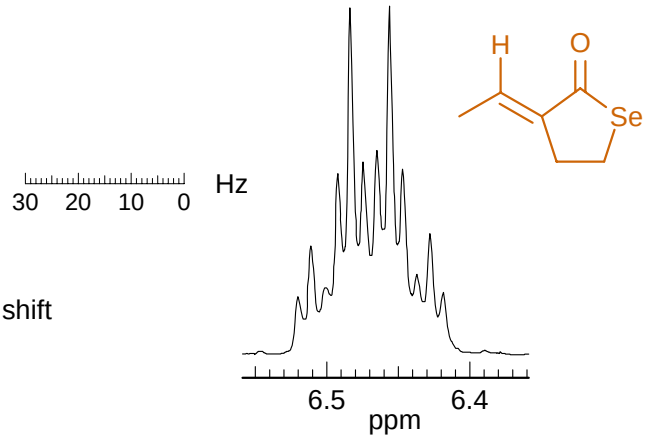
Problem R-55E. The basics.

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

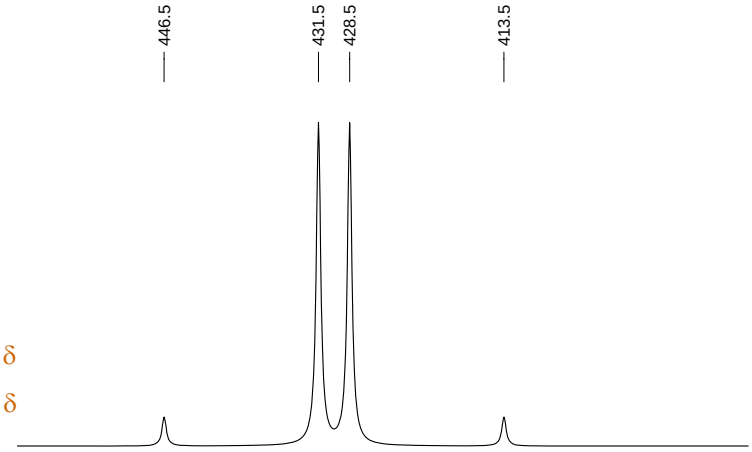


Type of multiplet: qt

Coupling constants: 7, 2.5 Hz

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)



This is an AB pattern

J_{AB} = 15 Hz

$\nu_{AB} = \sqrt{(446.5-413.5)(431.5-428.5)}$

= 9.9 Hz

Center = (428.5-431.5)/2 = 430 Hz

ν_A = 430 + 9.9/2 = 434.9 Hz = 2.17 δ

ν_A = 430 - 9.9/2 = 425.1 Hz = 2.12 δ

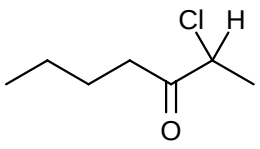
(c) One still occasionally sees ^{1}H NMR spectra reported in units, and the older literature uses this scale predominantly. If a signal appears at δ 7.46, what is its chemical shift in ? ___ (2 points)

δ = 10 - τ = 2.54

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

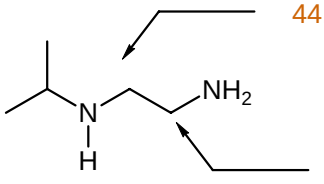
$$\text{Wave number} = \frac{10{,}000}{\nu} = 2314.8$$

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



Base:	1.55
α-Cl (CH)	2.55
α-Keto (CH)	0.95
	5.05

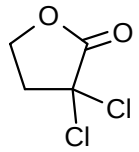
(h) The ^{13}C chemical shift of H_2N-CH_2-CH_2-NH_2 is δ 44.3. Estimate the chemical shifts of the underlined carbons in $(CH_3)_2CHNH$-$\underline{C}H_2$-$\underline{C}H_2$-NH_2. Show which parameters you used in your calculation. (6 points)



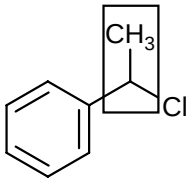
$44.3 + \beta_C + 2\gamma_C = 44.3 + 9.4 - 5.0 = 48.7$

$44.3 + \gamma_C + 2\,\delta_C = 44.3 - 2.5 - 0.6 = 42.4$

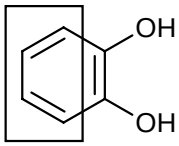
Problem R-13A: Identify the coupling pattern (e.g., AB_2, AA'BB', AMX) expected for the structures below. Make a rough estimate of chemical shifts to help in deciding between AB and AX assignment.



