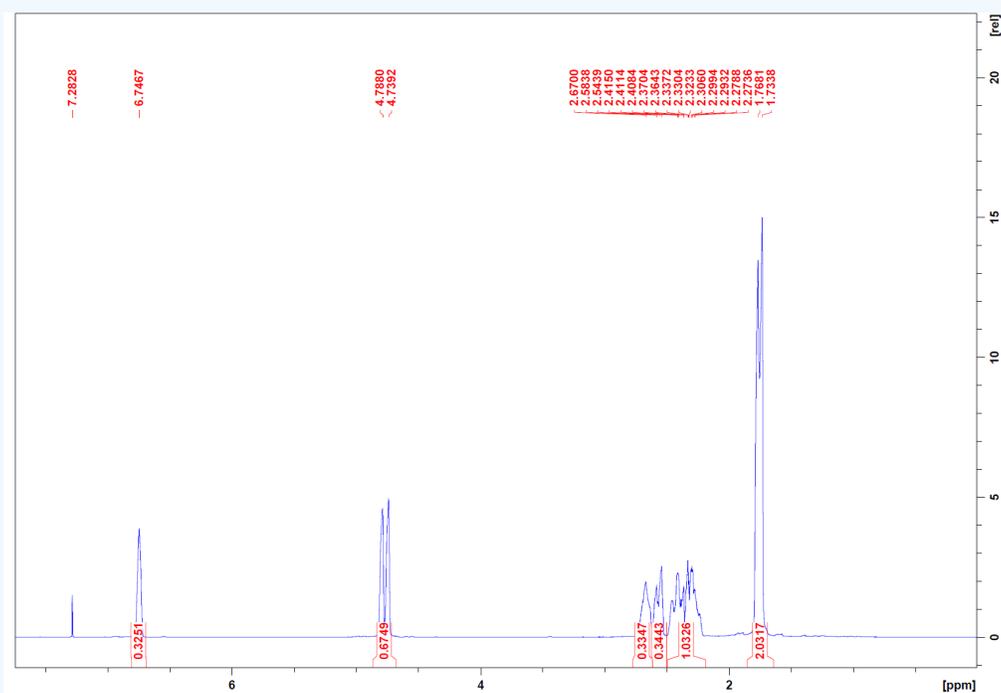
? Exercise 7.7.1

Propose a structure using the spectral data below for $C_{10}H_{14}O$. Note: You may need to check for solvent peaks. This sample was dissolved in $CDCl_3$.

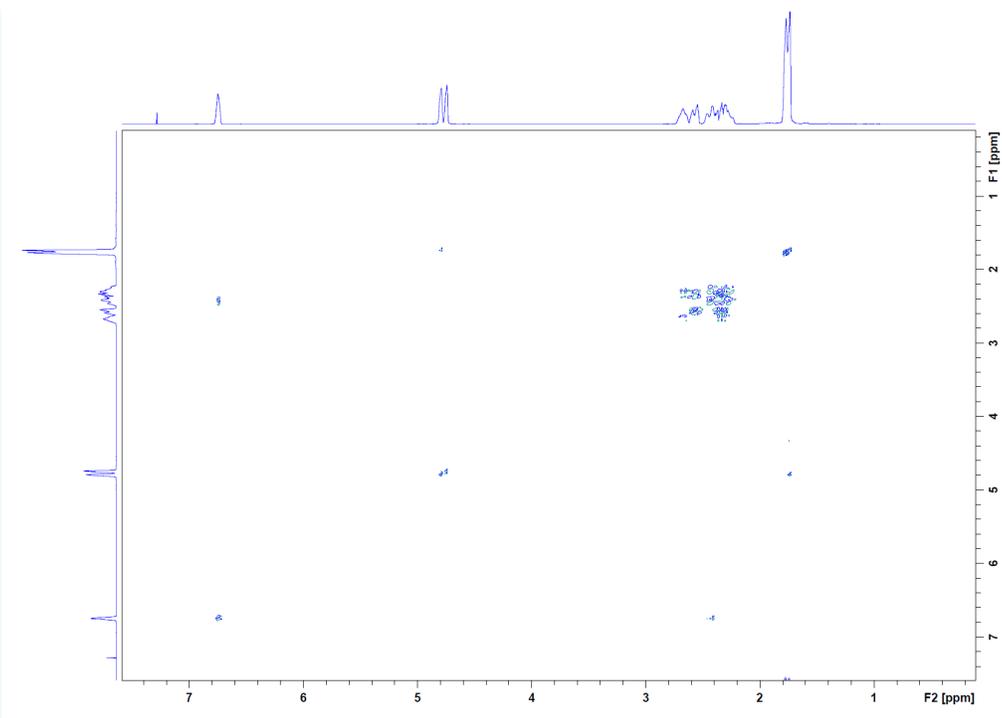
IR:



