Problem R-96J (C_{15}H_{20}O_{4})
300 MHz $^1$H NMR spectrum in CDCl$_3$
Source: Brian Austad/Burke 11/26 g
Problem R-96J \((C_{15}H_{20}O_4)\). Determine the structure of R-96J from the 300 MHz proton NMR spectrum provided. The compound contains a Ph and a \(\text{CO}_2\text{C(CH}_3)_3\) group.

(a) Analyze each of the proton signals, report multiplicity and coupling constants, and report any part structures you derived from the data.

\[\delta 1.4\]

\[\delta 3.0\]

\[\delta 3.9\]

\[\delta 7.3\]

\[\delta 9.7\]

(b) Draw a structure for R-96J. If more than one structure is possible, show them, but circle the one you prefer, and give reasons for your preference.
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**Problem R-96J** \((C_{15}H_{20}O_4)\). Determine the structure of **R-96J** from the 300 MHz proton NMR spectrum provided. The compound contains a Ph and a \(CO_2C(CH_3)_3\) group.

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\[
\begin{align*}
\delta 1.4 & \quad s, 9H, C(CH_3)_3 \\
\delta 3.0 & \quad AB of ABXY, J_{AB} = 14 \text{ Hz}, J_{AX} = 5 \text{ Hz}, J_{BX} = 8 \text{ Hz} \\
\delta 3.9 & \quad 3.85 \text{ and } 4.05, \text{ MN quartet, } J_{MN} = 16 \text{ Hz} \\
\delta 7.3 & \quad 5H, \text{ Ph} \\
\delta 9.7 & \quad d, J = 2 \text{ Hz}, 1H (Y \text{ of ABXY})
\end{align*}
\]

(b) Draw a structure for **R-96J**. If more than one structure is possible, show them, but circle the one you prefer, and give reasons for your preference.

The known groups are H-C-CH-CH_2-, O-CH_2-, Ph, CO_2-t-Bu. Quite a few ways of putting these together, some can be distinguished by chemical shift considerations.

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| Calc δ | 3.10 | 4.50 | 4.60 |
| Δδ (error) | 0.1 | 0.6 | 0.6 |
| Sum Δδ: | 1.3 |

Correct structure, and smallest error

These structures can probably be ruled out on the basis of the large shift error.