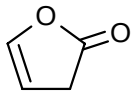
a AA'BB'



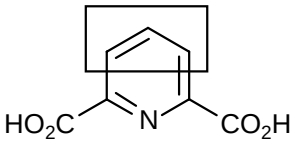
b AX_3



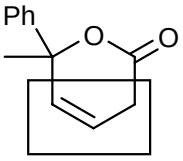
c AA'BB'



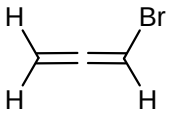
d AMX_2



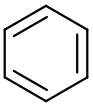
e AB_2



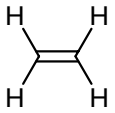
f ABXY



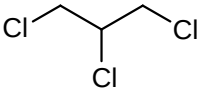
g AX_2



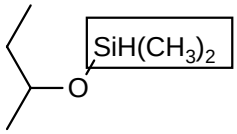
h AA'A''A''' ....



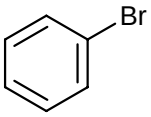
i AA'A''A'''



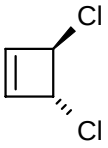
j AA'BB'X



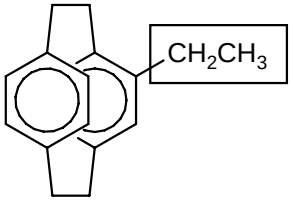
k A_3B_3X



l AA'BB'C



m AA'BB'



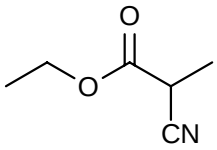
n ABX_3

o A_2X_2

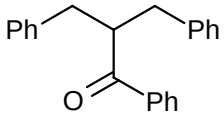
h, i: This would usually be assigned as A_6 (or A_4 for ethylene), but if you strictly apply the criteria, all the protons are magnetically inequivalent, and thus it is an AA'A''A'''.... system

j: Because the A and A', as well as B and B' protons are not coupled to each other, this could also be called an $(AB)_2X$ pattern