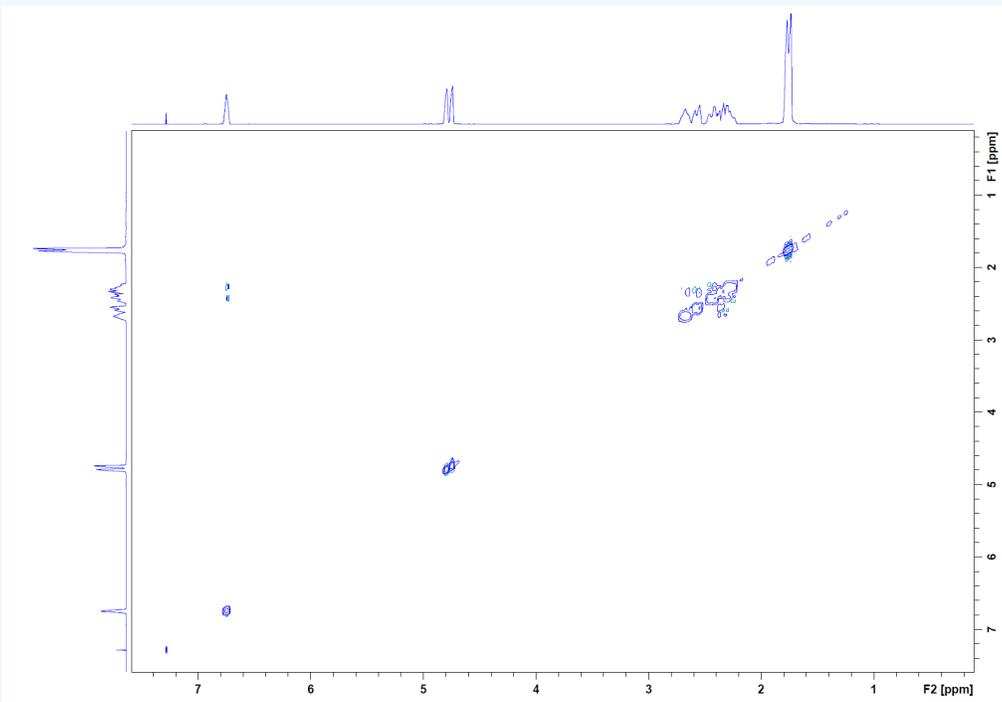
1H :



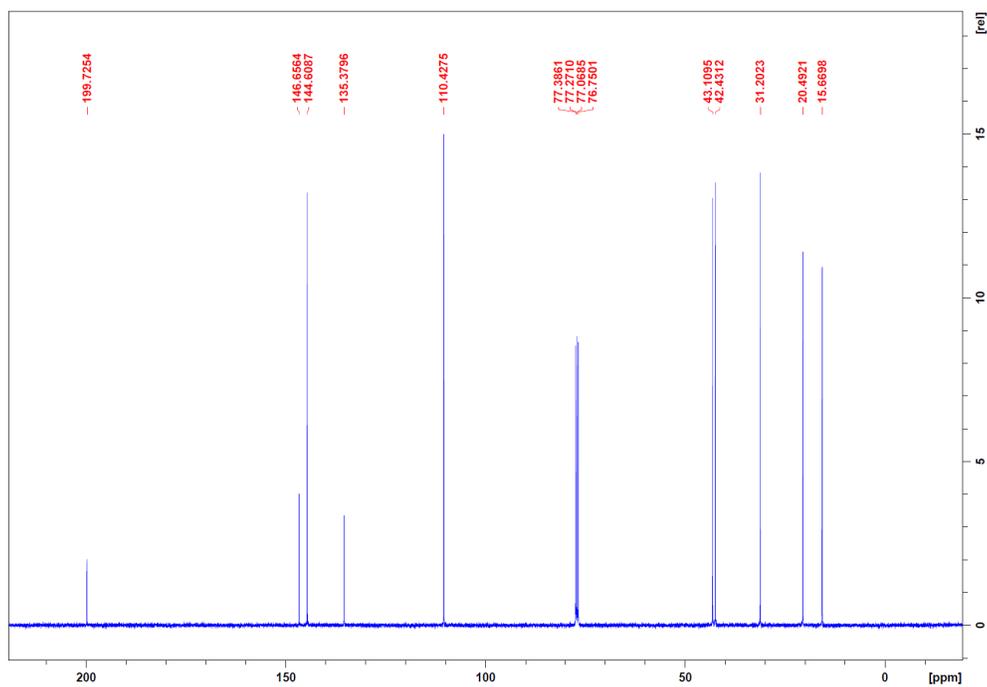
COSY:



