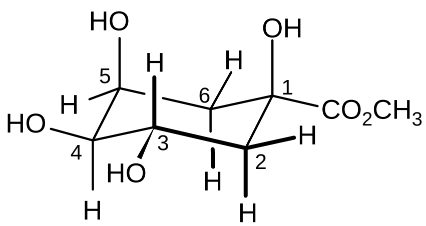
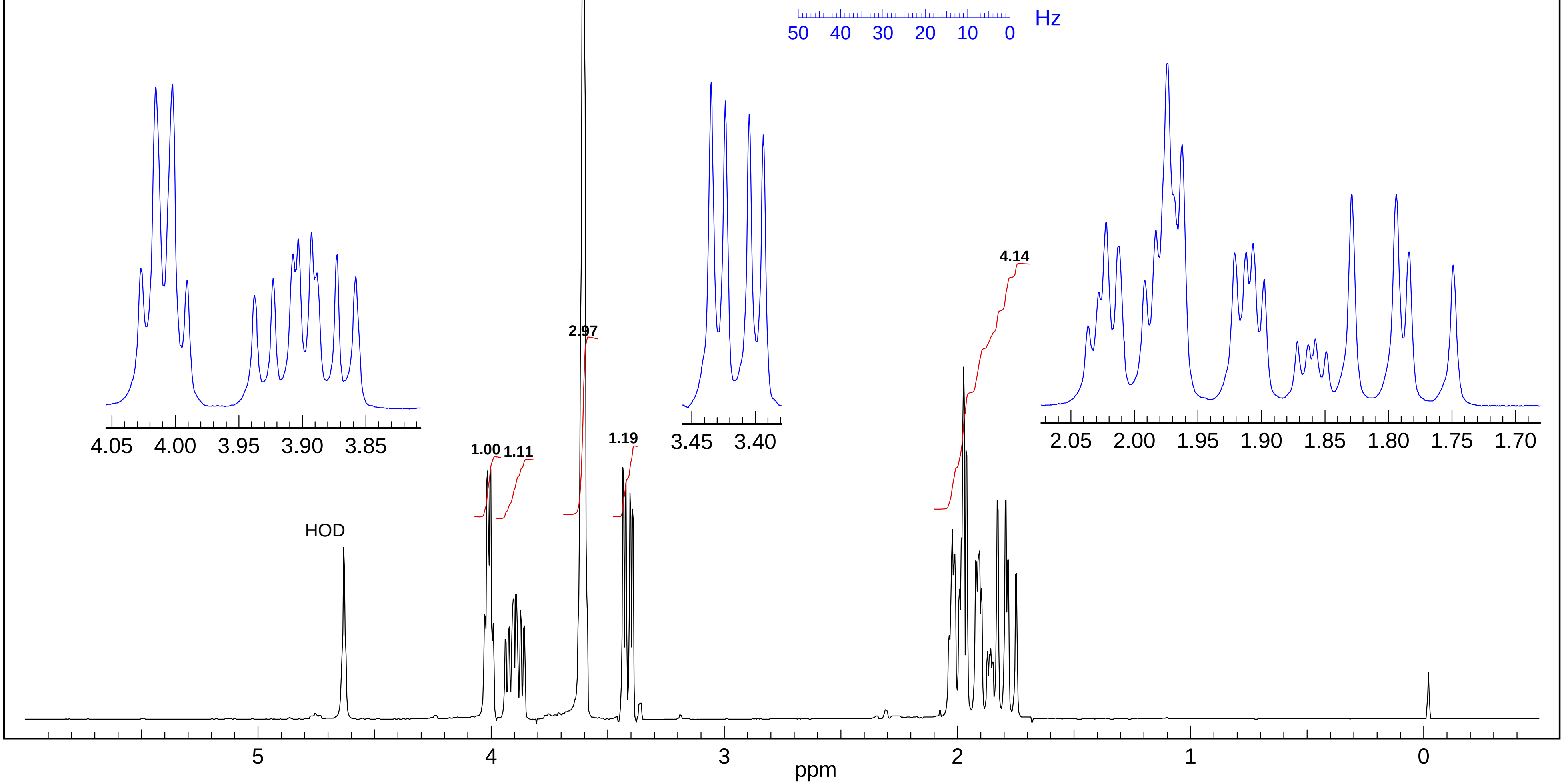
Problem R-06K. ($C_8H_{14}O_6$)
300 MHz ^1H NMR Spectrum in D_2O
Source: M. Schuster/Kiessling (Reich digitized hard copy) g





