

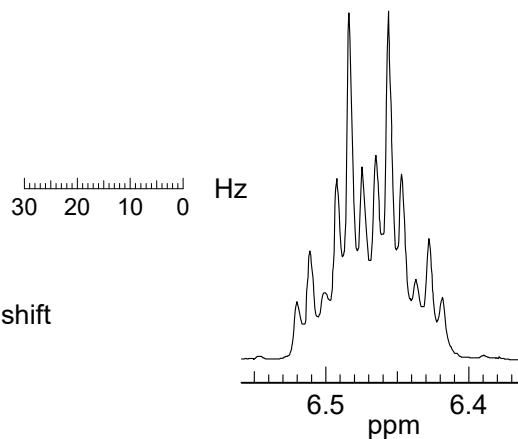
**Problem R-55E.** The basics.

(a) Analyze the one proton multiplet shown. (5 points)

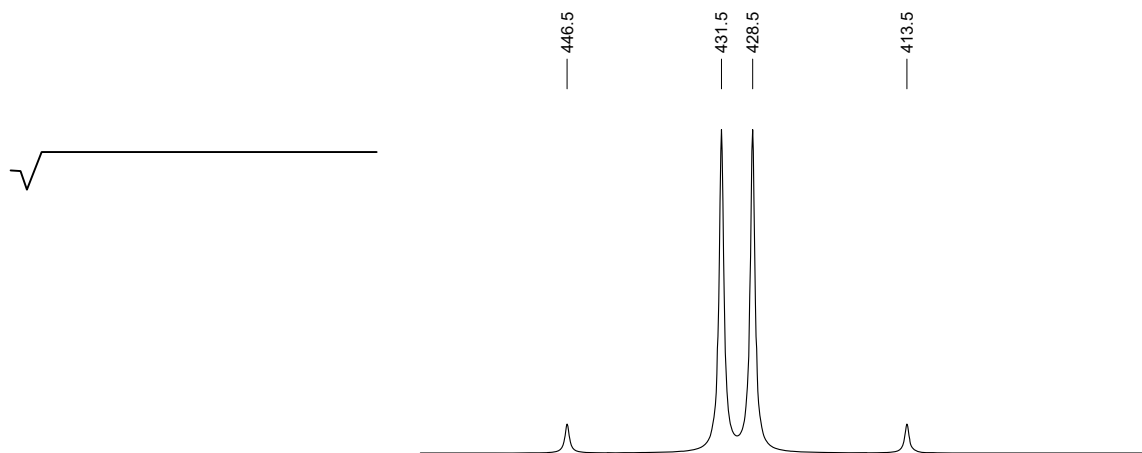
Type of multiplet: \_\_\_\_\_

Coupling constants: \_\_\_\_\_

Suggest a part structure, based on the coupling and chemical shift



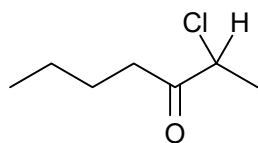
(b) Solve the two proton multiplet below. Determine J, and values from the peak positions given (200 MHz spectrometer) (5 points)



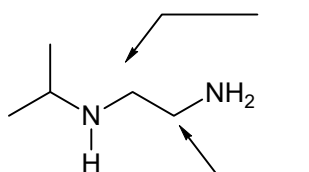
(c) One still occasionally sees  $^1\text{H}$  NMR spectra reported in units, and the older literature uses this scale predominantly. signal appears at  $\delta$  7.46, what is its chemical shift in ? \_\_\_\_\_ (2 points)

(d) A compound has an infrared peak at 4.32 microns. What is the position in  $\text{cm}^{-1}$ ? \_\_\_\_\_ (2 points)

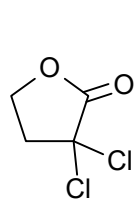
(g) Calculate the  $^1\text{H}$  chemical shift of H-2 of 2-chloro-3-heptanone. Show your work. (6 points)



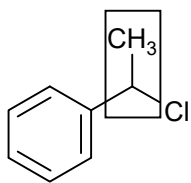
(h) The  $^{13}\text{C}$  chemical shift of  $\text{H}_2\text{N}-\text{CH}_2-\text{CH}_2-\text{NH}_2$  is  $\delta$  44.3. Estimate the chemical shifts of the underlined carbons in  $(\text{CH}_3)_2\text{CHNH}-\underline{\text{CH}_2}-\underline{\text{CH}_2}-\text{NH}_2$ . Show which parameters you used in your calculation. (6 points)



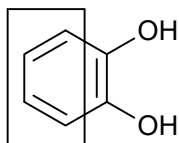
**Problem R-13A:** Identify the coupling pattern (e.g., AB<sub>2</sub>, AA'BB', AMX) expected for the structures below. Make a rough estimate of chemical shifts to help in deciding between AB and AX assignment.