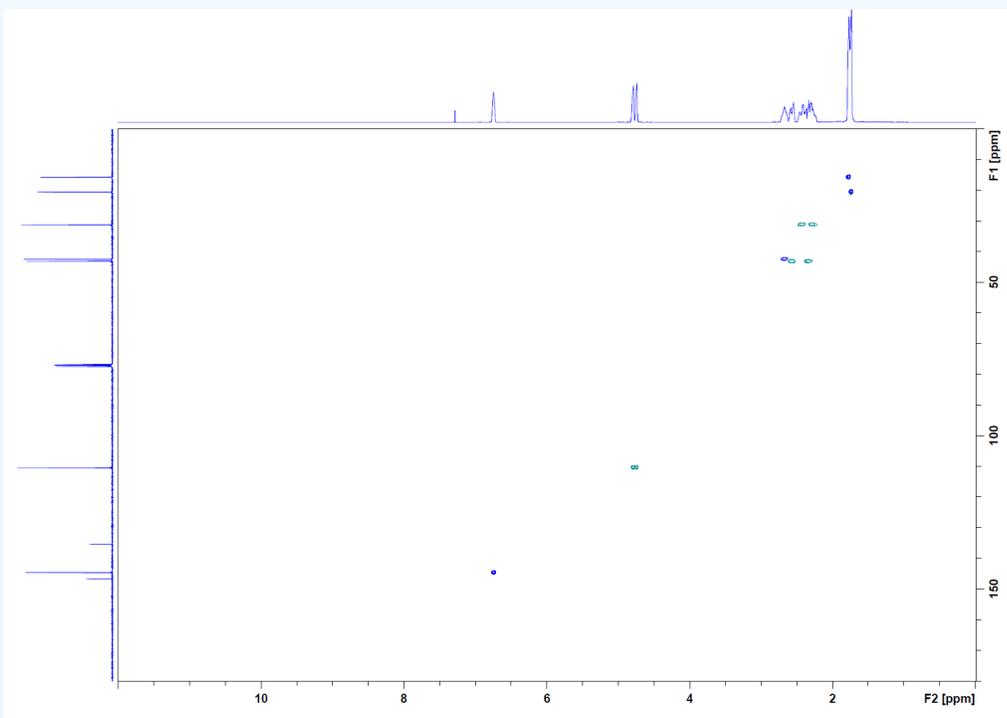
NOESY:



