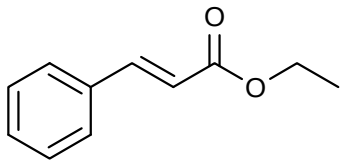
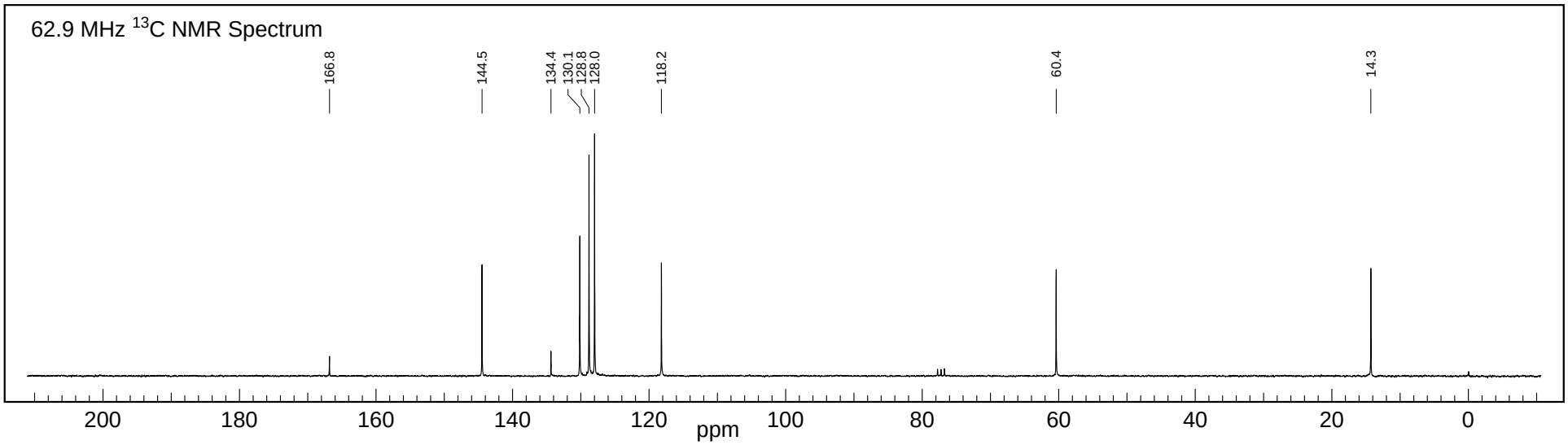
Problem R-99C ($C_{11}H_{12}O_2$).
250 MHz ^{1}H NMR Spectrum in $CDCl_3$
Source: Adam Fiedler/Reich 10/29 g



62.9 MHz ^{13}C NMR Spectrum



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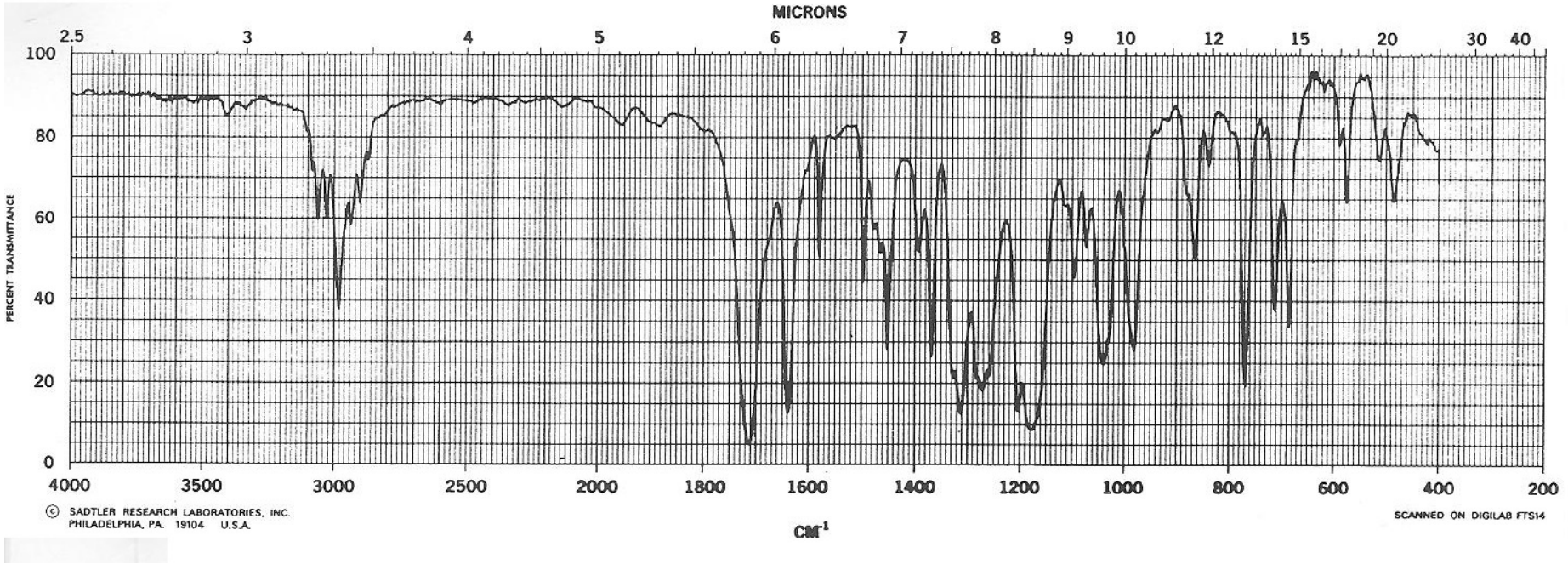
IR spectrum

