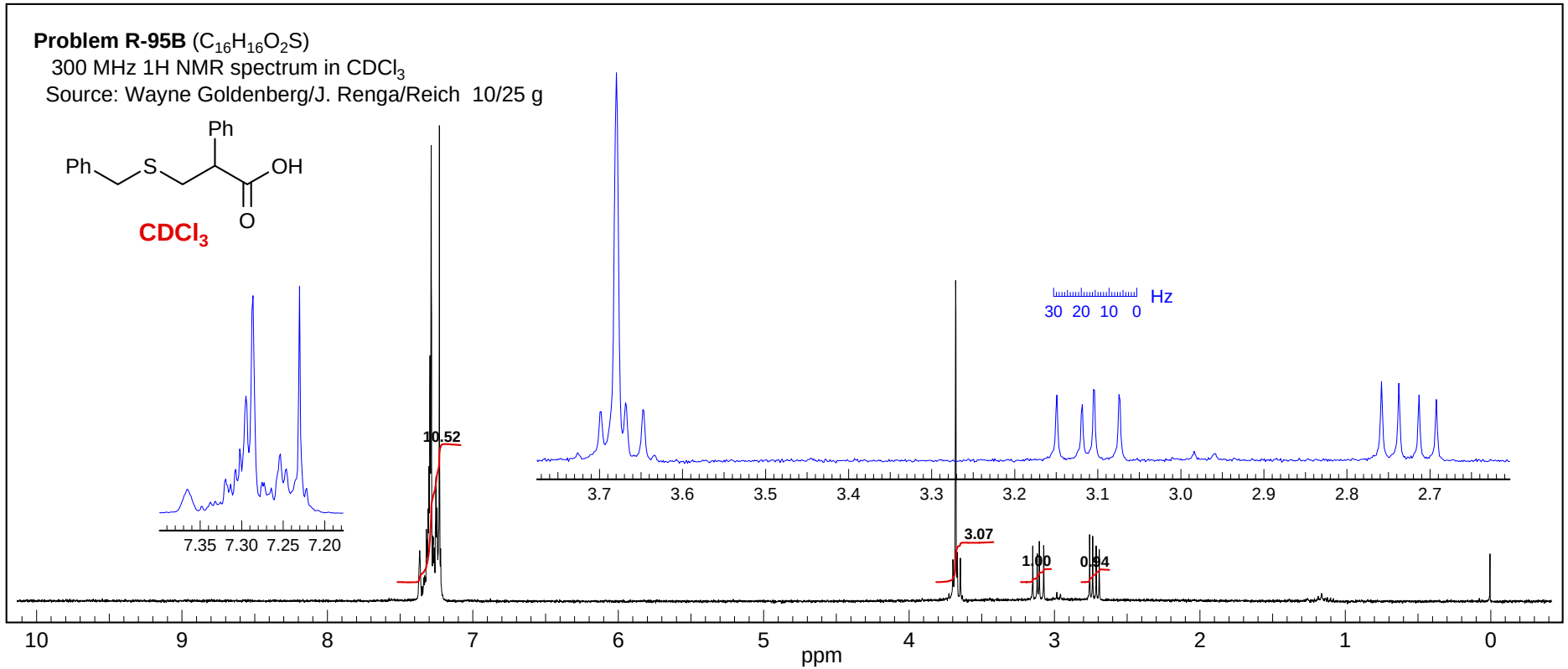
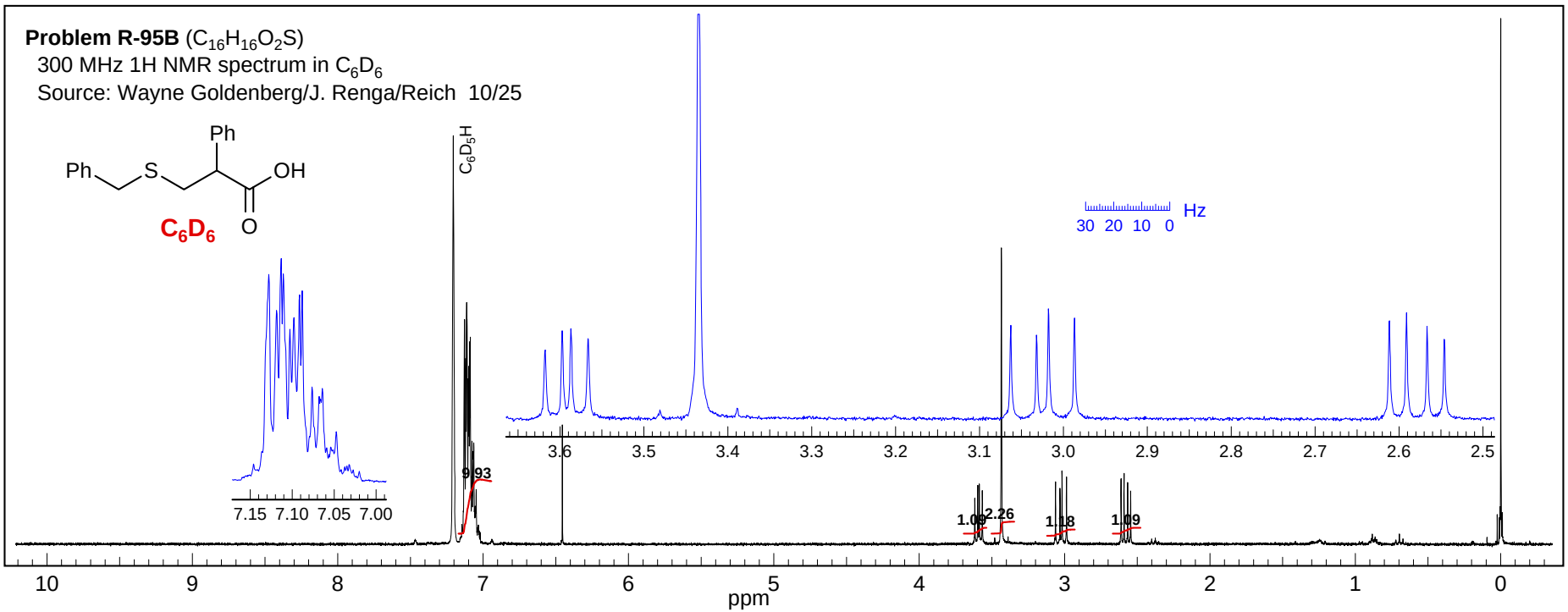