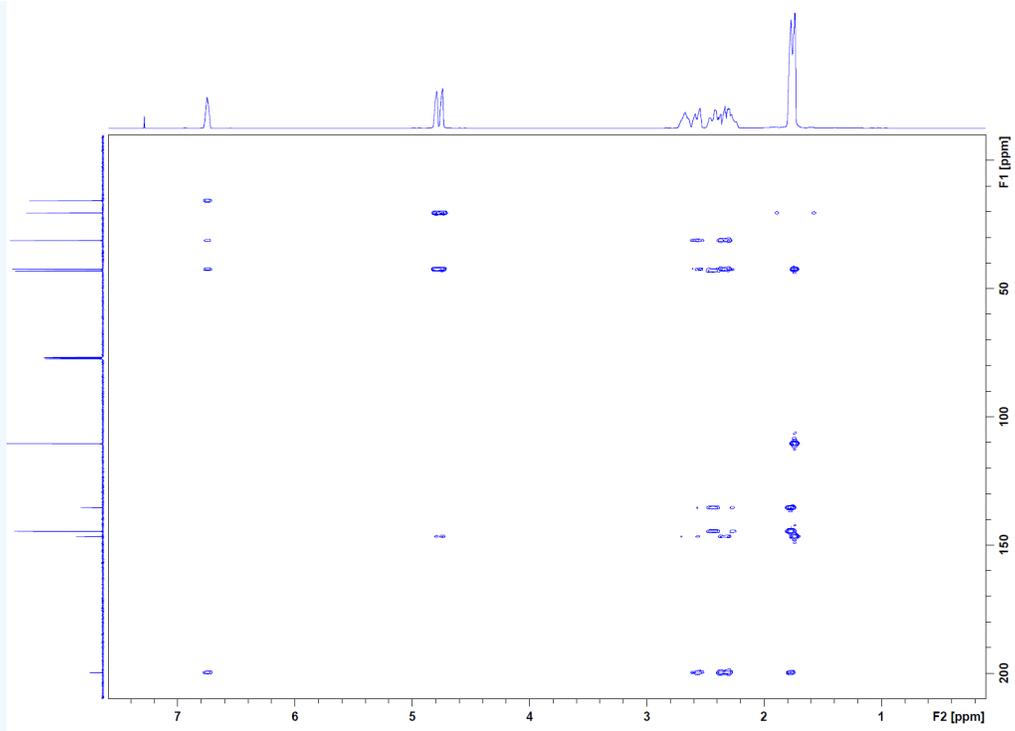
¹³C:



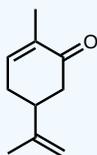
HSQC:



HMBC:



Answer

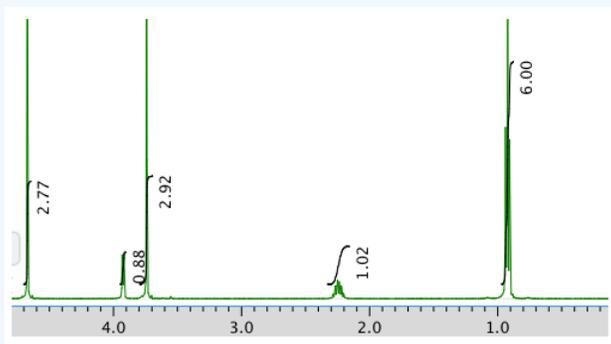


? Exercise 7.7.2

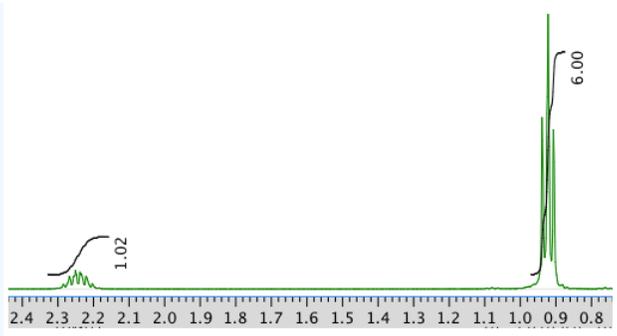
Present an analysis of the following data and propose a structure.

MW: 131 amu

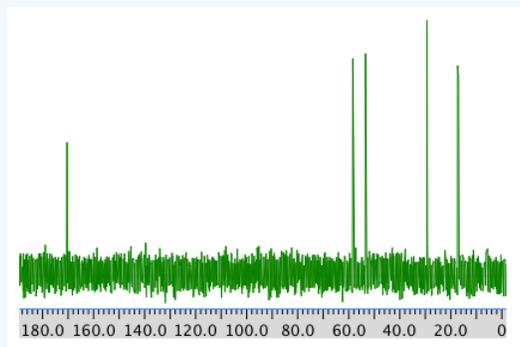
The full ^1H NMR spectrum in D_2O :