Problem R-77D

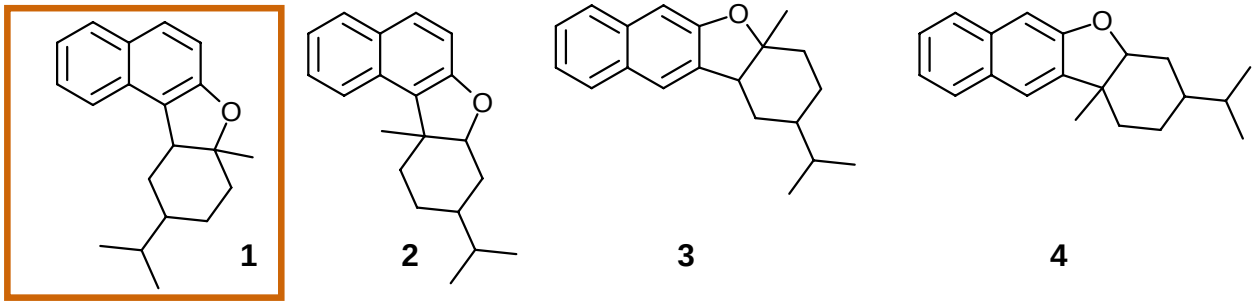


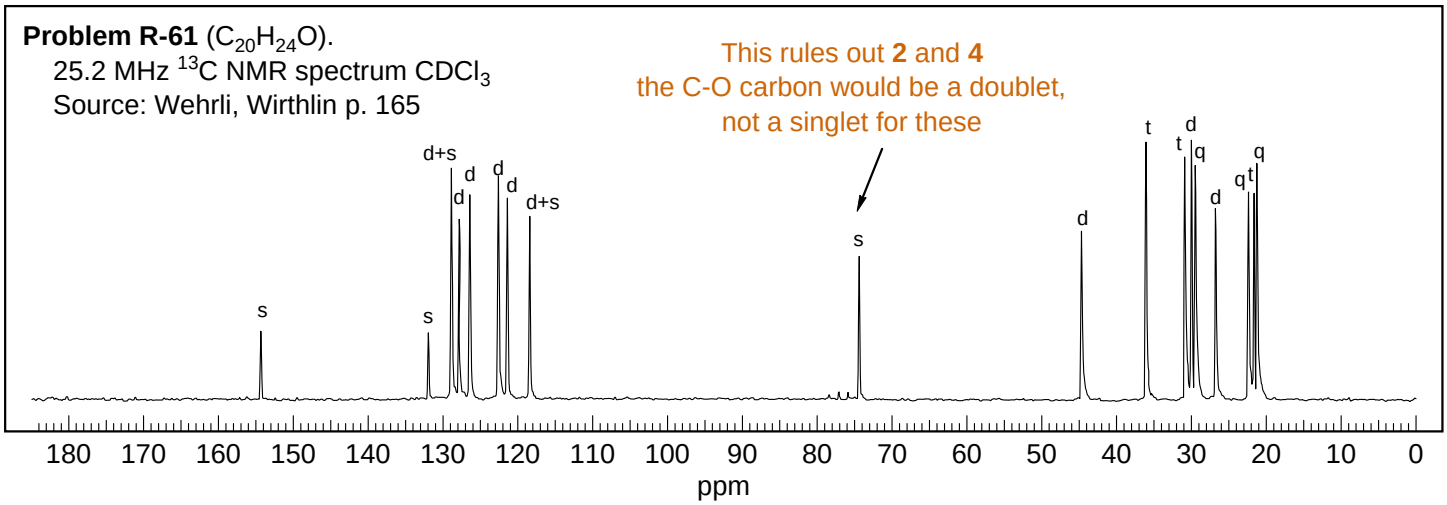
Problem R-256

