Additional NMR Examples

For each molecule, predict the number of signals in the $^1$H-NMR and the $^{13}$C-NMR spectra (do not count split peaks - eg. a quartet counts as only one signal). Assume that diastereotopic groups are non-equivalent.

a) \( \text{CH}_2=\text{CH}-\text{CO} \)  b) \( \text{CH}_2=\text{CH}-\text{CO} \)  c) \( \text{CH}_2=\text{CH}-\text{CO} \)  d) \( \text{CH}_2=\text{CH}-\text{OH} \)

e) \( \text{Cl} \)  f) \( \text{Cl} \)  g) \( \text{Cl} \)  h) \( \text{Cl} \)

i) \( \text{H} \text{C}=\text{C} \text{Cl} \)  j) \( \text{H} \text{C}=\text{C} \text{F} \)  k) \( \text{H}_3\text{C} \text{C}=\text{C} \text{OH} \)  l) \( \text{H}_3\text{C} \text{C}=\text{C} \text{OH} \)

m) \( \text{CH}_3 \)  n) \( \text{CH}_3 \)  o) \( \text{HO} \text{C} \text{H}_2 \text{OH} \)

**P5.2:** For each of the 20 common amino acids, predict the number of signals in the proton-decoupled $^{13}$C-NMR spectrum.

**P5.3:** Calculate the chemical shift value (expressed in Hz, to one decimal place) of each sub-peak on the $^1$H-NMR doublet signal below. Do this for:

a) a spectrum obtained on a 300 MHz instrument

b) a spectrum obtained on a 100 MHz instrument
P5.4: Consider a quartet signal in an $^1$H-NMR spectrum obtained on a 300 MHz instrument. The chemical shift is recorded as 1.7562 ppm, and the coupling constant is $J = 7.6$ Hz. What is the chemical shift, expressed to the nearest 0.1 Hz, of the furthest downfield sub-peak in the quartet? What is the resonance frequency (again expressed in Hz) of this sub-peak?

P5.5: One easily recognizable splitting pattern for the aromatic proton signals from disubstituted benzene structures is a pair of doublets. Does this pattern indicate ortho, meta, or para substitution?

P5.6: Match spectra below to their corresponding structures A-F.

**Structures:**

![Structures A-F](image)

**Spectrum 1**
<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.13</td>
<td>q</td>
<td>2</td>
</tr>
<tr>
<td>2.45</td>
<td>t</td>
<td>2</td>
</tr>
<tr>
<td>1.94</td>
<td>quintet</td>
<td>1</td>
</tr>
<tr>
<td>1.27</td>
<td>t</td>
<td>3</td>
</tr>
</tbody>
</table>

**Spectrum 2**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.68</td>
<td>s</td>
<td>3</td>
</tr>
<tr>
<td>2.99</td>
<td>t</td>
<td>2</td>
</tr>
<tr>
<td>1.95</td>
<td>quintet</td>
<td>1</td>
</tr>
</tbody>
</table>

**Spectrum 3**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.14</td>
<td>q</td>
<td>1</td>
</tr>
<tr>
<td>2.62</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>1.26</td>
<td>t</td>
<td>1.5</td>
</tr>
</tbody>
</table>
### Spectrum 4

<table>
<thead>
<tr>
<th>δ splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.14 q</td>
<td>4</td>
</tr>
<tr>
<td>3.22 s</td>
<td>1</td>
</tr>
<tr>
<td>1.27 t</td>
<td>6</td>
</tr>
<tr>
<td>1.13 s</td>
<td>9</td>
</tr>
</tbody>
</table>

### Spectrum 5

<table>
<thead>
<tr>
<th>δ splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.18 q</td>
<td>1</td>
</tr>
<tr>
<td>1.92 q</td>
<td>1</td>
</tr>
<tr>
<td>1.23 t</td>
<td>1.5</td>
</tr>
<tr>
<td>0.81 t</td>
<td>1.5</td>
</tr>
</tbody>
</table>

### Spectrum 6

<table>
<thead>
<tr>
<th>δ splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.69 s</td>
<td>1.5</td>
</tr>
<tr>
<td>2.63 s</td>
<td>1</td>
</tr>
</tbody>
</table>
P5.7: Match spectra 7-12 below to their corresponding structures G-L.