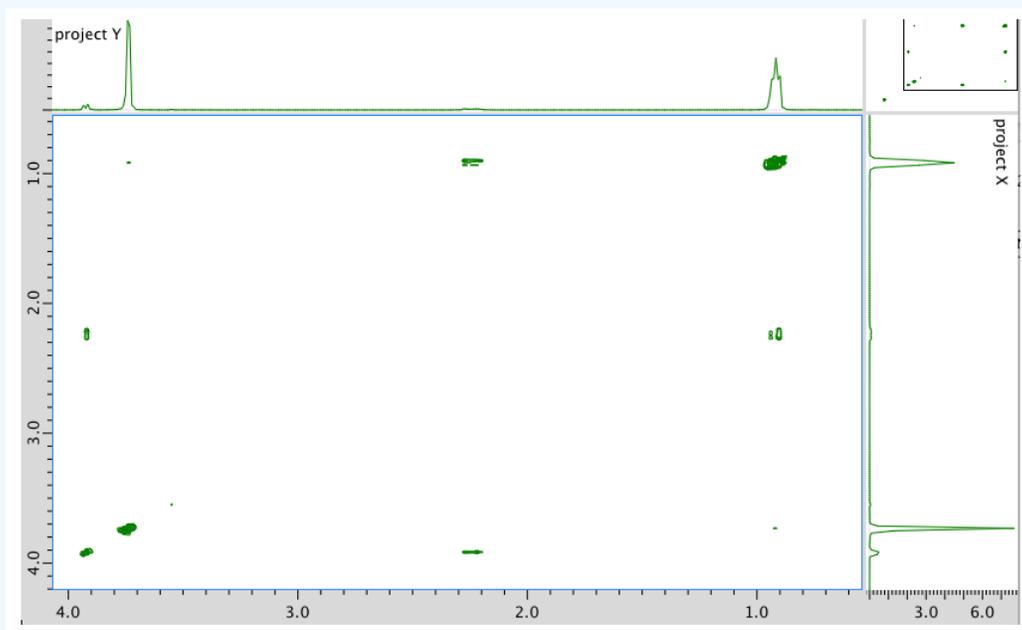
An expansion:



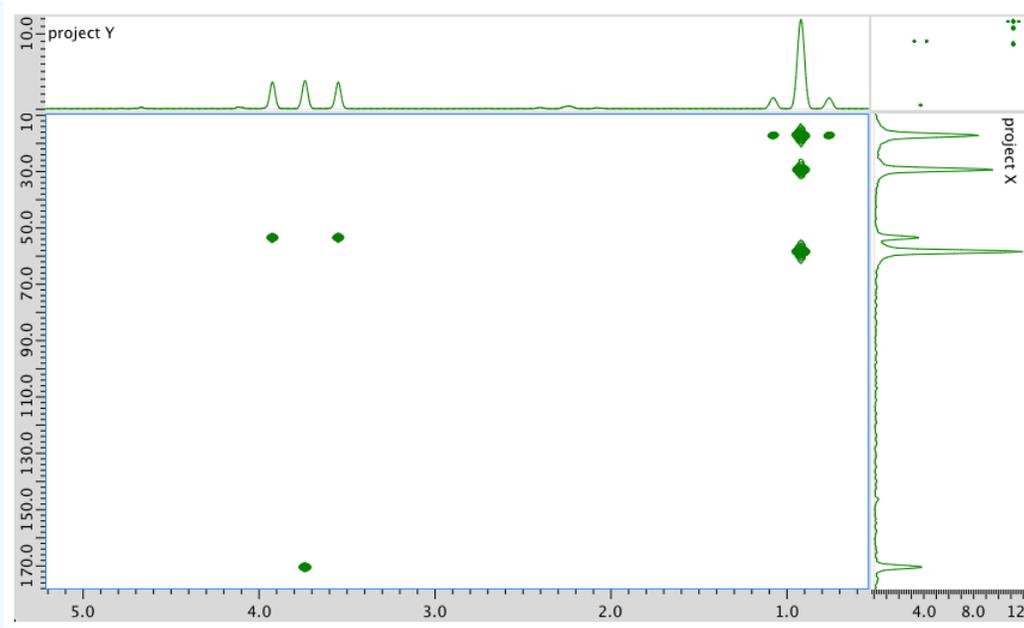
^{13}C NMR:



