"It is illegal to give someone food in which has been found a dead mouse or weasel."

- from Ireland's ancient Brehon laws
1. Given that you have a compound found to be 65.1 %C, 6.71 %H, 8.47 %N and had the following spectroscopic information, answer the questions below.

**MS**

![MS spectrum graph]

**IR**

![IR spectrum graph]

**$^{13}$C NMR**

![$^{13}$C NMR spectrum graph]
a. What is the molecular formula? (2 pts)

C₉H₁₁NO₂

b. What specific information did you get from the mass spectrum? (2 pts)

MW = 165, odd MW – there is a N present. [No halogens. Base peak 150. Peak at 91 indicates substituted benzene.]

c. How many units of unsaturation do you have? (2 pts)

UU = 9 + 1 – 1/2 (11 – 1) = 10 – 5 = 5

d. What information did you get from the IR spectrum? Be specific and list stretching frequencies and what they told you. (5 pts)

Stretches above 3000 cm⁻¹ indicate C-H on sp² hybridized carbons. Stretches at 1500 and 1600 cm⁻¹ indicate an aromatic ring. [No stretch at 1700 cm⁻¹ so no C=O.]
e. What information did you obtain from the $^{13}$C NMR spectrum? Your answer should include interpretation of the chemical shift and coupling data. (5 pts)

$\delta = 155$ ppm, s (aromatic C, no H's)
$\delta = 145$ ppm, s (aromatic C, no H's)
$\delta = 128$ ppm, d (aromatic C, 1H)
$\delta = 123$ ppm, d (aromatic C, 1H) All this indicates a p substituted aromatic ring
$\delta = 35$ ppm, d (aliphatic C, 1H), CH
$\delta = 23$ ppm, q (aliphatic C, 3H's), CH$_3$

Lots of symmetry in molecule, no C=O.

f. What specific information have you gotten from the $^1$H NMR spectrum? Include details such as the interpretation of integration, coupling constants, and chemical shifts in your answer in order to receive full credit. (10 pts)

$\delta = 8.2$ ppm, d, 2H (CH's next to CH on para substituted aromatic)
$\delta = 7.4$ ppm, d, 2H (CH's next to CH on para substituted aromatic)
$\delta = 3.0$ ppm, septuplet, 1H (CH next to two CH$_3$'s in isopropyl group)
$\delta = 1.3$ ppm, d, 6H (CH$_3$'s next to CH in isopropyl group)

g. What do you think the compound is? (4 pts)

\[
\begin{align*}
\text{X} &\text{-} \text{Y} &+& \text{N and 2O's (NO}_2) \\
\text{O}_2\text{N} &\text{-} \text{Y} 
\end{align*}
\]
2. Given that you have a compound found to be 47.1 %C, 3.93 %H, 34.9 %X and had the following spectroscopic information, answer the questions below.

**MS**

![MS spectrum](image)

**IR**

![IR spectrum](image)

**$^{13}$C NMR**

![$^{13}$C NMR spectrum](image)
a. What is the molecular formula? (2 pts)

\[ C_9H_9BrO_2 \]

b. What specific information did you get from the mass spectrum? (2 pts)

MW = 224 and \( X = \text{Br} \) (two isotopes in equal abundance)

c. How many units of unsaturation do you have? (2 pts)

\[ UU = 9 + 1 - \frac{1}{2}(10) = 10 - 5 = 5 \]

d. What information did you get from the IR spectrum? Be specific and list stretching frequencies and what they told you. (5 pts)

Stretches above 3000 cm\(^{-1}\) indicate C-H on sp\(^2\) hybridized carbons. Stretches at 1500 and 1600 cm\(^{-1}\) indicate an aromatic ring. Strong stretch at 1720 cm\(^{-1}\) which indicates a C=O.
e. What information did you obtain from the $^{13}$C NMR spectrum? Your answer should include interpretation of the chemical shift and coupling data. (5 pts)

\[ \delta = 165 \text{ ppm}, \text{s} \text{ (in carbonyl region, no H's on it, not CHO – ketone, ester possible)} \]
\[ \delta = 122 - 135 \text{ ppm}, \text{ssdddd} \text{ (aromatic C's, six unique signals, two C's no H's, four C's one H), ortho or meta substituted aromatic ring.} \]
\[ \delta = 61 \text{ ppm}, \text{t} \text{ (aliphatic C, 2H, next to X, O, or N), CH}_2 \text{ probably O-CH}_2 \]
\[ \delta = 15 \text{ ppm}, \text{q} \text{ (aliphatic C, 3H's), CH}_3 \]

f. What specific information have you gotten from the $^1$H NMR spectrum? Include details such as the interpretation of integration, coupling constants, and chemical shifts in your answer in order to receive full credit. (10 pts)

\[ \delta = 7.5 - 8.2 \text{ ppm}, \text{tdds, 1H each (CH's on aromatic ring indicating a meta substituted system, 1H with no H's next door, 2H's with one H next door, and 1H with two H's next door – can only be meta)} \]
\[ \delta = 4.3 \text{ ppm}, \text{q, 2H (CH}_2 \text{ next to CH}_3 \text{ in ethyl group, next door to X, O, N) probably An O-CH}_2 \]
\[ \delta = 1.4 \text{ ppm}, \text{t, 3H (CH}_3 \text{ next to CH}_2 \text{ in ethyl group)} \]

g. What do you think the compound is? (4 pts)

\[
\begin{align*}
\text{Ar} & + \text{Br} + \text{CO} & = & -\text{O-CH}_2\text{CH}_3 \\
\text{Ar} & + \text{Br} + \text{CO} & = & \text{Br}
\end{align*}
\]
3. Circle the answer that is most correct for **four** of the **five** the following questions.  
(4 pts each)

a. The DEPT spectrum shown is for this compound.

![DEPT spectrum](image)

3-methyl-1-pentyne  OR  cyclohexene  OR  3-methyl-cyclopentene

b. This bond will have the larger stretching frequency.

![Bonds](image)

C=C  OR  C=N  OR  C=O

c. The UV-Vis spectrum shown is for this compound.

![UV-Vis spectrum](image)

cyclohexene  OR  3-penten-1-yne  OR  octatetraene

d. This compound will have the most number of $^{13}$C signals.

ortho t-butyl phenol  OR  **meta sec-butyl phenol**  OR  para isoropyl phenol
Given the DEPT spectrum below, which of the statements is most correct?

There are 7 CH₃’s. OR There are 3 C’s with no H’s. OR There are 3 CH₂’s.

(12) 4. Assistant Beaker was working in the laboratory and added a Grignard reagent to the wrong ketone (OOPS!). The molecular formula of his resulting alcohol was C₁₀H₁₄O. What are the structures of his alcohol, his ketone, and his Grignard reagent?

Incorrect alcohols with the correct Grignard reagent and ketone which would give rise to that alcohol were given six points.

Correct alcohol:

Ketone/Grignard Pairs which would give this alchol:
5. Following are several IR spectra for monofunctional compounds. The possibilities for these are: acid halide; anhydride; alcohol; ketone; and nitrile (you should have one left over!). Determine which spectrum belongs to which functional group. Identify the stretch (or stretches) that allowed you to make this determination.

- **Anhydride**, two stretches at 1800 and 1750 cm\(^{-1}\)
- **Acid chloride**, stretch at 1800 cm\(^{-1}\)
- **Nitrile**, stretch at 2250 cm\(^{-1}\)
- **Alcohol**, stretch at 3350 cm\(^{-1}\)

(3) **BONUS**: Briefly describe either a fat or olestra.

Any reasonable answer accepted