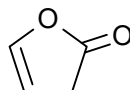
a \_\_\_\_\_



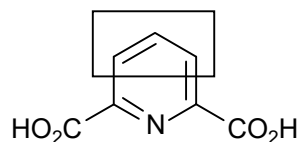
b \_\_\_\_\_



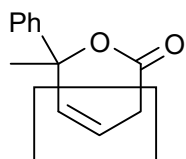
c \_\_\_\_\_



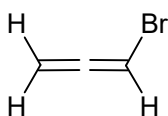
d \_\_\_\_\_



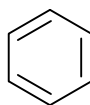
e \_\_\_\_\_



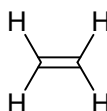
f \_\_\_\_\_



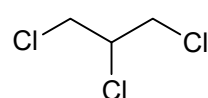
g \_\_\_\_\_



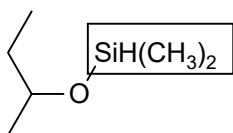
h \_\_\_\_\_



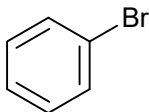
i \_\_\_\_\_



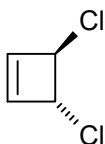
j \_\_\_\_\_



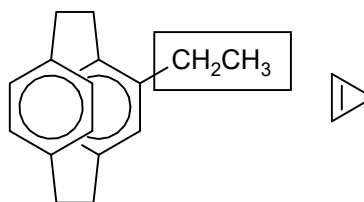
k \_\_\_\_\_



l \_\_\_\_\_



m \_\_\_\_\_



n \_\_\_\_\_



o \_\_\_\_\_

**Problem R-256** ( $C_{22}H_{20}O$ ). The 200 MHz  $^1H$  spectrum of R-256 is provided.

(a) DBE \_\_\_\_\_

(b) For each of the multiplets at  $\delta$  4.0, 3.1 and 2.8 show a "coupling tree" (work on the spectrum), indicate the type of multiplet and the coupling constants derived from each multiplet. Report them in the standard format