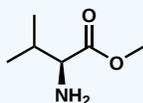
COSY:



HMBC:



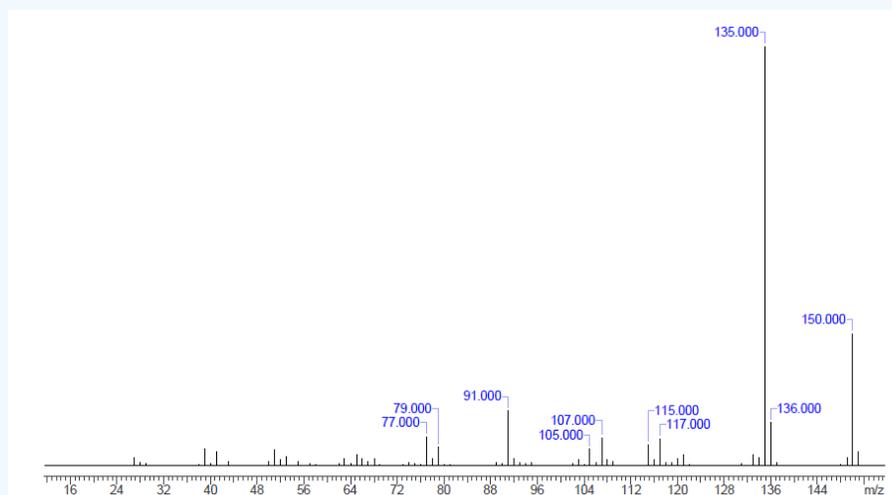
Answer



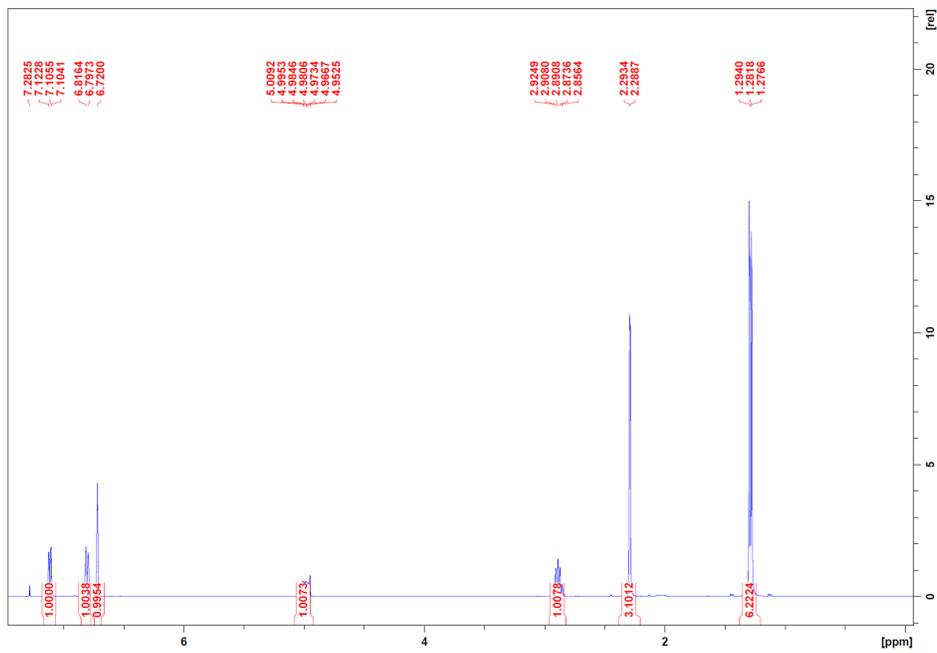
✓ Example 7.7.3

Propose a structure using the spectral data below for $C_{10}H_{14}O$. Note: You may need to check for solvent peaks. This sample was dissolved in $CDCl_3$.