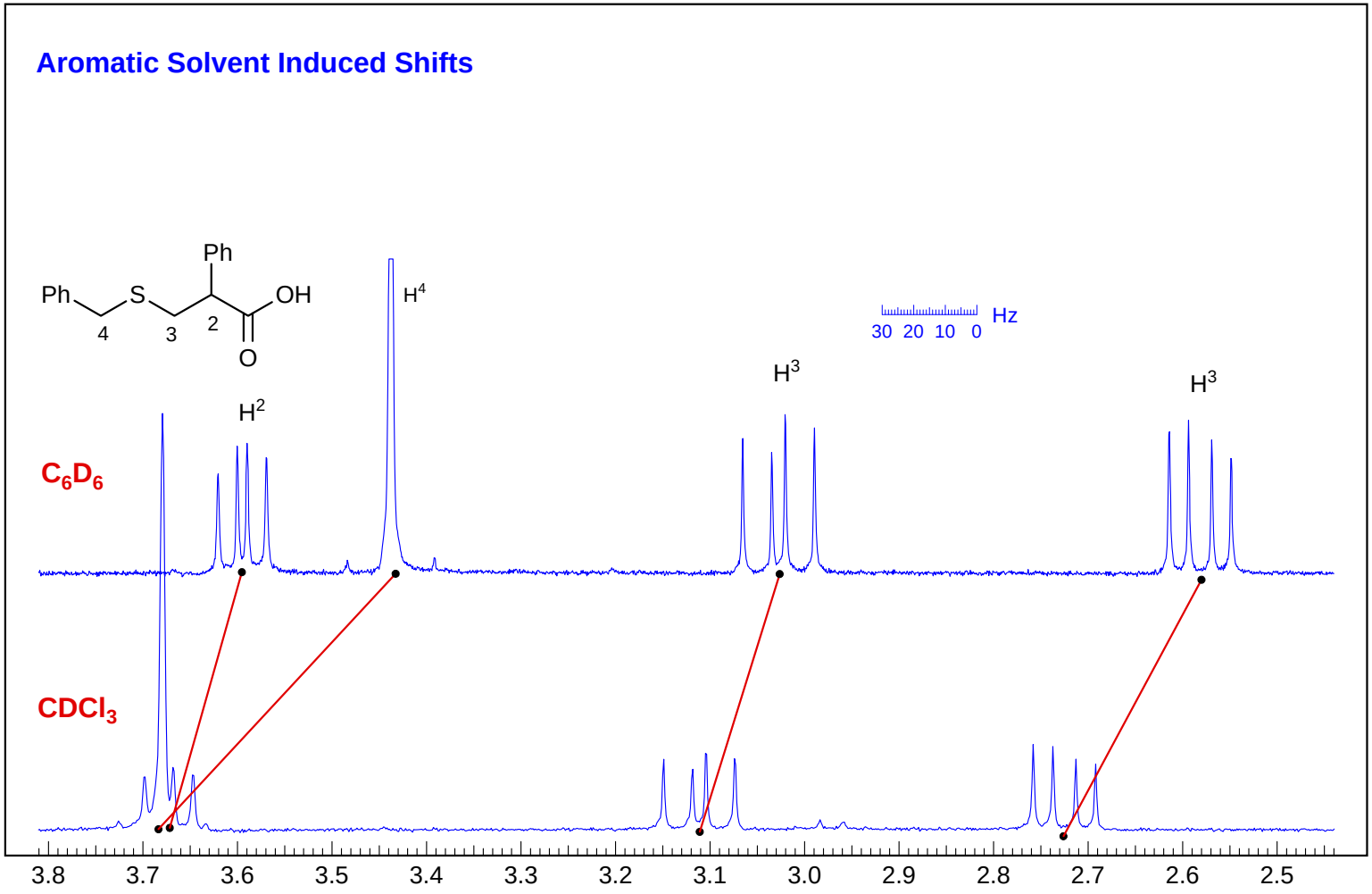