$\delta$  4.0 \_\_\_\_\_

$\delta$  3.1 \_\_\_\_\_

$\delta$  2.8 \_\_\_\_\_

(c) What type of pattern is this (e.g., AA'BB')? \_\_\_\_\_

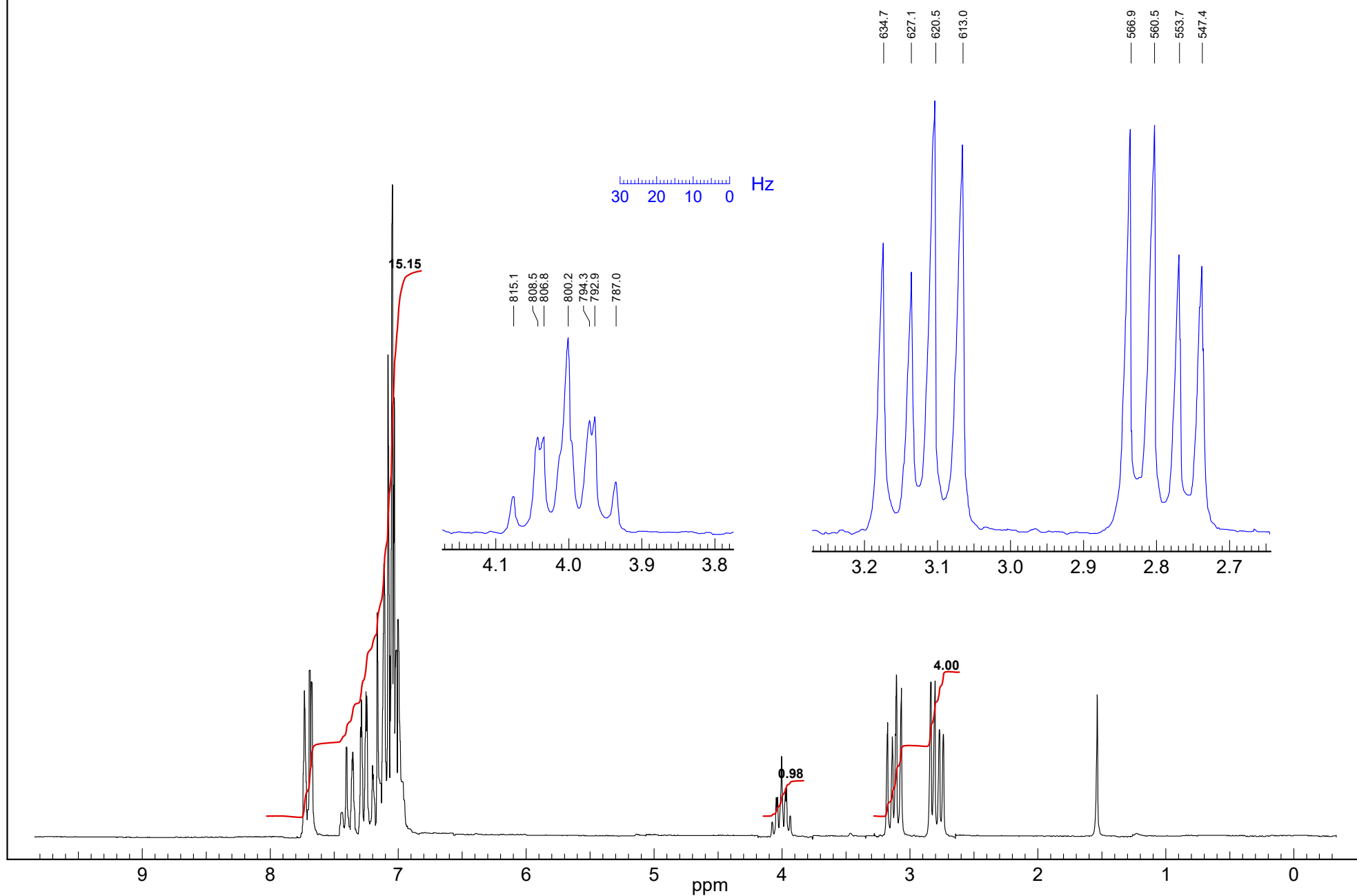
(d) Suggest a partial structure for the molecular fragment which includes these protons.

(e) There is a strong IR absorption at  $1695\text{ cm}^{-1}$ . Suggest a structure for compound **R-256**. If you have more than one possible structure, circle the one you like best.

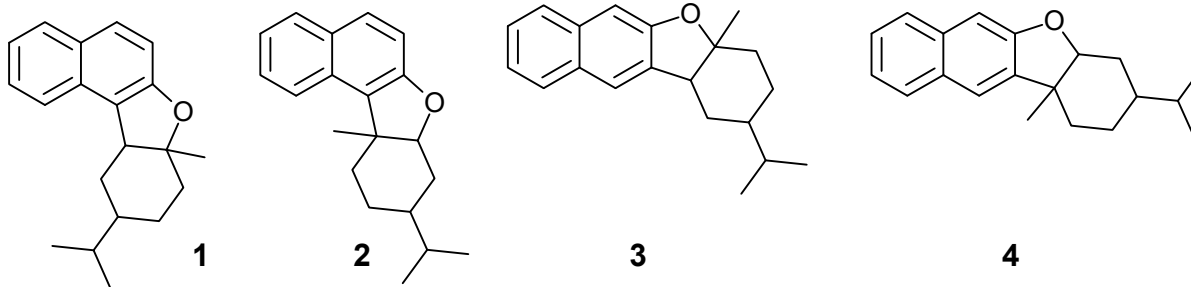
Problem R-256 (C<sub>22</sub>H<sub>20</sub>O)