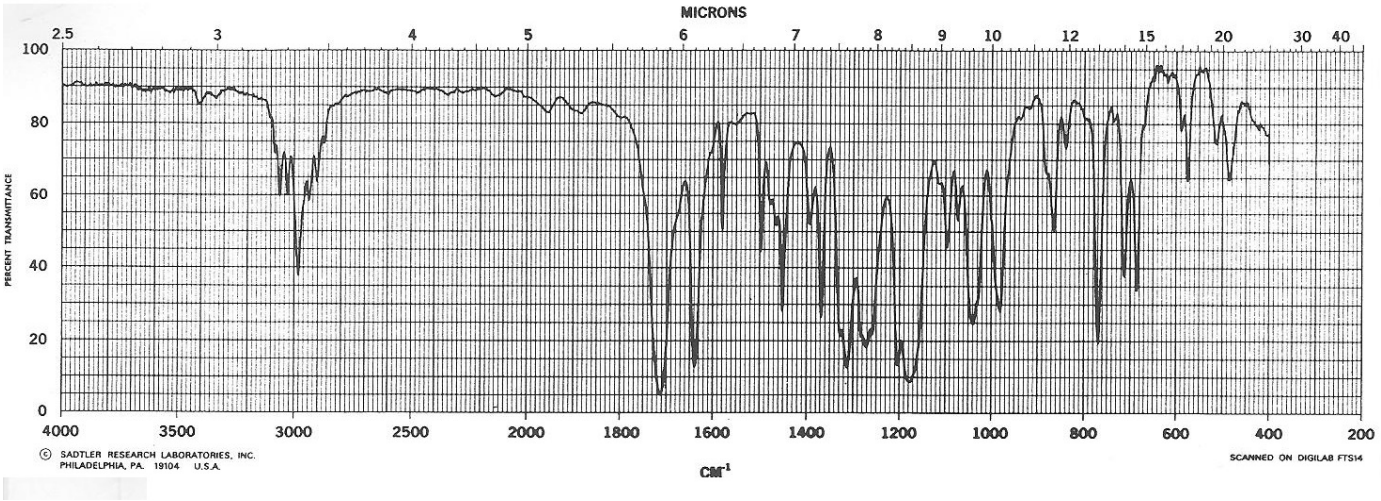


PLT ex-1-1999a-g.plt

Problem R-99C ($C_{11}H_{12}O_2$). Determine the structure of **R-99C** from the ^{1}H NMR, ^{13}C NMR and IR spectra provided.

(a) DBE__

(b) What information can you obtain from the IR spectrum?



(c) Analyze the signals in the ^{1}H NMR spectrum. Report multiplicity, coupling constants and part structure you could obtain from each signal or set of signals.