PLT pr-087-to-95.plt

Aromatic Solvent Induced Shifts



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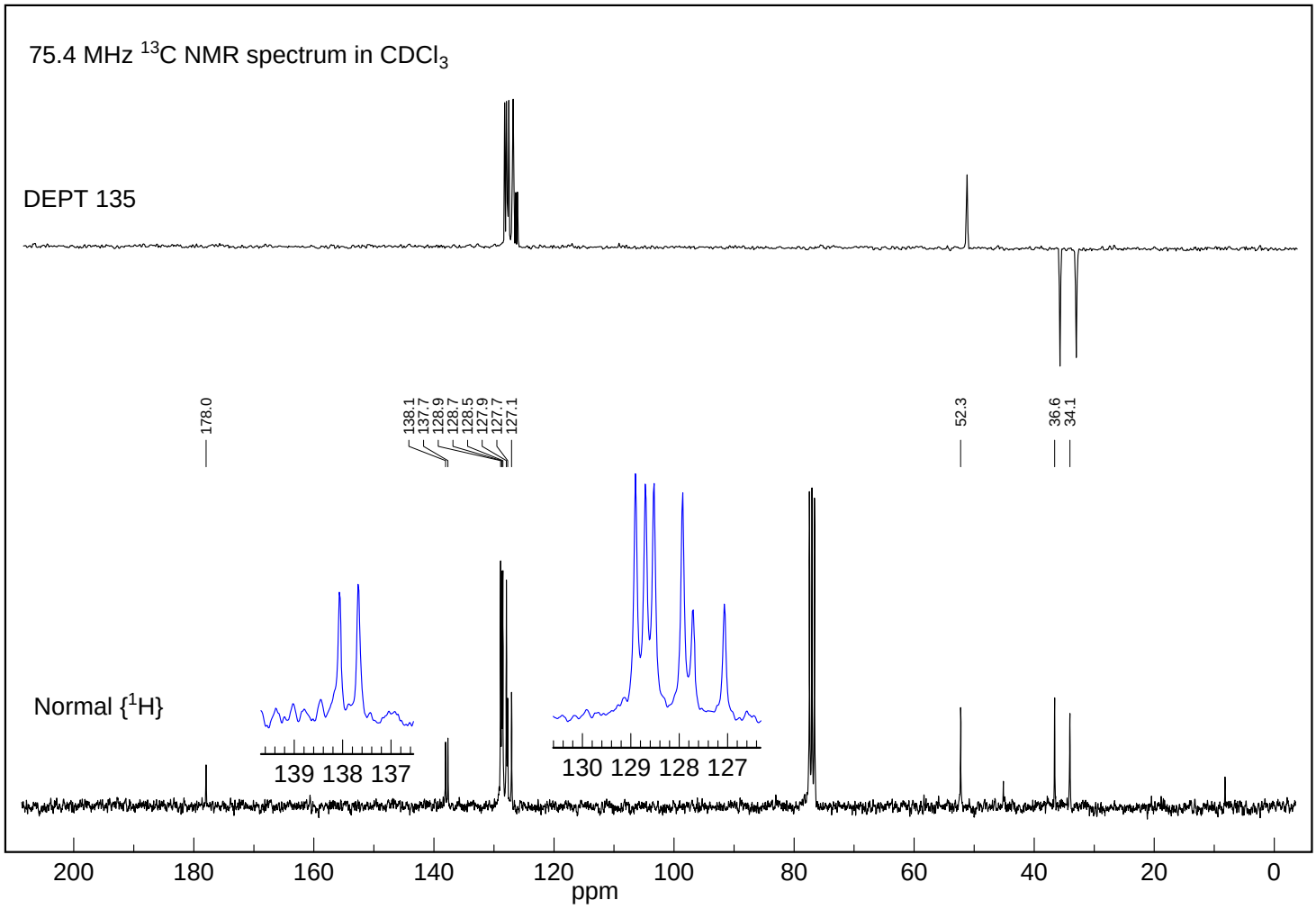
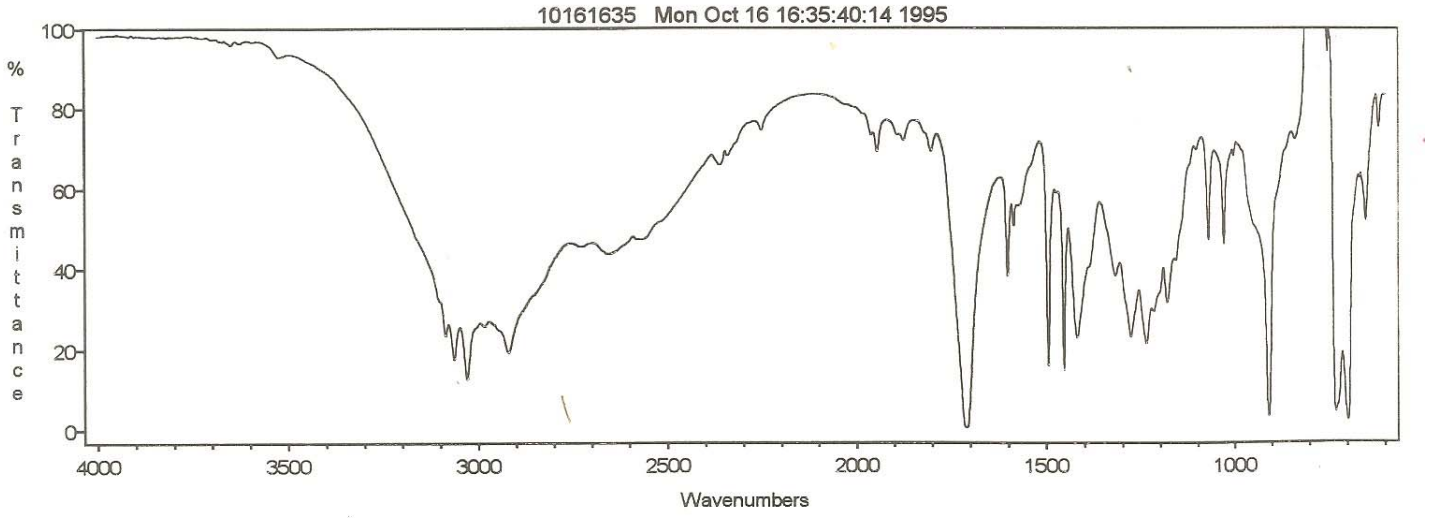


IR Spectrum



PLT pr-087-to-95.plt

Problem R-95B ($C_{16}H_{16}O_2S$). Determine the structure (or part structure) of R-95B 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) Interpret the ^{13}C NMR spectrum. The DEPT 135 spectrum shows all CH and CH_3 peaks as positive, and CH_2 peaks negative. Identify what kind of carbon each signal corresponds to, and write possible part structures.