200 MHz NMR Spectrum (CDCl<sub>3</sub>)

Source: Carl Hoeger/Reich 8-14 (digitized hard copy) g



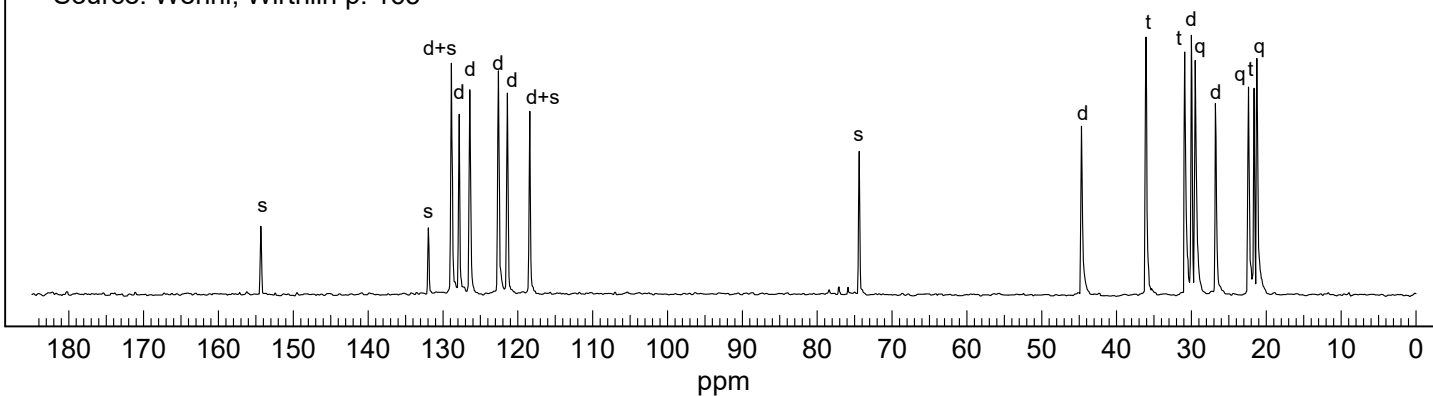
**Problem R-61** ( $C_{20}H_{24}O$ ). An adduct of  $\alpha$ -phellandrene and  $\beta$ -naohtl is expected to possess one of the structures **1** to **4**. Select the proper structure using the 100 MHz proton NMR spectrum and the 25.2 MHz proton noise decoupled  $^{13}C$  NMR spectrum