δ 1.3_____ δ 7.3_____

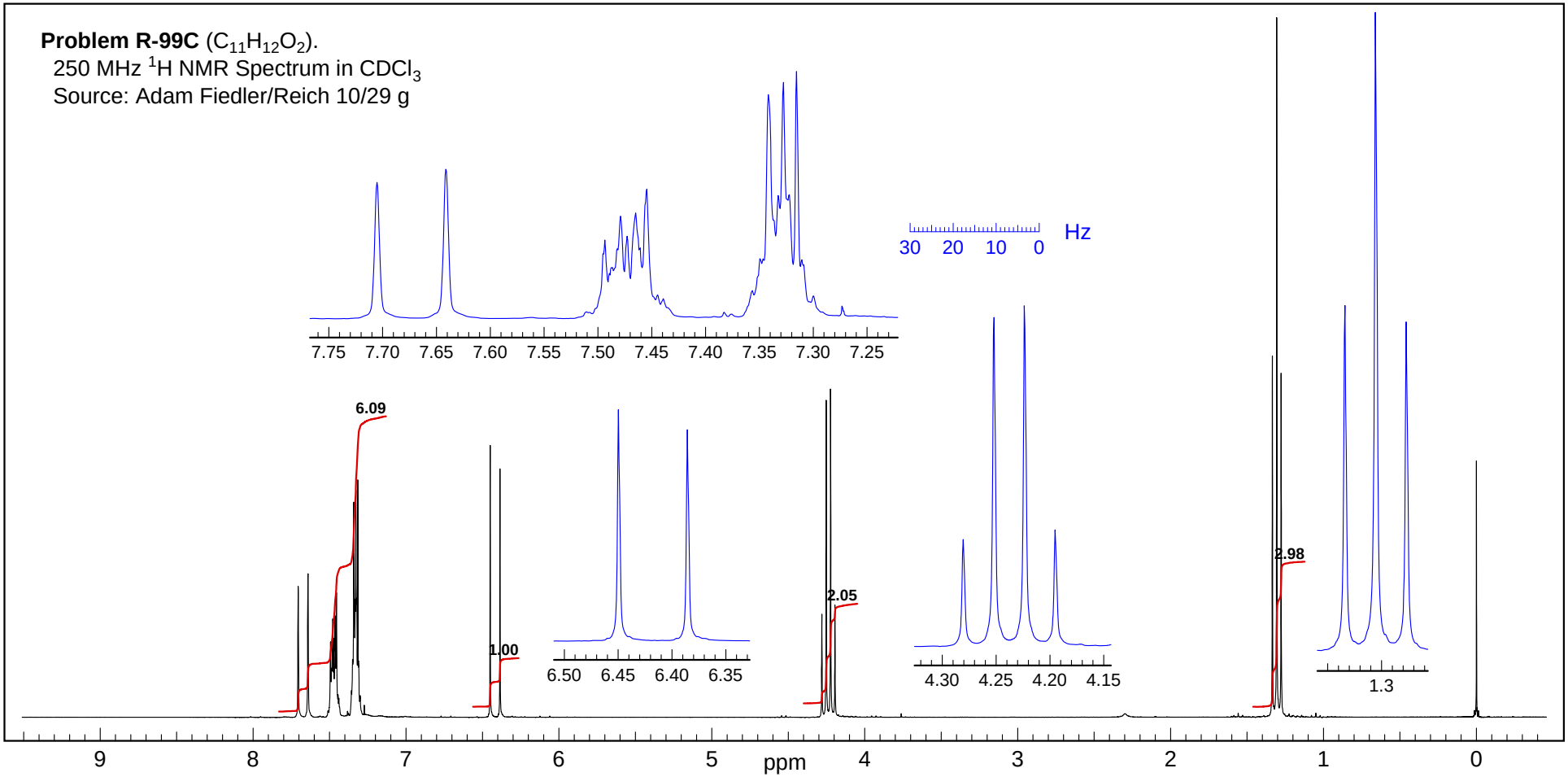
δ 4.3_____ δ 7.5_____

δ 6.4_____ δ 7.7_____

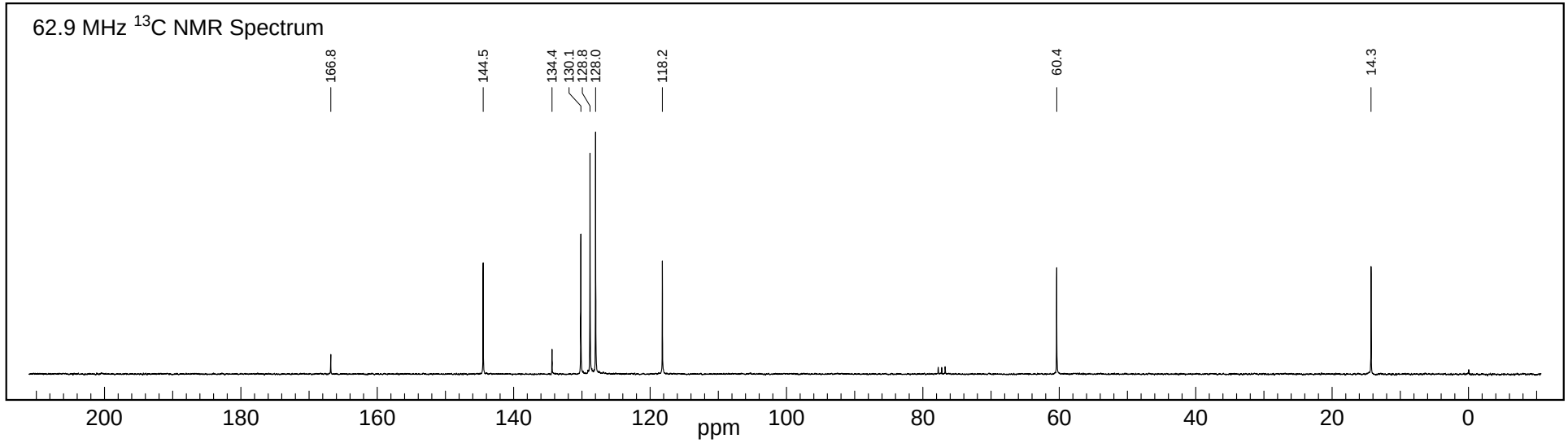
(d) Summarize the information you obtained from the ^{13}C NMR spectrum. **Assign the ^{13}C signals by placing the chemical shift number on your structure in part (e) below** (you don't need to write any numbers past the decimal point).

(e) Draw the structure of **R-99C**. If more than one structure fit the data, show them, and circle the one you think fits best and give your reasons for choosing it.

Problem R-99C ($C_{11}H_{12}O_2$).
250 MHz ^{1}H NMR Spectrum in $CDCl_3$
Source: Adam Fiedler/Reich 10/29 g



