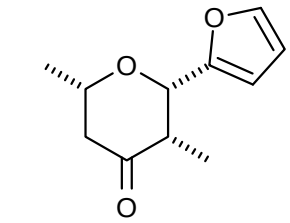
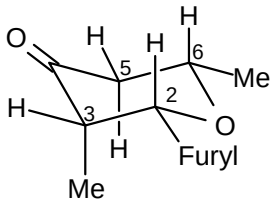
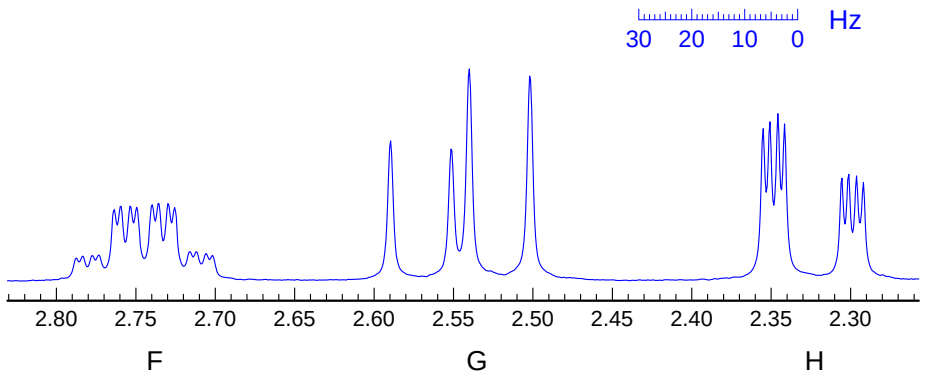
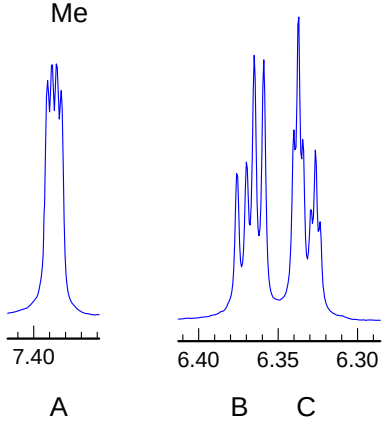
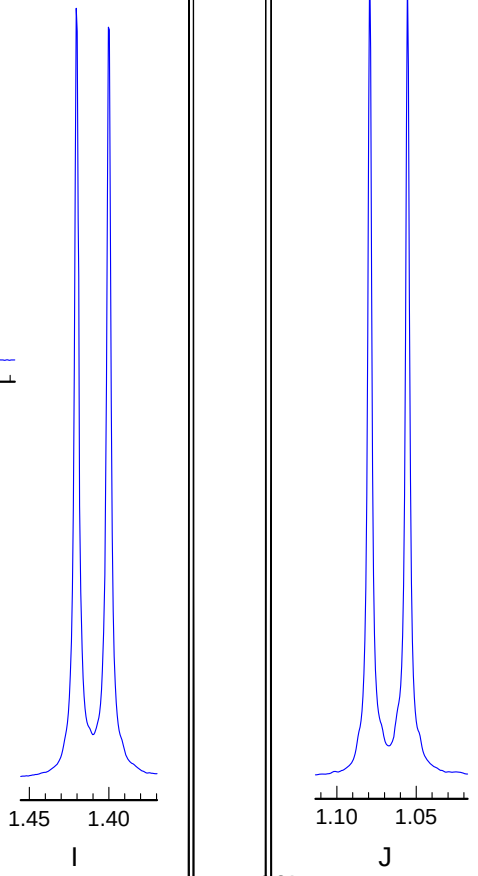
Problem R-08G ($C_{11}H_{14}O_3$)
300 MHz ^{1}H NMR Spectrum in $CDCl_3$
Source: Andrew Dilger/Burke g