Structures:

G

H

I

(J = 0 for geminal vinylic protons)

J

K

L

Spectrum 7:

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.96</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>5.88</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>2.17</td>
<td>s</td>
<td>3</td>
</tr>
<tr>
<td>1.98</td>
<td>s</td>
<td>3</td>
</tr>
</tbody>
</table>

Spectrum 8:
<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.36</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>6.55</td>
<td>q</td>
<td>1</td>
</tr>
<tr>
<td>2.26</td>
<td>q</td>
<td>2</td>
</tr>
<tr>
<td>1.99</td>
<td>d</td>
<td>3</td>
</tr>
<tr>
<td>0.96</td>
<td>t</td>
<td>3</td>
</tr>
</tbody>
</table>

**Spectrum 9:**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.57</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>6.30</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>6.00</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>1.84</td>
<td>s</td>
<td>3</td>
</tr>
</tbody>
</table>

**Spectrum 10:**
<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.83</td>
<td>t</td>
<td>1</td>
</tr>
<tr>
<td>2.27</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>1.07</td>
<td>s</td>
<td>9</td>
</tr>
</tbody>
</table>

**Spectrum 11:**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.75</td>
<td>t</td>
<td>1</td>
</tr>
<tr>
<td>2.30</td>
<td>dd</td>
<td>2</td>
</tr>
<tr>
<td>2.21</td>
<td>m</td>
<td>1</td>
</tr>
<tr>
<td>0.98</td>
<td>d</td>
<td>6</td>
</tr>
</tbody>
</table>

**Spectrum 12:**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.08</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>4.13</td>
<td>t</td>
<td>2</td>
</tr>
</tbody>
</table>
P5.8: Match the $^1$H-NMR spectra 13-18 below to their corresponding structures M-R.

Structures:

- **M**
- **N**
- **O**
- **P**
- **Q**
- **R**

**Spectrum 13:**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.15</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>6.33</td>
<td>d</td>
<td>1</td>
</tr>
</tbody>
</table>
### Spectrum 14: 1-723C (structure O)

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.05</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>2.24</td>
<td>s</td>
<td>3</td>
</tr>
</tbody>
</table>

### Spectrum 15:

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.57</td>
<td>s (b)</td>
<td>1</td>
</tr>
<tr>
<td>7.89</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>6.30</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>2.28</td>
<td>s</td>
<td>3</td>
</tr>
</tbody>
</table>

### Spectrum 16:

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.05</td>
<td>s (b)</td>
<td>1</td>
</tr>
</tbody>
</table>
8.03  s  1
6.34  s  1
5.68  s (b)  1
4.31  s  2

Spectrum 17:

\[\delta \quad \text{splitting} \quad \text{integration}\]

7.76  d  1
7.57  s (b)  1
6.44  d  1
2.78  q  2
1.25  t  3

Spectrum 18:

\[\delta \quad \text{splitting} \quad \text{integration}\]
P5.9: Match the $^1$H-NMR spectra 19-24 below to their corresponding structures S-X.

Structures:

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.94</td>
<td>s</td>
<td>1</td>
</tr>
</tbody>
</table>

Spectrum 19:
<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.77</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>7.31</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>2.43</td>
<td>s</td>
<td>3</td>
</tr>
</tbody>
</table>

*Spectrum 20:*

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.14</td>
<td>s</td>
<td>2</td>
</tr>
<tr>
<td>8.38</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>8.17</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>7.75</td>
<td>t</td>
<td>1</td>
</tr>
</tbody>
</table>

*Spectrum 21:*

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.98</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>7.81</td>
<td>d</td>
<td>2</td>
</tr>
</tbody>
</table>
7.50  d  2