**Problem R-61** ( $C_{20}H_{24}O$ ).

25.2 MHz  $^{13}C$  NMR spectrum  $CDCl_3$

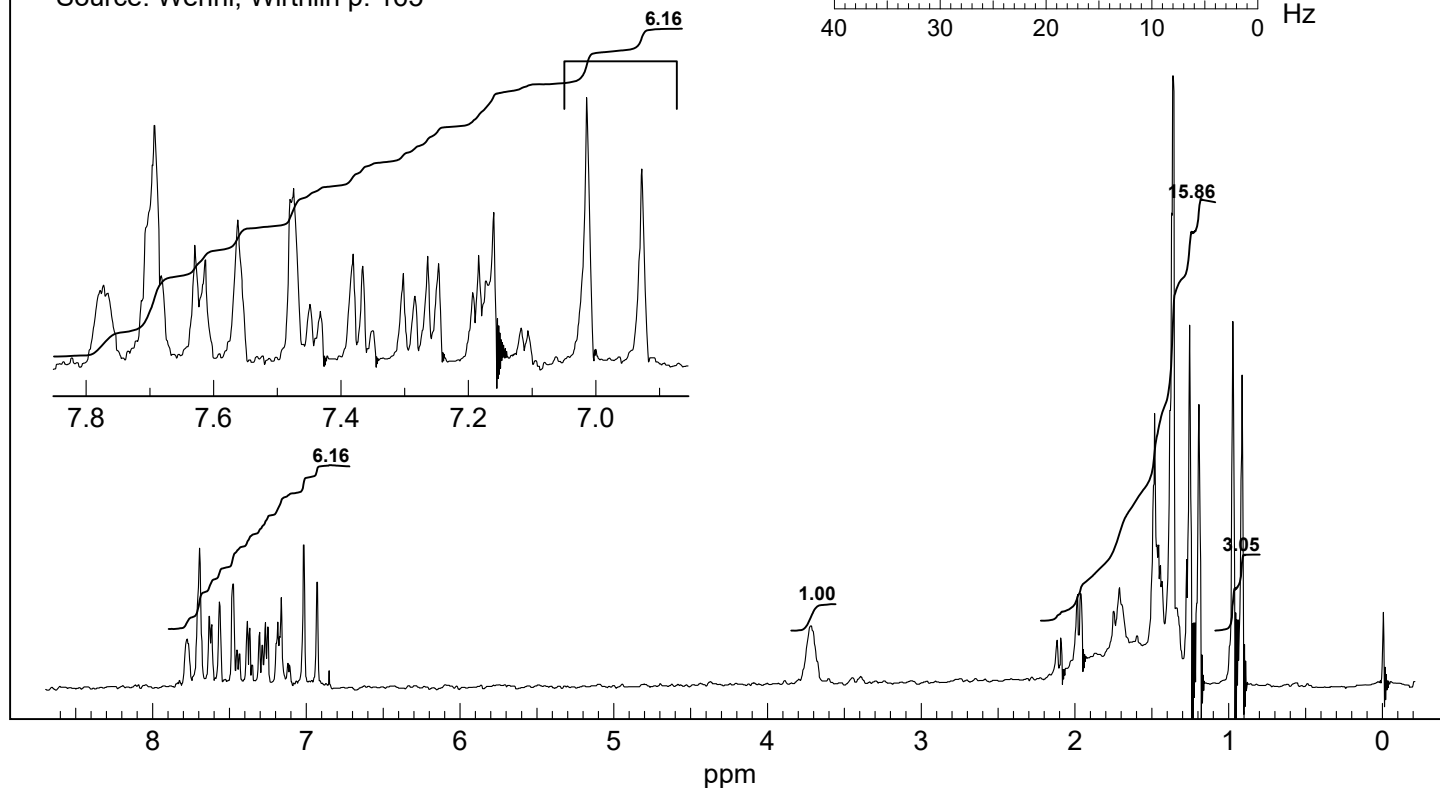
Source: Wehrli, Wirthlin p. 165



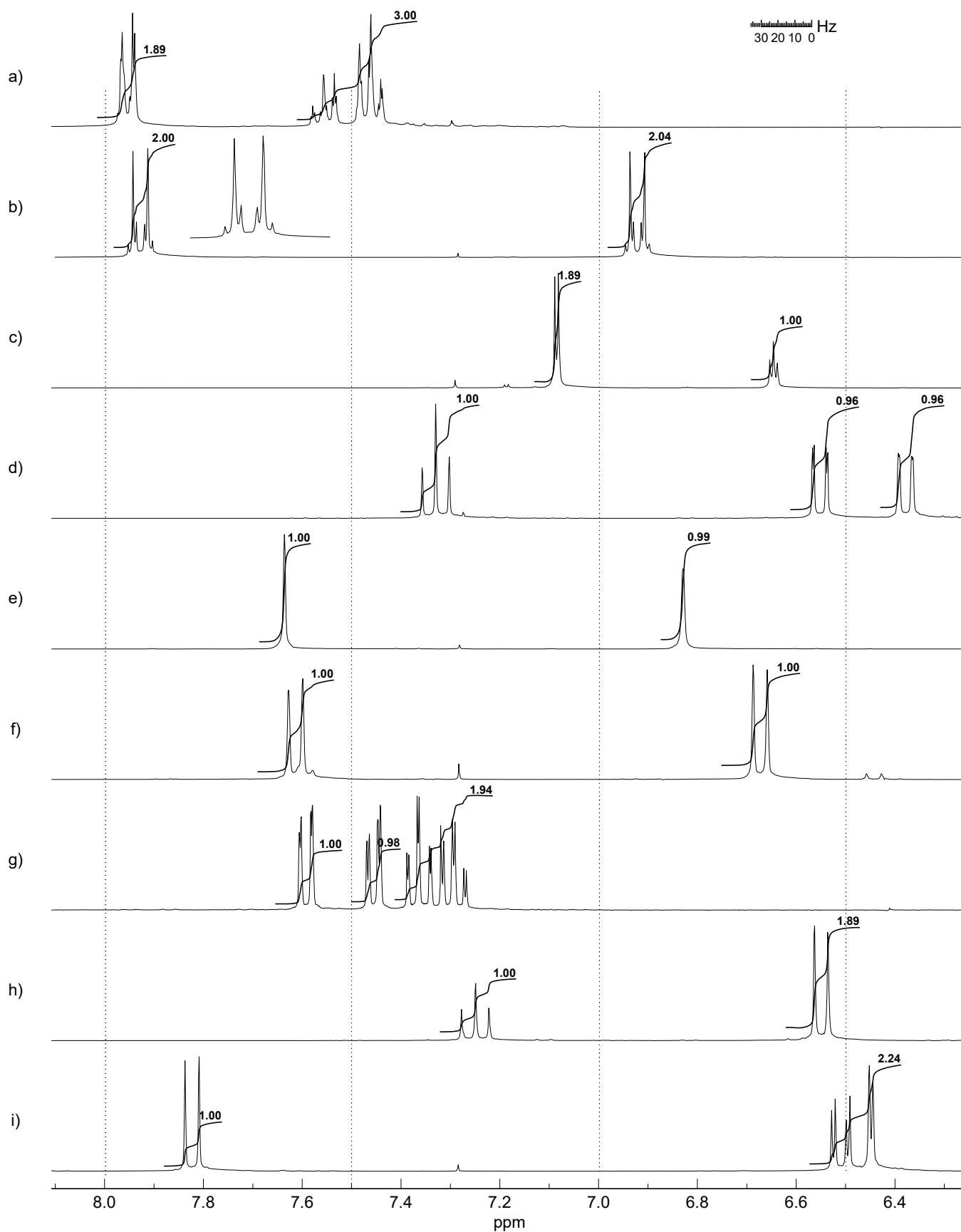
**Problem R-61** ( $C_{20}H_{24}O$ ).