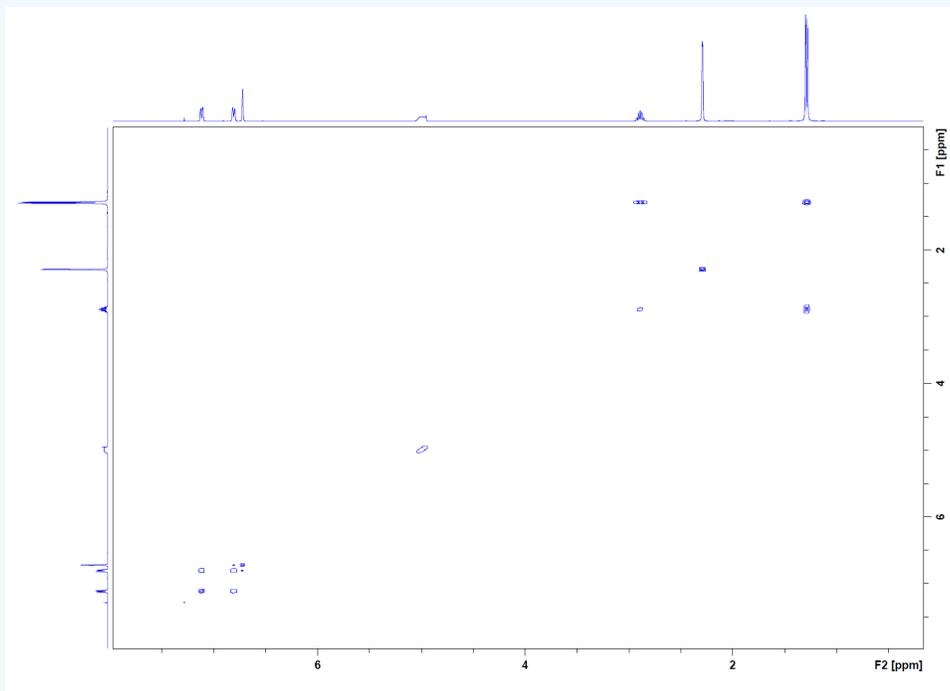
Mass Spectrum:



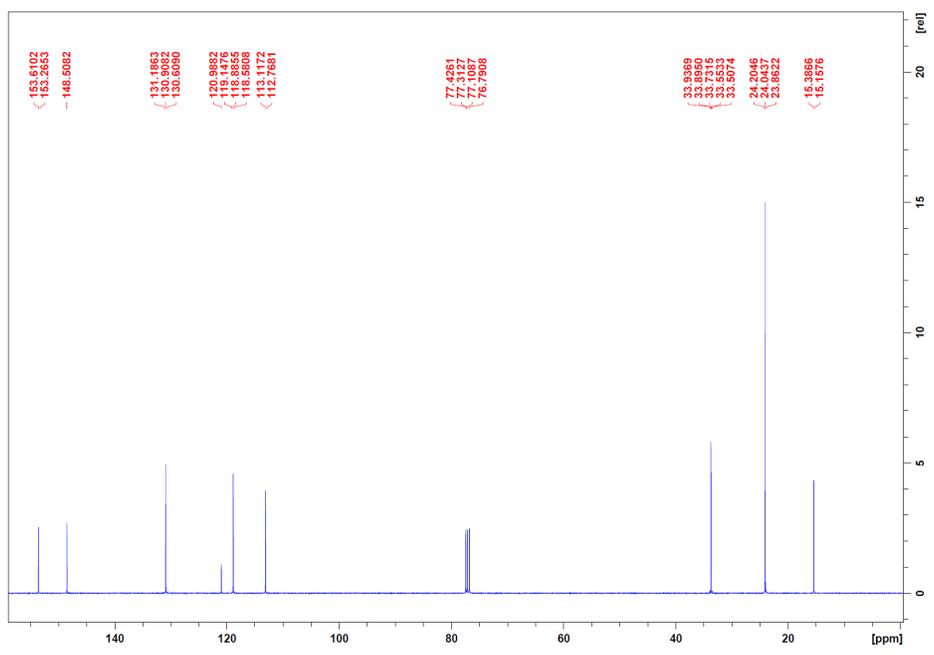
1H :