Type of C (e.g. sp^3 CH_2) and/or part structures (e.g. N-CH_2)

δ 34-36 _____

δ 52 _____

δ 127-129 _____

δ 137-138 _____

δ 178 _____

What are the three peaks at δ 77?_____

(d) Analyze the multiplets in the 300 MHz ^{1}H NMR spectrum in C_6D_6. Report multiplicity, coupling constants and part structure you could obtain from each signal. Be sure to fully interpret the signal at δ 3.4.

δ 2.6

δ 3.0

δ 3.4

δ 3.6

(e) Draw possible structures for R-95B. If more than one structure is possible, show them. Circle the one you think fits the data best and give your reasons for choosing it.

Problem R-95B ($C_{16}H_{16}O_2S$). Determine the structure (or part structure) of R-95B from the ^{1}H NMR, ^{13}C NMR and IR spectra provided.

2 (a) DBE 9

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

3 1710 cm^{-1} Carbonyl stretch, ketone or carboxylic acid
2500-3500 broad peak, often characteristic of the OH stretch of CO_2H

(c) Interpret the ^{13}C NMR spectrum. The DEPT 135 spectrum shows all CH and CH_3 peaks as positive, and CH_2 peaks negative. Identify what kind of carbon each signal corresponds to, and write possible part structures.

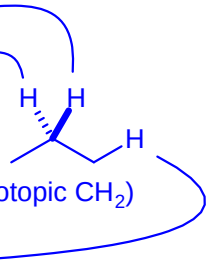
	Type of C (e.g. sp^3 CH_2) and/or part structures (e.g. N-CH_2)
δ 34-36	2 aliphatic sp^3 CH_2
δ 52	CH - some electronedative substituent(s)
δ 127-129	4 double intensity aromatic CH (2 sets ortho, meta), 2 single intensity - probably two phenyl groups
δ 137-138	2 Quaternary sp^2 C (ipso carbon of two phenyls)
δ 178	C=O carbon of ester or carboxylic acid

4

What are the three peaks at δ 77? **C**DCl_3

(d) Analyze the multiplets in the 300 MHz ^{1}H NMR spectrum in C_6D_6. Report multiplicity, coupling constants and part structure you could obtain from each signal. Be sure to fully interpret the signal at δ 3.4.

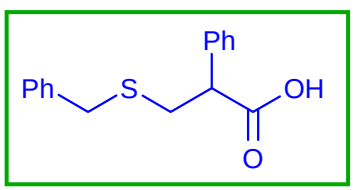
δ 2.6	dd, *J* = 13.4, 6 Hz (coupled to3.0 and 3.6)
δ 3.0	dd, *J* = 13.4, 9 Hz (coupled to 2.6 and 3.6)
δ 3.4	AB quartet (very closely spaced), $J_{AB} \approx 14$ Hz (Isolated diastereotopic CH_2)
δ 3.6	dd, *J* = 9, 6 Hz (coupled to 2.6 and 3.9)

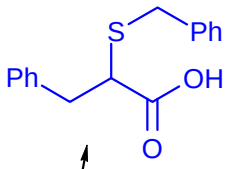


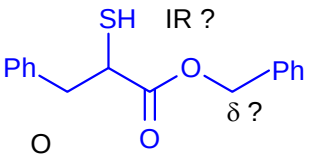
5

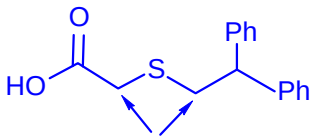
(e) Draw possible structures for R-95B. If more than one structure is possible, show them. Circle the one you think fits the data best and give your reasons for choosing it.

Groups identified are 2 Ph, CH_2-CH, CH_2, S, CO_2H. Many ways to put these pieces together which fit the NMR patterns, the actual structure fits best.





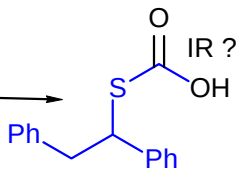


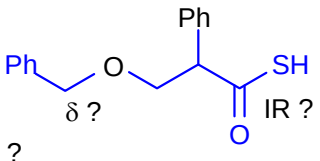


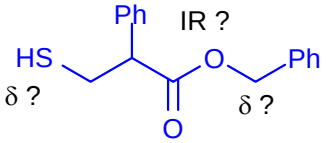
Would not be diastereotopic

6

These also fit pretty well







Unfortunately, the α and β proton shift increments of Ph, CO_2R and SR are rather similar, so chemical shift calculations do not provide a very clear distinction between the various possible structures.