**Spectrum 22:**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.15-7.29</td>
<td>m</td>
<td>2.5</td>
</tr>
<tr>
<td>2.86</td>
<td>t</td>
<td>1</td>
</tr>
<tr>
<td>2.73</td>
<td>t</td>
<td>1</td>
</tr>
<tr>
<td>2.12</td>
<td>s</td>
<td>1.5</td>
</tr>
</tbody>
</table>

**Spectrum 23:**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.10</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>6.86</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>3.78</td>
<td>s</td>
<td>1.5</td>
</tr>
<tr>
<td>3.61</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>2.12</td>
<td>s</td>
<td>1.5</td>
</tr>
</tbody>
</table>

**Spectrum 24:**
**P5.10:** Match the $^1$H-NMR spectra 25-30 below to their corresponding structures AA-FF.

**Structures:**

**Spectrum 25:**

- **AA**
- **BB**
- **CC**

(spectrum does not show acid proton)

- **DD**
- **EE**
- **FF**
<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.96</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>7.79</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>7.33</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>2.72</td>
<td>q</td>
<td>2</td>
</tr>
<tr>
<td>1.24</td>
<td>t</td>
<td>3</td>
</tr>
</tbody>
</table>

**Spectrum 26:**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.73</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>7.71</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>6.68</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>3.06</td>
<td>s</td>
<td>6</td>
</tr>
</tbody>
</table>

**Spectrum 27:**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>δ</td>
<td>splitting</td>
<td>integration</td>
</tr>
<tr>
<td>-----</td>
<td>-----------</td>
<td>-------------</td>
</tr>
<tr>
<td>8.08</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>7.29</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>6.87</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>5.11</td>
<td>s</td>
<td>2</td>
</tr>
<tr>
<td>3.78</td>
<td>s</td>
<td>3</td>
</tr>
</tbody>
</table>

**Spectrum 28:**

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.18</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>6.65</td>
<td>m</td>
<td>1.5</td>
</tr>
</tbody>
</table>

**Spectrum 29:**
3.2 q 2
1.13 t 3

Spectrum 30:

δ splitting integration

8.32 s 1
4.19 t 2
2.83 t 2
2.40 s 3

P5.11: Match the $^1$H-NMR spectra 31-36 below to their corresponding structures GG-LL

Structures:
Spectrum 31:

δ  splitting  integration

6.98  d  1
6.64  d  1
6.54  s  1
4.95  s  1
2.23  s  3
2.17  s  3
### Spectrum 32:

<table>
<thead>
<tr>
<th>( \delta )</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.08</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>6.72</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>6.53</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>4.81</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>3.15</td>
<td>7-tet</td>
<td>1</td>
</tr>
<tr>
<td>2.24</td>
<td>s</td>
<td>3</td>
</tr>
<tr>
<td>1.22</td>
<td>d</td>
<td>6</td>
</tr>
</tbody>
</table>

### Spectrum 33:

<table>
<thead>
<tr>
<th>( \delta )</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.08</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>6.71</td>
<td>d</td>
<td>2</td>
</tr>
<tr>
<td>6.54</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>3.69</td>
<td>s</td>
<td>3</td>
</tr>
</tbody>
</table>
### Spectrum 34:

<table>
<thead>
<tr>
<th>δ splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.63 s</td>
<td>1</td>
</tr>
<tr>
<td>7.45 d</td>
<td>2</td>
</tr>
<tr>
<td>6.77 d</td>
<td>2</td>
</tr>
<tr>
<td>3.95 q</td>
<td>2</td>
</tr>
<tr>
<td>2.05 s</td>
<td>3</td>
</tr>
<tr>
<td>1.33 t</td>
<td>3</td>
</tr>
</tbody>
</table>