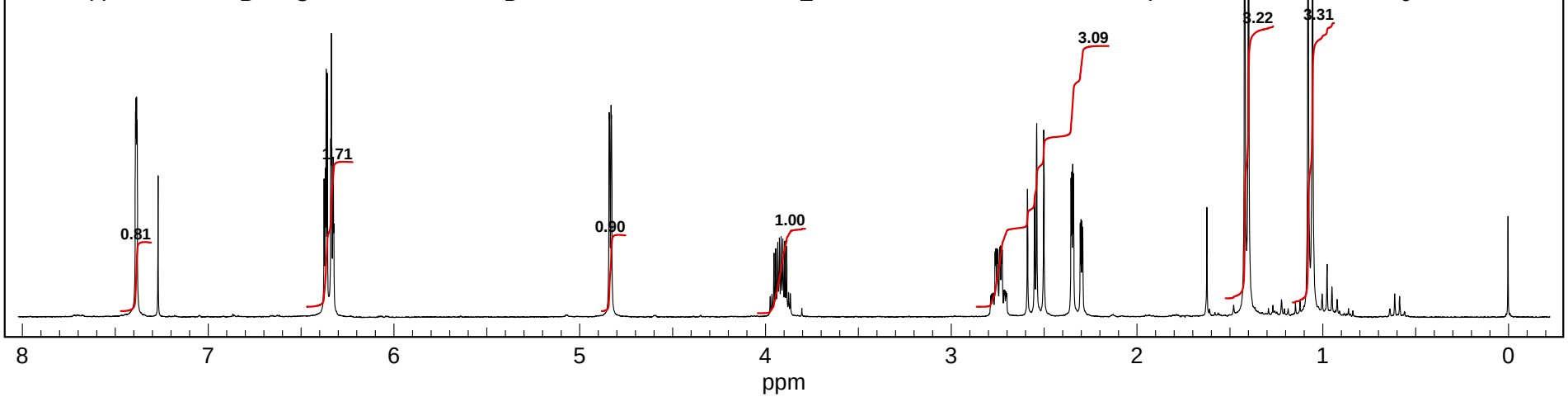






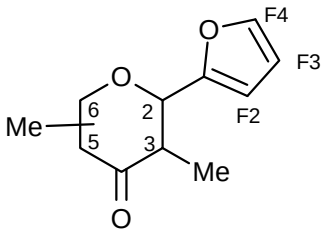






PLT ex-2-2008-09-gq.plt

Problem R-08G ($C_{11}H_{14}O_3$). In this problem you are given the part structure of a tetrahydropyran. Your task is to completely assign the ^{1}H NMR spectrum, determine the position of the second methyl group, which is either at position 5 or 6, and determine the relative stereochemistry of the three substituents on the ring. You may assume that the ring adopts a chair-like conformation. Please use the peak labelling (A-J) shown on the spectrum and the position labelling (1-6, F2-F4, 3Me, 5/6Me) shown on the structure. You may use first order analysis.

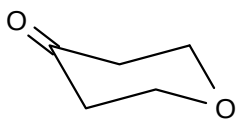


(a) Analyze the multiplets A-J. Report your results in the standard format: δ 9.3, dt, J = 14, 6 Hz, 3H. For each proton indicate which other protons (A-J), are coupled to it. You may use first order analysis.

		A-J		1-6, F_2-F_4 3Me, 5/6Me
A	_____ Coupled to:	_____	Assigned to:	_____
B	_____ Coupled to:	_____	Assigned to:	_____
C	_____ Coupled to:	_____	Assigned to:	_____
D	_____ Coupled to:	_____	Assigned to:	_____
E	_____ Coupled to:	_____	Assigned to:	_____
F	_____ Coupled to:	_____	Assigned to:	_____
G	_____ Coupled to:	_____	Assigned to:	_____
H	_____ Coupled to:	_____	Assigned to:	_____
I	_____ Coupled to:	_____	Assigned to:	_____
J	_____ Coupled to:	_____	Assigned to:	_____

(b) Briefly describe how you determined the position of the methyl group

(c) Using the structure below, draw a good representation of the molecule, clearly indicating stereochemistry (axial or equatorial substituents).



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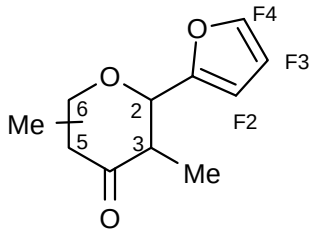