PLT ex-2-2006-07-gq.plt

Problem R-06K. Determine the stereochemistry at the three indicated carbons from the 300 MHz ^1H NMR spectrum presented on the next page

(a) Analyze the individual signals and show coupling constants in the standard format. Assign them to the extent possible. Use the numbering system given on the structure in part (b).

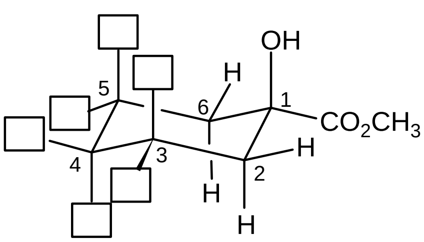
δ 1.7 - 2.1

δ 3.4

δ 3.9

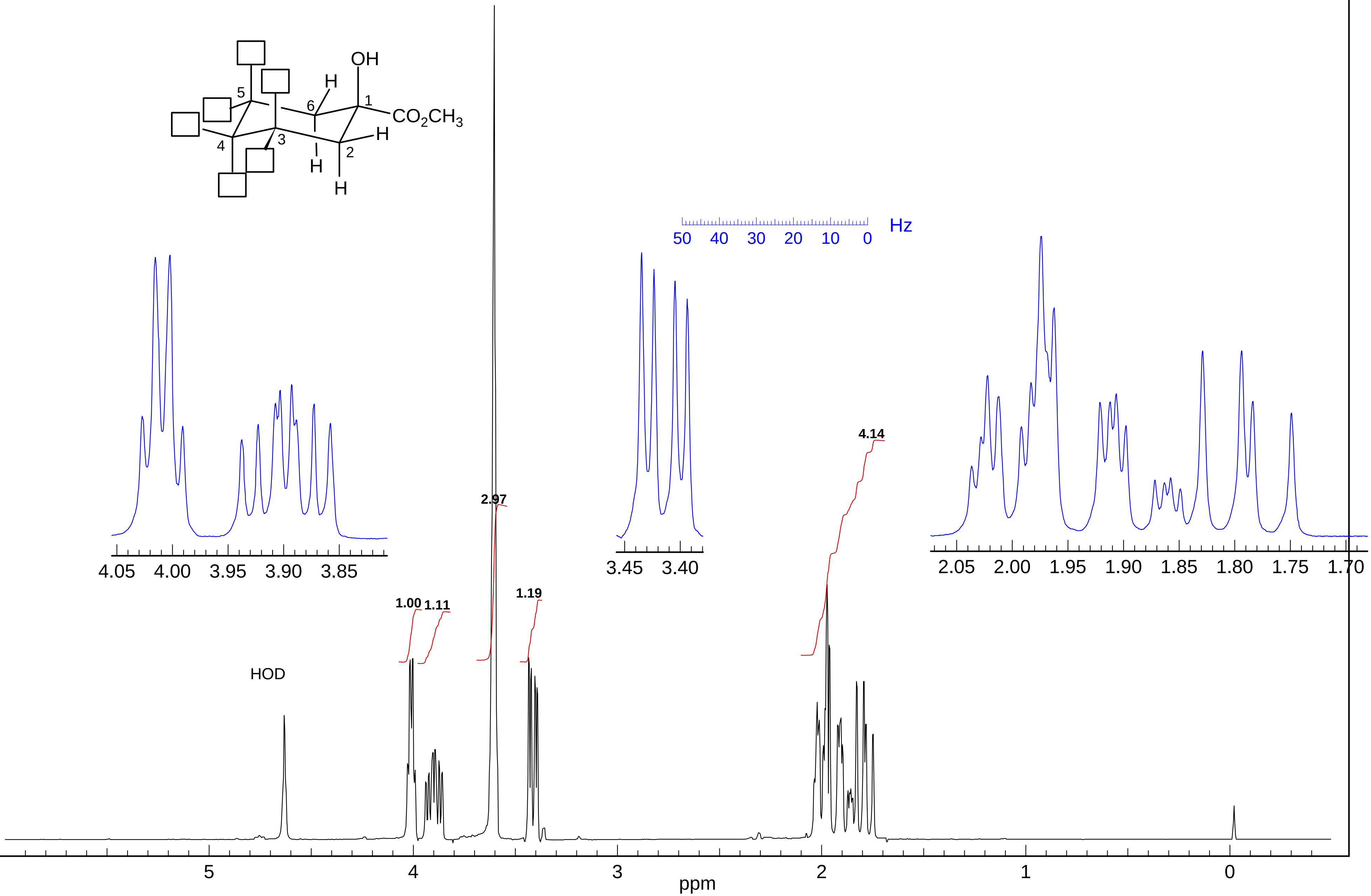
δ 4.0

(b) Determine the stereochemistry of **R-06K**. Place the appropriate substituents (H and OH) in each of the boxes on the structure below.



At each carbon 3, 4, and 5 there is a H and an OH group

Problem R-06K. ($C_8H_{14}O_6$)
300 MHz ^1H NMR Spectrum in D_2O
Source: M. Schuster/Kiessling (Reich digitized hard copy) g



PLT ex-2-2006-07-gq.plt

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Problem R-06K. Determine the stereochemistry at the three indicated carbons from the 300 MHz ^{1}H NMR spectrum presented on the next page