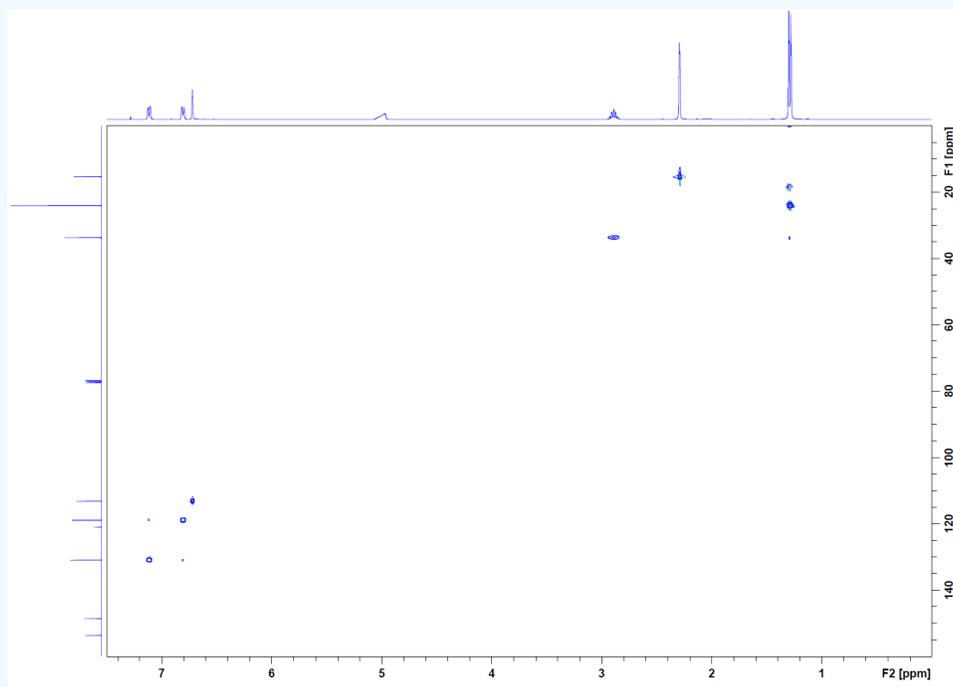
COSY:



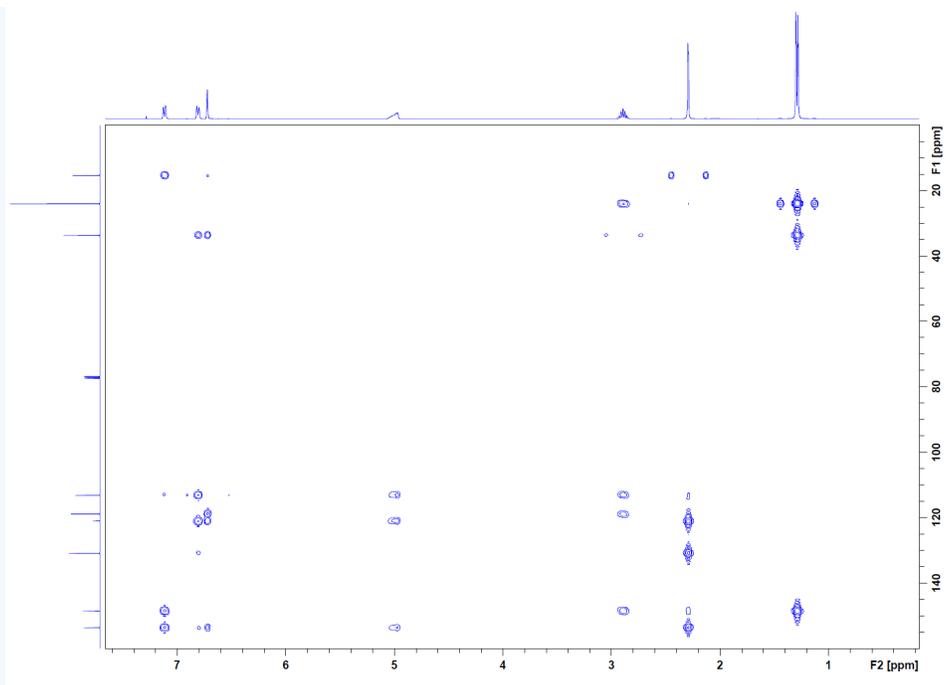
¹³C:



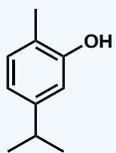
HSQC:



HMBC:



Solution



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