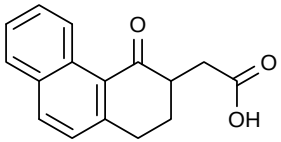
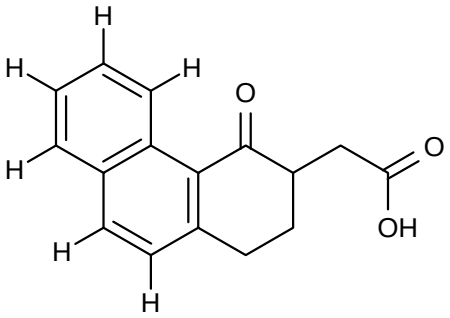
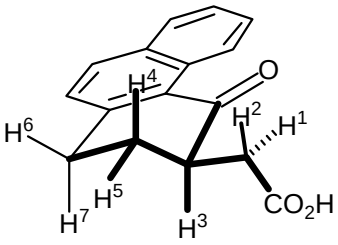
Problem R-05F ($C_{16}H_{14}O_3$)
300 MHz ^{1}H NMR spectrum in $CDCl_3$
Source: Chris Marvin/Charlie Fry g

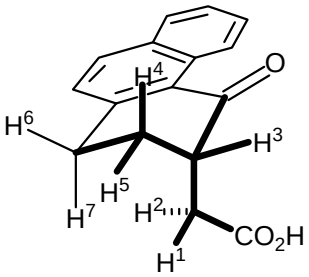


PLT ex-2-2005-06-gq.plt

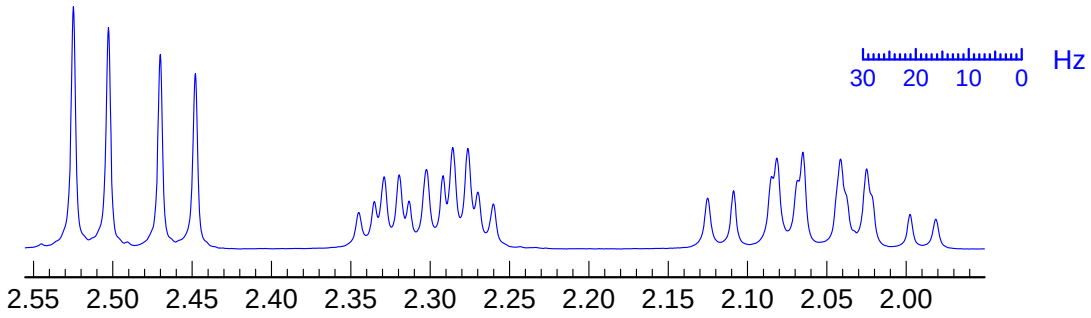
Problem R-05FK ($C_{16}H_{14}O_3$) This problem requires you to assign some of the protons of a substituted naphthalene, and determine the conformation. You may use first order analysis.



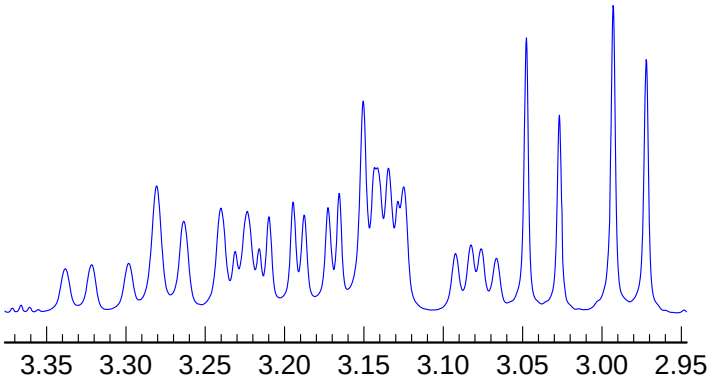




(a) For each proton give the chemical shift (δ), the multiplicity (e.g. dtq) and the coupling constants. To help you pick apart the overlapping peaks between δ 2.95 and 3.35 the signals for H^3 have been identified for you.