### Spectrum 35:

<table>
<thead>
<tr>
<th>δ splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.49 s</td>
<td>1</td>
</tr>
<tr>
<td>7.20 d</td>
<td>2</td>
</tr>
<tr>
<td>6.49 d</td>
<td>2</td>
</tr>
</tbody>
</table>
Spectrum 36:

\[ \begin{array}{ccc}
\delta & \text{splitting} & \text{integration} \\
9.58 & \text{s(b)} & 1 \\
9.31 & \text{s} & 1 \\
7.36 & \text{d} & 1 \\
6.67 & \text{s} & 1 \\
6.55 & \text{d} & 1 \\
2.21 & \text{s} & 3 \\
2.11 & \text{s} & 3 \\
\end{array} \]

**P5.12**: Use the NMR data given to deduce structures.

a ) Molecular formula: C\textsubscript{5}H\textsubscript{8}O

\[^1\text{H-NMR}:\]
<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.56</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>6.25</td>
<td>d (J~1 Hz)</td>
<td>1</td>
</tr>
<tr>
<td>5.99</td>
<td>d (J~1 Hz)</td>
<td>1</td>
</tr>
<tr>
<td>2.27</td>
<td>q</td>
<td>2</td>
</tr>
<tr>
<td>1.18</td>
<td>t</td>
<td>3</td>
</tr>
</tbody>
</table>

\[ ^{13}\text{C-NMR} \]

<table>
<thead>
<tr>
<th>δ</th>
<th>DEPT</th>
</tr>
</thead>
<tbody>
<tr>
<td>194.60</td>
<td>CH</td>
</tr>
<tr>
<td>151.77</td>
<td>C</td>
</tr>
<tr>
<td>132.99</td>
<td>CH_2</td>
</tr>
<tr>
<td>20.91</td>
<td>CH_2</td>
</tr>
<tr>
<td>11.92</td>
<td>CH_3</td>
</tr>
</tbody>
</table>

b) Molecular formula: C\_7H\_14O\_2
\[ ^1\text{H-NMR:} \]

\[
\begin{array}{ccc}
\delta & \text{splitting} & \text{integration} \\
3.85 & d & 2 \\
2.32 & q & 2 \\
1.93 & m & 1 \\
1.14 & t & 3 \\
0.94 & d & 6 \\
\end{array}
\]

\[ ^{13}\text{C-NMR} \]

\[
\begin{array}{cc}
\delta & \text{DEPT} \\
174.47 & C \\
70.41 & \text{CH}_2 \\
27.77 & \text{CH} \\
27.64 & \text{CH}_2 \\
19.09 & \text{CH}_3 \\
\end{array}
\]
c) Molecular formula: C₅H₁₂O

^{1}H-NMR:

<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.38</td>
<td>s</td>
<td>2H</td>
</tr>
<tr>
<td>2.17</td>
<td>s</td>
<td>1H</td>
</tr>
<tr>
<td>0.91</td>
<td>s</td>
<td>9H</td>
</tr>
</tbody>
</table>

^{13}C-NMR

<table>
<thead>
<tr>
<th>δ</th>
<th>DEPT</th>
</tr>
</thead>
<tbody>
<tr>
<td>73.35</td>
<td>CH₂</td>
</tr>
<tr>
<td>32.61</td>
<td>C</td>
</tr>
<tr>
<td>26.04</td>
<td>CH₃</td>
</tr>
</tbody>
</table>

d) Molecular formula: C₁₀H₁₂O

^{1}H-NMR:
<table>
<thead>
<tr>
<th>δ</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.18-7.35</td>
<td>m</td>
<td>2.5</td>
</tr>
<tr>
<td>3.66</td>
<td>s</td>
<td>1</td>
</tr>
<tr>
<td>2.44</td>
<td>q</td>
<td>1</td>
</tr>
<tr>
<td>1.01</td>
<td>t</td>
<td>1.5</td>
</tr>
</tbody>
</table>