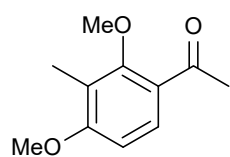
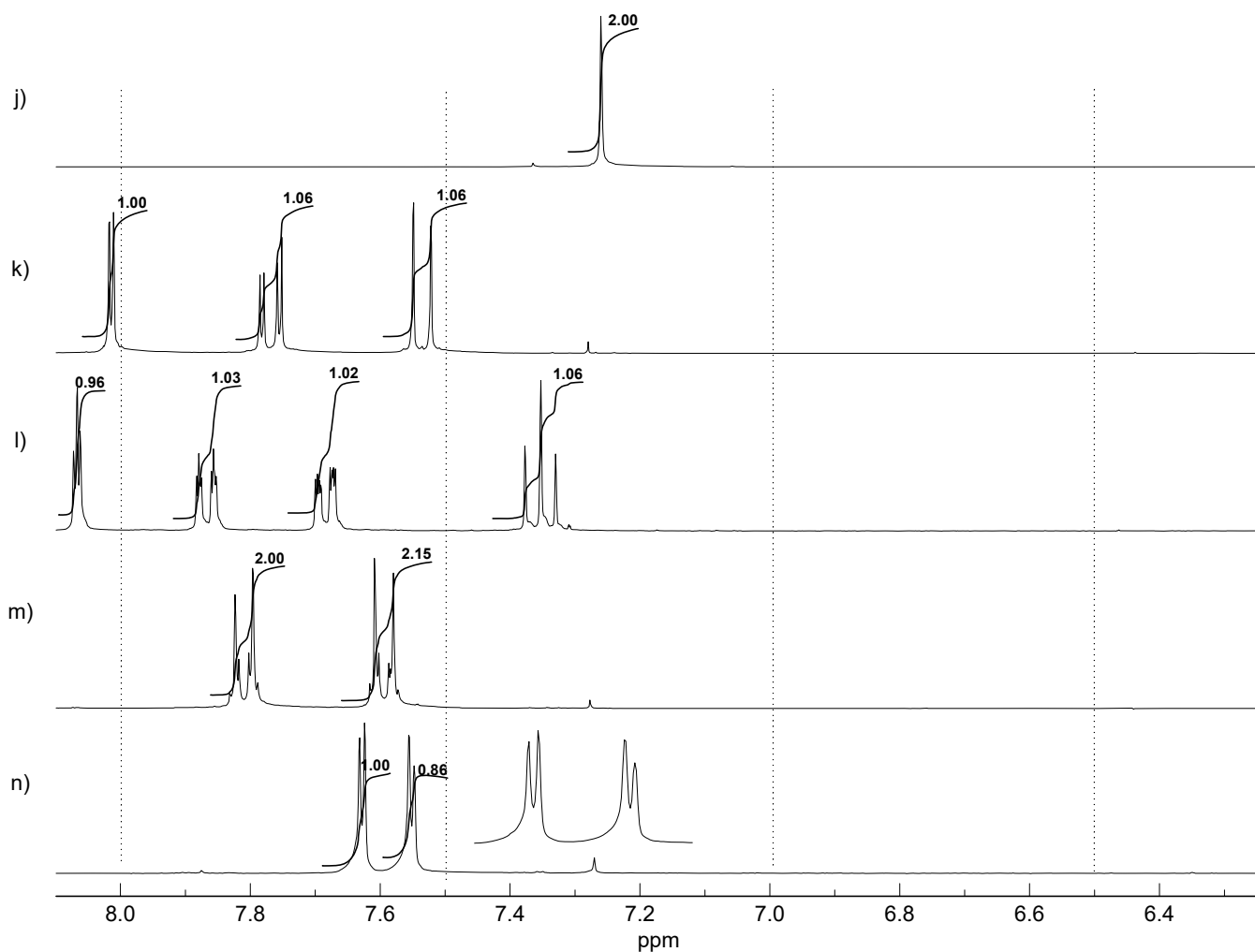
100 MHz  $^1H$  NMR spectrum  $CDCl_3$