(a) Analyze the individual signals and show coupling constants in the standard format. Assign them to the extent possible. Use the numbering system given on the structure in part (b).

8 δ 1.7 - 2.1

H_{2-ax}: 1.78 dd, J = 14, 10.5 Hz — The 10.5 Hz coupling must be ax-ax, so H_3 must be axial

H_{2-eq}: 2.00 ddd, J = 14, 4, 2.5 Hz — The 2.5 Hz coupling is a "W" coupling - H_{2-eq} - H_{6-eq}

H_{6-ax}: 1.98 dd, J = 15, 3.5 Hz — The 3.5 Hz coupling must be ax-eq, so H_5 must be equatorial

H_{6-eq}: 1.89 ddd, J = 15, 4, 2.5 Hz — The 2.5 Hz coupling is a "W" coupling - H_{2-eq} - H_{6-eq}

3 δ 3.4

δ 3.42, dd, J =9, 3.2 Hz

H_4 - only one of the downfield protons with just two couplings. It must be axial, with H_3 axial and H_5 equatorial

3 δ 3.9

δ 3.90, ddd, J =10, 9, 4.5 Hz

H_3 - coupled twice with large couplings to axial protons at H_2 and H_4, and once to equatorial proton at H_2

2 δ 4.0

δ 4.02, apparent quartet, J =3.5 Hz (actually a ddd)

H_5 - equatorial proton, coupled eq-ax to protons H_4 and H_6, and eq-eq to H_6

(b) Determine the stereochemistry of **R-06K**. Place the appropriate substituents (H and OH) in each of the boxes on the structure below.