\(^{13}\)C-NMR

<table>
<thead>
<tr>
<th>δ</th>
<th>DEPT</th>
</tr>
</thead>
<tbody>
<tr>
<td>208.79</td>
<td>C</td>
</tr>
<tr>
<td>134.43</td>
<td>C</td>
</tr>
<tr>
<td>129.31</td>
<td>CH</td>
</tr>
<tr>
<td>128.61</td>
<td>CH</td>
</tr>
<tr>
<td>126.86</td>
<td>CH</td>
</tr>
<tr>
<td>49.77</td>
<td>CH(_2)</td>
</tr>
<tr>
<td>35.16</td>
<td>CH(_2)</td>
</tr>
</tbody>
</table>
P5.13:

$^{13}$C-NMR data is given for the molecules shown below. Complete the peak assignment column of each NMR data table.

a)

\[ \begin{array}{cccc}
\delta & \text{DEPT} & \text{carbon #} \\
161.12 & CH & \\
65.54 & CH_2 & \\
21.98 & CH_2 & \\
10.31 & CH_3 & \\
\end{array} \]

b)
δ  DEPT  carbon #

194.72  C
149.10  C
146.33  CH
16.93   CH₂
14.47   CH₃
12.93   CH₃

c)

δ  DEPT  carbon #

171.76  C
60.87   CH₂
58.36   C
d) 

\[
\begin{align*}
&\text{δ} & \text{DEPT} & \text{carbon #} \\
&173.45 & \text{C} \\
&155.01 & \text{C} \\
&130.34 & \text{CH} \\
&125.34 & \text{C} \\
&115.56 & \text{CH} \\
&52.27 & \text{CH}_3 \\
&40.27 & \text{CH}_2 \\
\end{align*}
\]
P5.14: You obtain the following data for an unknown sample. Deduce its structure.

$^1$H-NMR:
\(^{13}\text{C-NMR}:\)

Mass Spectrometry:
P5.15: You take a $^1$H-NMR spectrum of a sample that comes from a bottle of 1-bromopropane. However, you suspect that the bottle might be contaminated with 2-bromopropane. The NMR spectrum shows the following peaks:

<table>
<thead>
<tr>
<th>$\delta$</th>
<th>splitting</th>
<th>integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.3</td>
<td>septet</td>
<td>0.0735</td>
</tr>
<tr>
<td>3.4</td>
<td>triplet</td>
<td>0.661</td>
</tr>
<tr>
<td>1.9</td>
<td>sextet</td>
<td>0.665</td>
</tr>
<tr>
<td>1.7</td>
<td>doublet</td>
<td>0.441</td>
</tr>
<tr>
<td>1.0</td>
<td>triplet</td>
<td>1.00</td>
</tr>
</tbody>
</table>

How badly is the bottle contaminated? Specifically, what percent of the molecules in the bottle are 2-bromopropane?
Challenge problems

C5.1: All of the $^{13}\text{C}$-NMR spectra shown in this chapter include a signal due to CDCl$_3$, the solvent used in each case. Explain the splitting pattern for this signal.

C5.2: Researchers wanted to investigate a reaction which can be catalyzed by the enzyme alcohol dehydrogenase in yeast. They treated 4'-acylpyridine (1) with living yeast, and isolated the alcohol product(s) (some combination of 2A and 2B).

\[
\text{I} \xrightarrow{\text{yeast alcohol dehydrogenase}} \begin{array}{c}
\text{2A} \\
\text{2B}
\end{array}
\]

a) Will the products 2A and 2B have identical or different $^1\text{H}$-NMR spectra? Explain.

b) Suggest a $^1\text{H}$-NMR experiment that could be used to determine what percent of starting material (1) got turned into product (2A and 2B).

c) With purified 2A/2B, the researchers carried out the subsequent reaction shown below to make 3A and 3B, known as 'Mosher's esters'. Do 3A and 3B have identical or different $^1\text{H}$-NMR spectra? Explain.
d) Explain, very specifically, how the researchers could use $^1$H-NMR to determine the relative amounts of 2A and 2B formed in the reaction catalyzed by yeast enzyme.