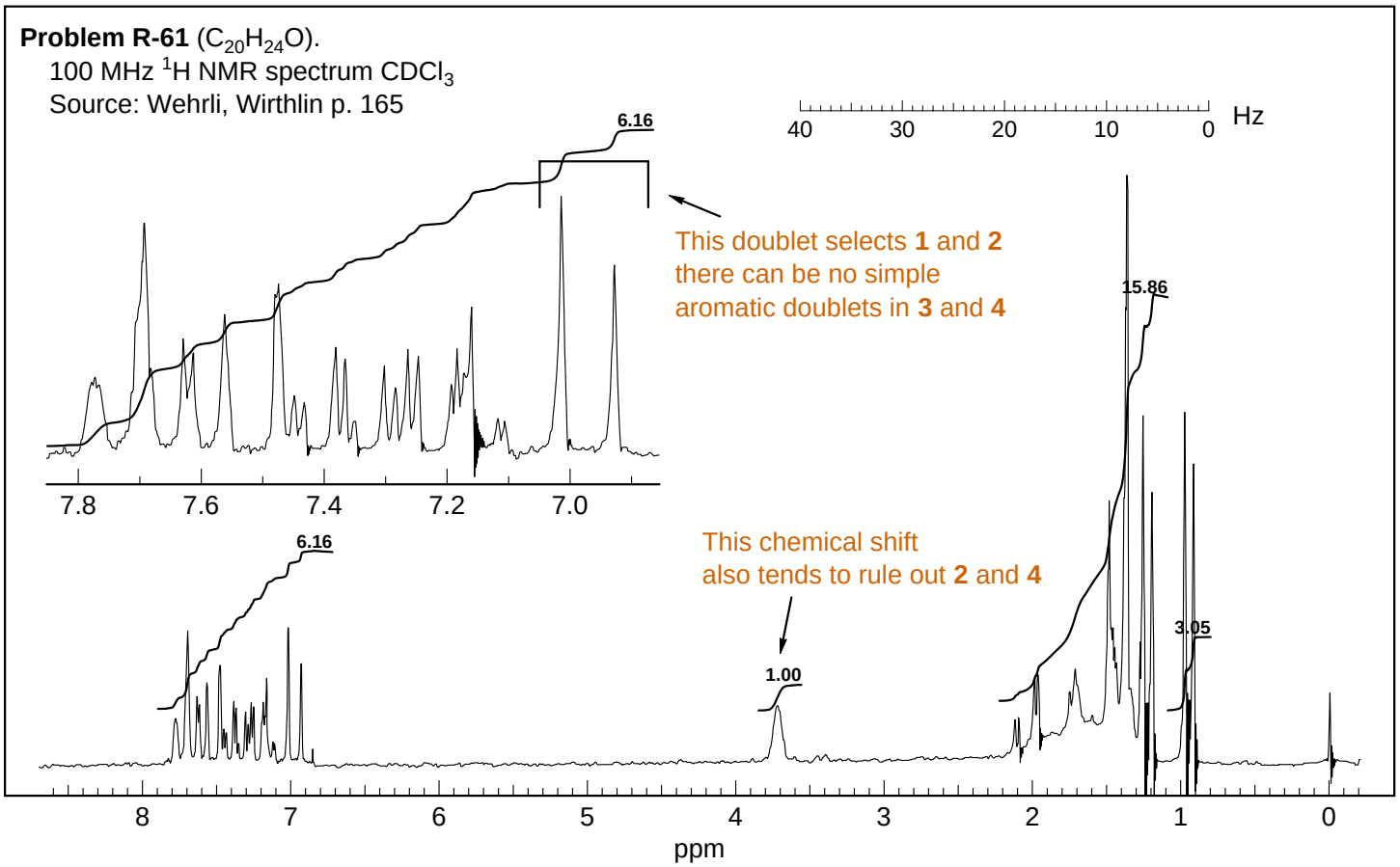


AA'MM'X (or perhaps better $(AM)_2X$ since A is not coupled to A' and B is not coupled to B')