62.9 MHz ^{13}C NMR Spectrum

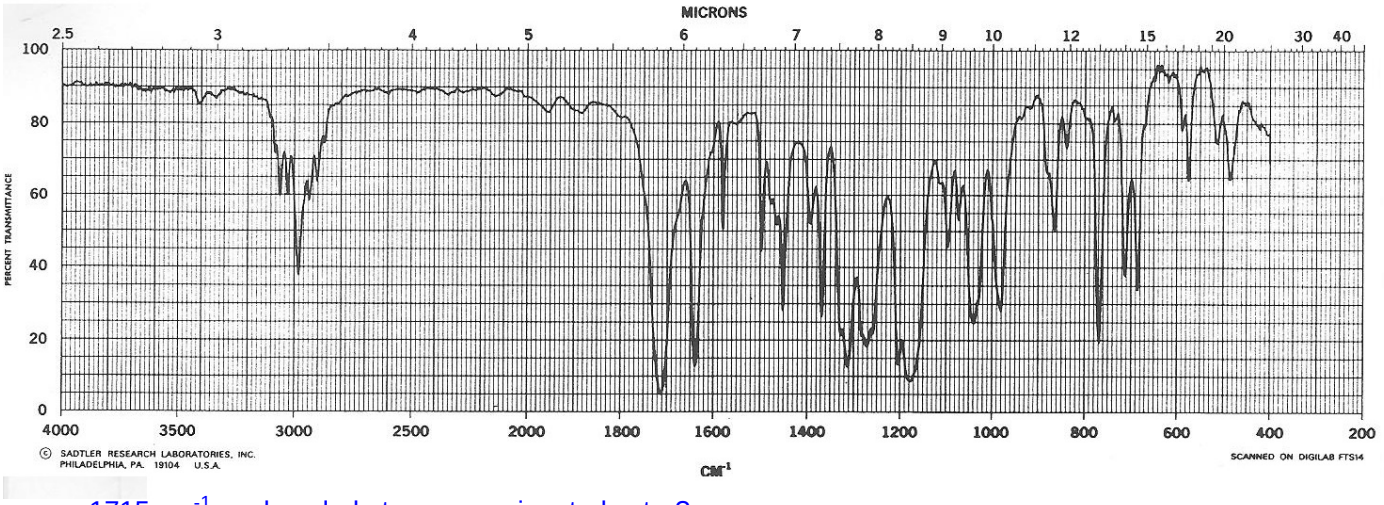


PLT ex-1-1999a-g.plt

Problem R-99C ($C_{11}H_{12}O_2$). Determine the structure of **R-99C** from the ^{1}H NMR, ^{13}C NMR and IR spectra provided.

2 (a) DBE 6

(b) What information can you obtain from the IR spectrum?

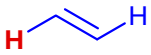
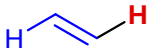


1715 cm^{-1}: carbonyl - ketone or conjugated ester?

3 2130, 2150 cm^{-1}: vinyl/aryl CH

No OH stretch 3500 cm^{-1}

(c) Analyze the signals in the ^{1}H NMR spectrum. Report multiplicity, coupling constants and part structure you could obtain from each signal or set of signals.

δ 1.3	t, *J* = 7 Hz, 3H	C**H**$_3$-CH$_2$-O	δ 7.3	m, ArH, 3H (meta, para protons)	
5 δ 4.3	q, *J* = 7 Hz, 2H	CH$_3$-C**H**$_2$-O	δ 7.5	m, ArH, 2H (ortho aryl protons?)	
δ 6.4	d, *J* = 16 Hz, 1H		δ 7.7	d, *J* = 16 Hz, 1H	

(d) Summarize the information you obtained from the ^{13}C NMR spectrum. **Assign the ^{13}C signals by placing the chemical shift number on your structure in part (e) below** (you don't need to write any numbers past the decimal point).

δ 166: ester carbonyl, maybe conjugated

There is monosubstituted phenyl group: 1:1:1:1 in sp^2 region

4 δ 60: **C**-O

δ 118, 144: two additional sp^2 carbons - C=C

(e) Draw the structure of **R-99C**. If more than one structure fit the data, show them, and circle the one you think fits best and give your reasons for choosing it.

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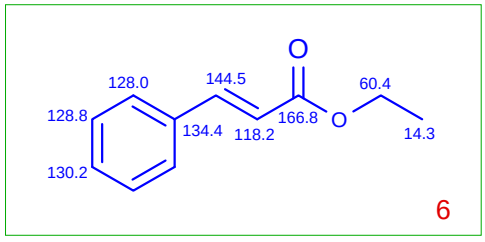
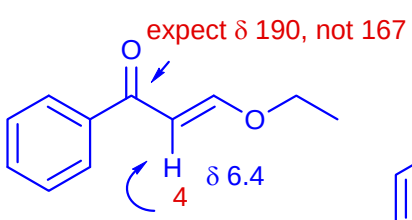


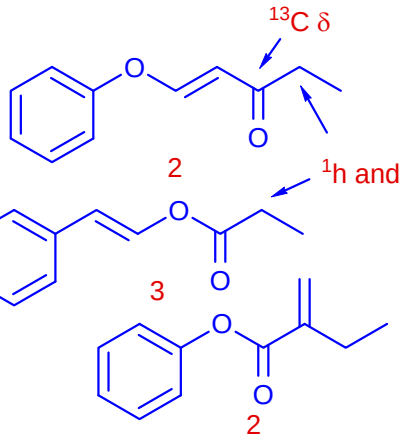
6 6

Other structures proposed:



expect δ 190, not 167

Calc: base: 5.25
cis OR: -1.07
α ARC=O: 1.10
5.64
Error ^{1}H calc: 0.8 ppm



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