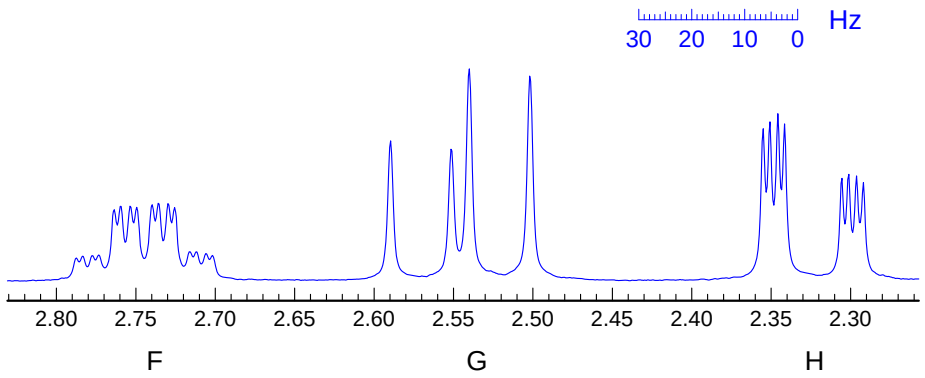

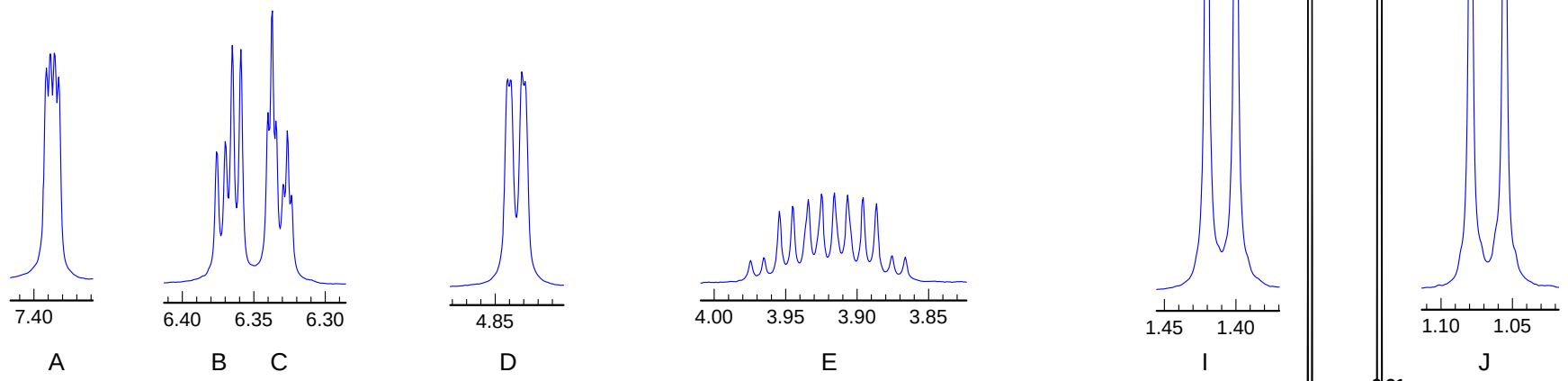

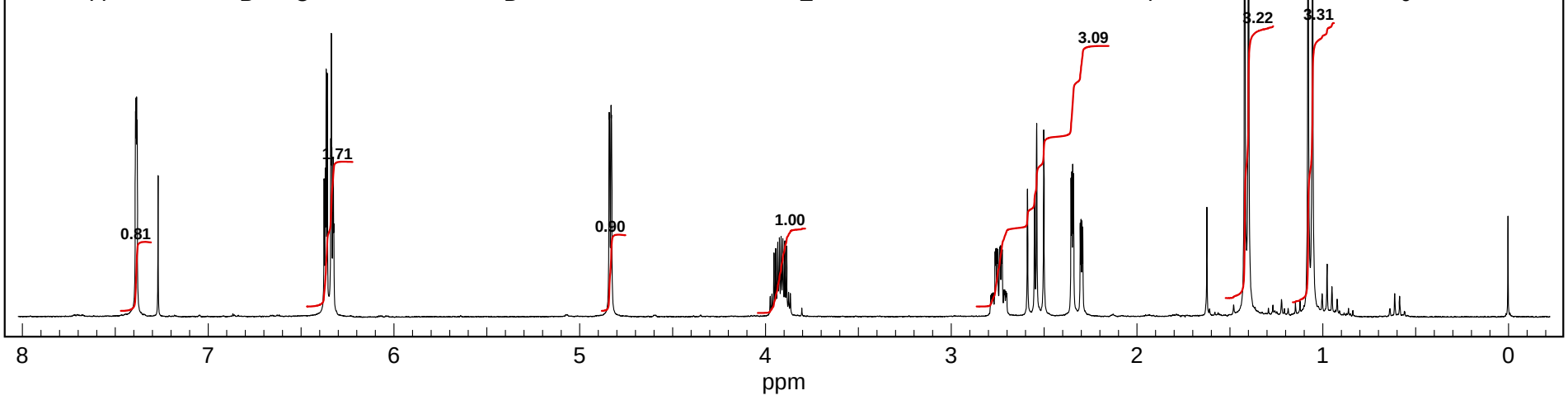

PLT ex-2-2008-09-gq.plt

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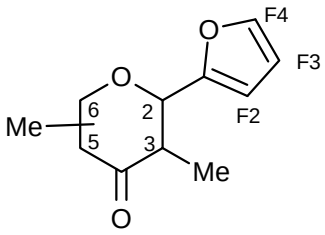