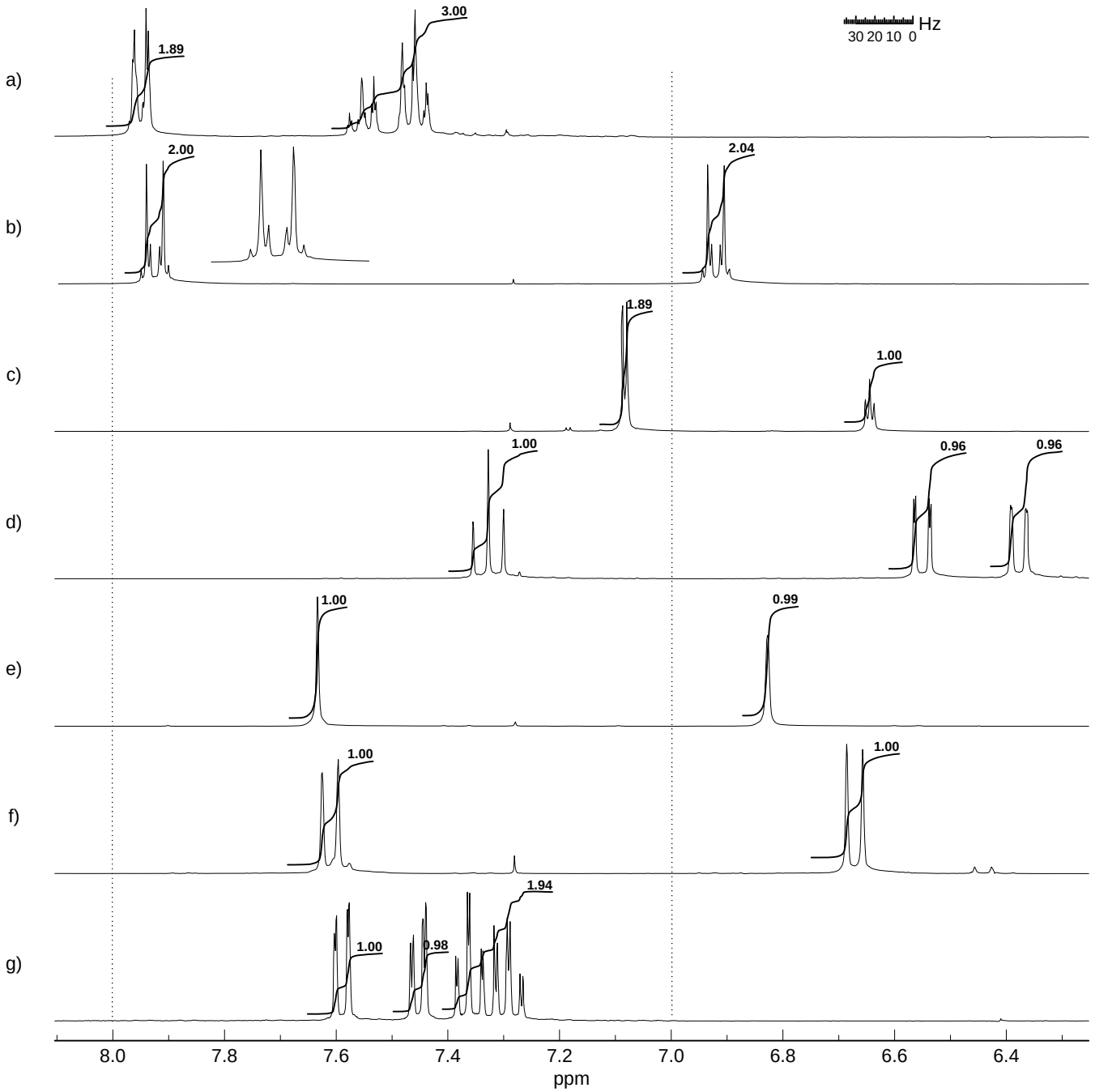
Problem R-61 ($C_{20}H_{24}O$). An adduct of α-phellandrene and β-naohthl is expected to possess one of the structures **1** to **4**. Select the proper structure using the 100 MHz proton NMR spectrum and the 25.2 MHz proton noise decoupled ^{13}C NMR spectrum



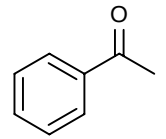




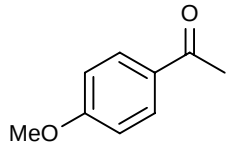
Problem R-02A. Select the correct structure from the list of possible substituted benzenes provided. You should not have to do more than the occasional chemical shift calculation to identify the correct structure (Source: Aldrich Spectra Viewer).