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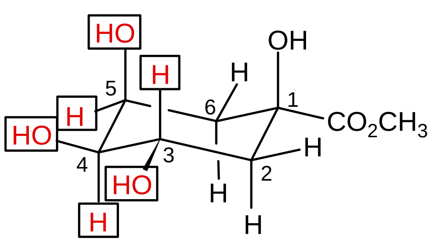

At each carbon 3, 4, and 5 there is a H and an OH group

Problem R-06K. ($C_8H_{14}O_6$)

300 MHz ^{1}H NMR Spectrum in D_2O

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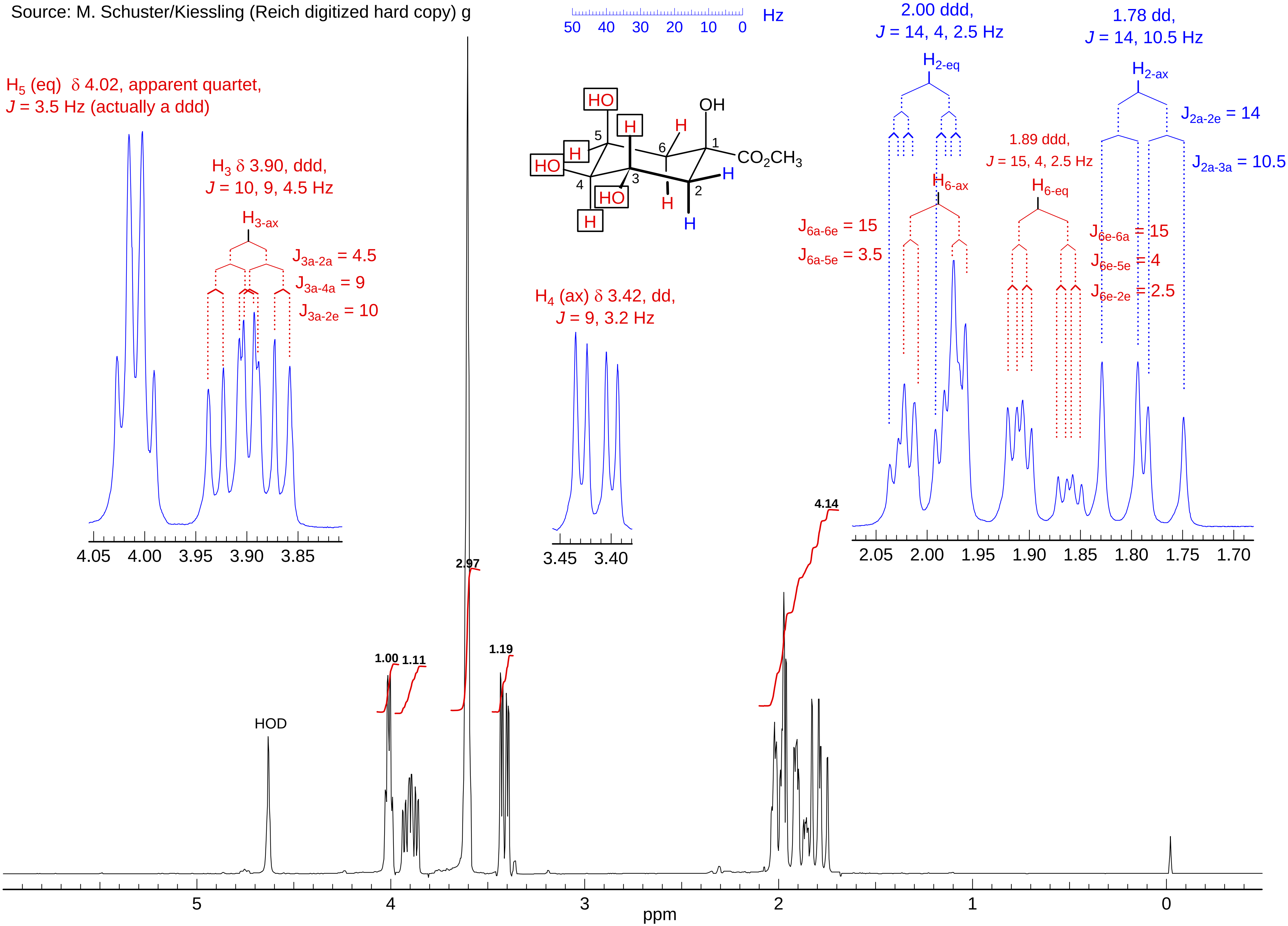

PLT ex-2-2006-07-gq.plt