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		A-J	1-6, F_2-F_4 3Me, 5/6Me
A	δ 7.39, dd, J = 2, 1 Hz, 1H	Coupled to: B, C	Assigned to: F4
B	δ 6.36, dd, J = 3.5, 2 Hz, 1H	Coupled to: A, C	Assigned to: F3
C	δ 6.33, dt, J = 3.5, 1 Hz, 1H	Coupled to: A, B, D	Assigned to: F2
D	δ 4.84, dd, J = 3.5, 1 Hz, 1H	Coupled to: C, F	Assigned to: 2
E	δ 3.92, dqd, J = 12, 6, 3 Hz, 1H	Coupled to: H, I, G	Assigned to: 6
F	δ 3.92, qdd, J = 7, 3, 1.5 Hz, 1H	Coupled to: J, D, H	Assigned to: 3
G	δ 2.54, dd, J = 15, 12 Hz, 1H	Coupled to: H, E	Assigned to: 5
H	δ 2.33, ddd, J = 15, 3, 1.5 Hz, 1H	Coupled to: G, E, F	Assigned to: 5
I	δ 1.41, d, J = 6 Hz, 3H	Coupled to: E	Assigned to: 6Me
J	δ 1.07, d, J = 7 Hz, 3H	Coupled to: F	Assigned to: 3Me

(b) Briefly describe how you determined the position of the methyl group

If Me were at C-5 then here should have been a quartet splitting of a proton near 2.8, similar to the H-3 signal F. Since the proton at 3.9 (E) has the quartet splitting, the methyl group must be at position 6

4

A number of other criteria can be used - e.g. the large ^2J between G and H (15 Hz) argues that the CH_2 must be next to a carbonyl not an oxygen, as does the chemical shift.

(c) Using the structure below, draw a good representation of the molecule, clearly indicating stereochemistry (axial or equatorial substituents).

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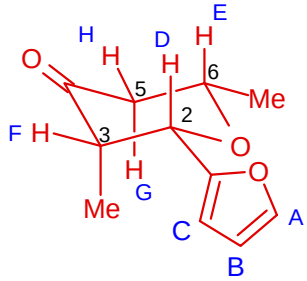
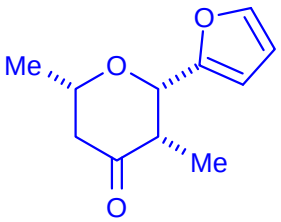
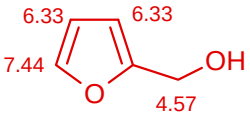
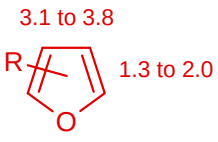




Note long range (allylic) coupling between C and D, and W-couping between F and H

Assignment of furan protons based on shift and coupling comparisons with models:





Large coupling (4Hz) should be between F2 and F3

Can't actually tell whether Fu is ax or eq, except that if it were axial, the ring would flip

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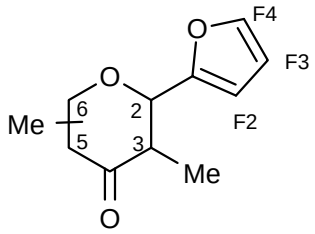