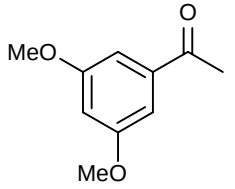
14
13



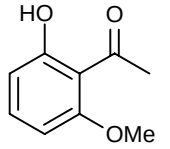
3
4
8



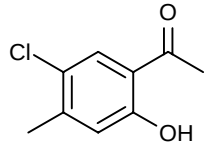
12



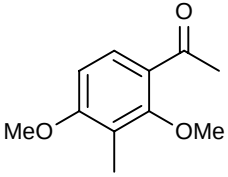
10



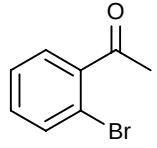
19

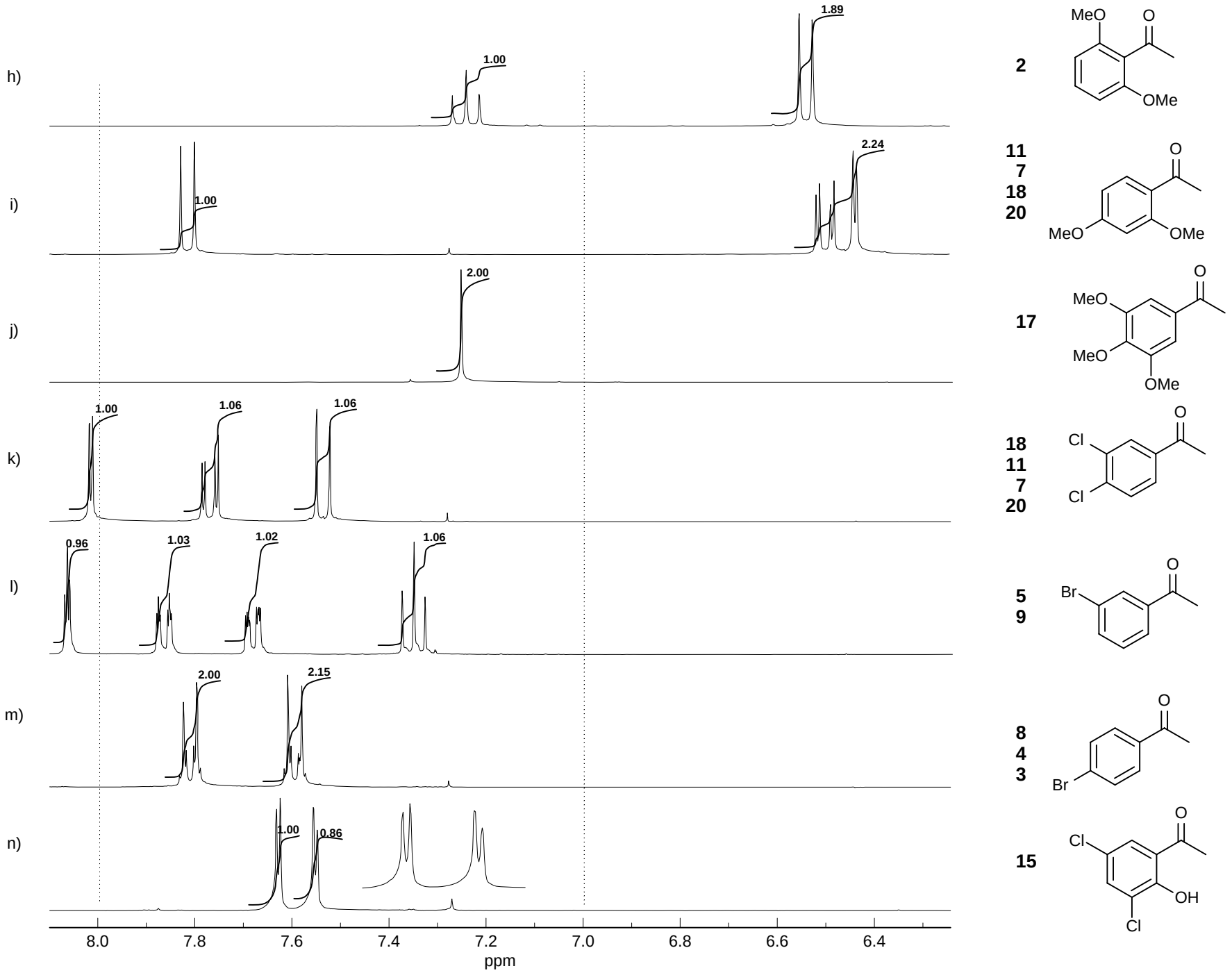


1



16




h)
1.00
1.89
i)
1.00
2.24
j)
2.00
k)
1.00
1.06
1.06
l)
0.96
1.03
1.02
1.06
m)
2.00
2.15
n)
1.00
0.86
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
ppm
2
MeO
O
OMe
11
7
18
20
O
MeO
OMe
17
O
MeO
MeO
OMe
18
11
7
20
O
Cl
Cl
5
9
O
Br
8
4
3
O
Br
15
O
Cl
OH
Cl