Source: Wehrli, Wirthlin p. 165

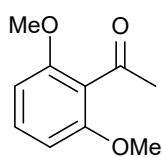


**Problem R-02A.** Select the correct structure from the list of possible substituted benzenes provided. You should not have to do more than the occasional chemical shift calculation to identify the correct structure (Source: Aldrich Spectra Viewer).

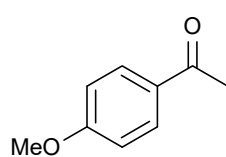




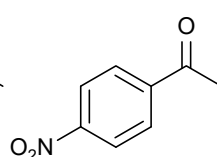
**1**



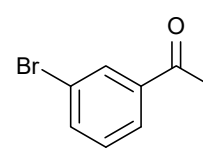
**2**



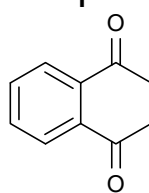
**3**



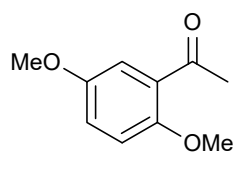
**4**



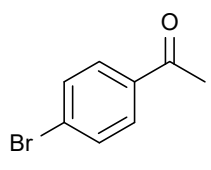
**5**



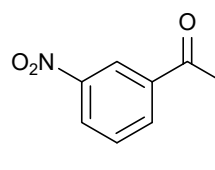
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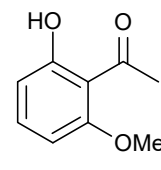
**7**



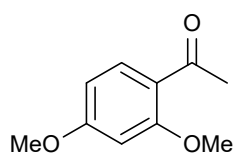
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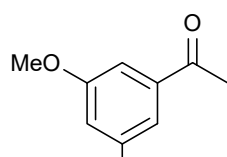
**9**



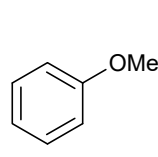
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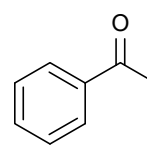
**11**



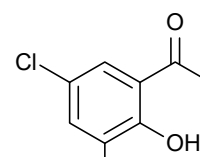
**12**



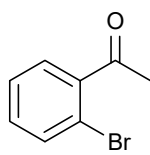
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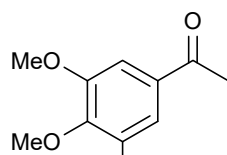
**14**



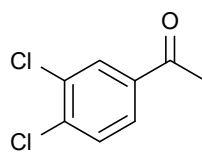
**15**



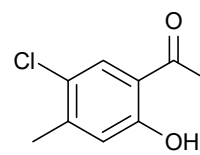
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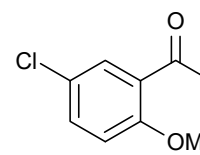
**17**



**18**



**19**



**20**