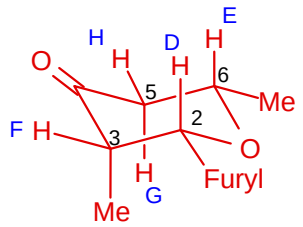

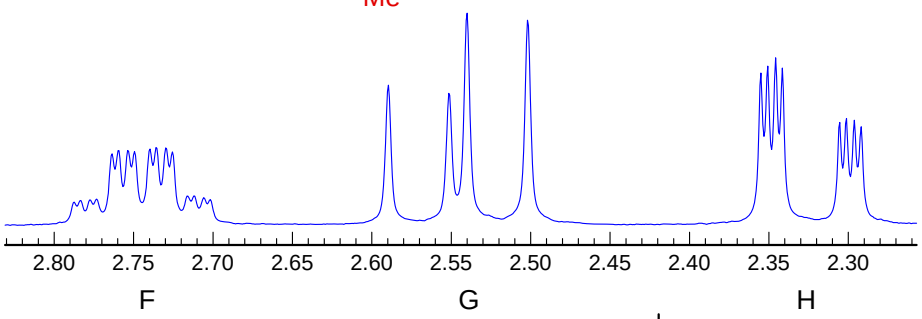

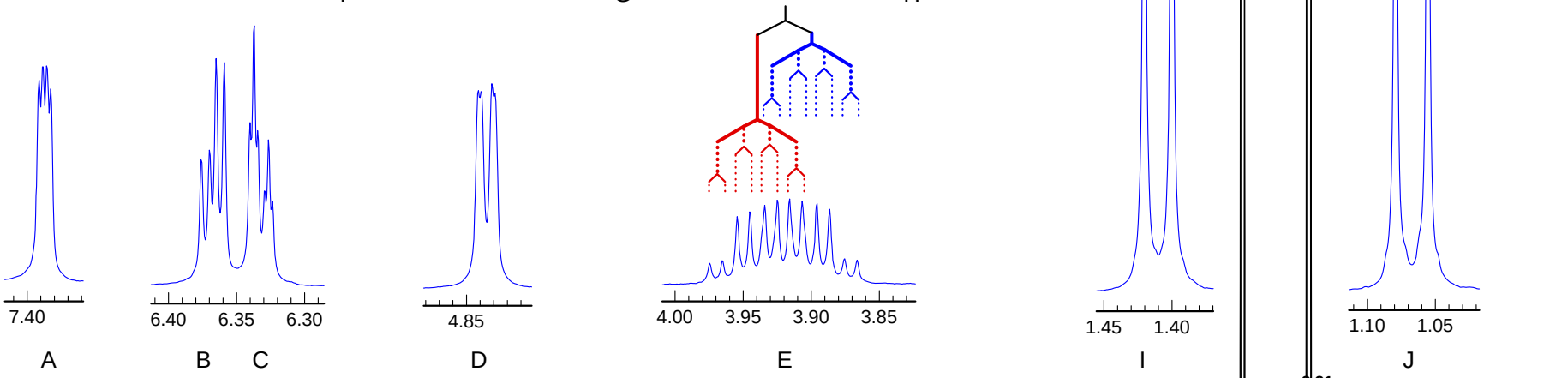

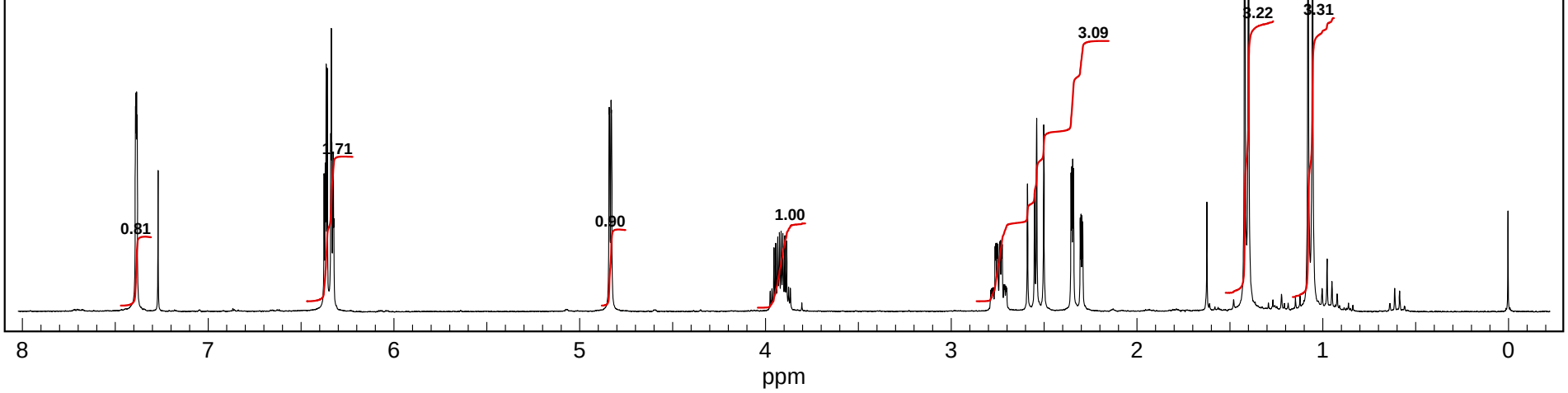

PLT ex-2-2008-09-gq.plt