	δ	mult.	Coupling constants
H^1			
H^2			
H^3			
H^4			
H^5			
H^6			
H^7			



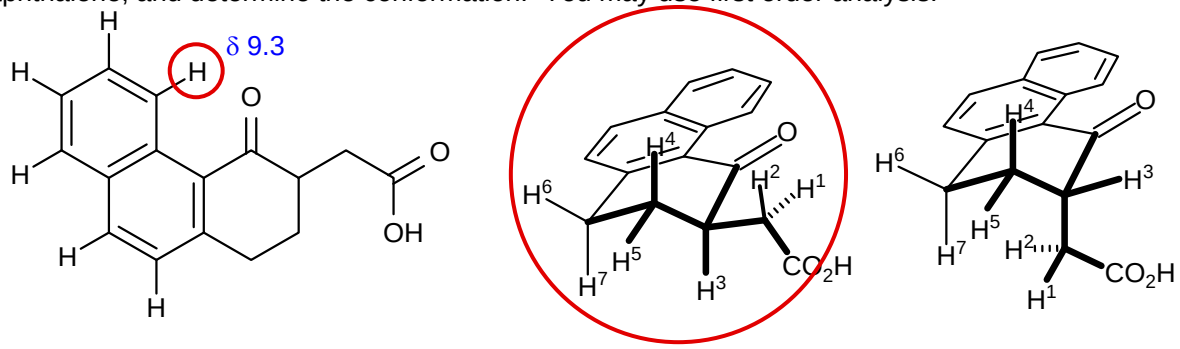
(b) A key signal is the one for H^3. Draw a stick diagram (with correct intensities) of the multiplet for H^3 above or below the appropriate peaks.

(c) **Circle** the correct conformation, and briefly explain how you made the assignment. Be specific.

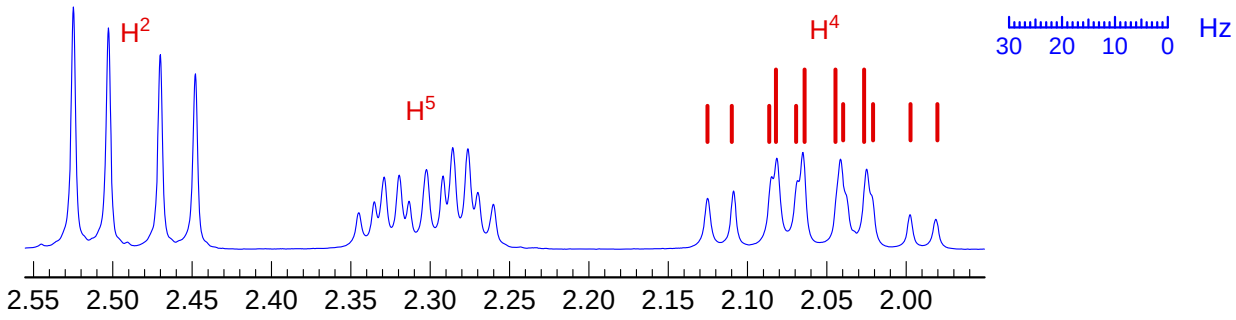
(d) Assign the proton at δ 9.3 (circle it on the structure).

20

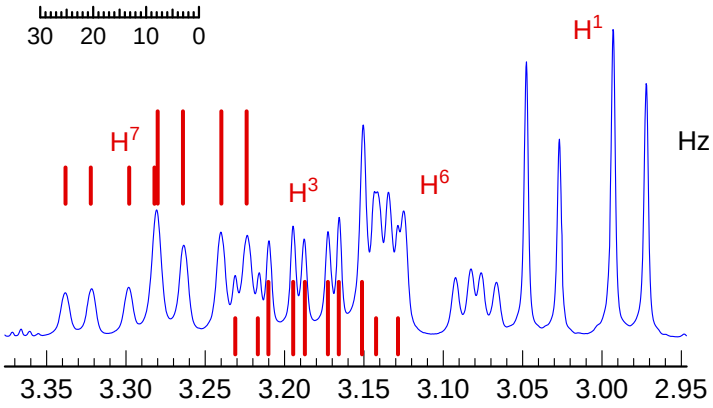
Problem R-05F ($C_{16}H_{14}O_3$) This problem requires you to assign some of the protons of a substituted naphthalene, and determine the conformation. You may use first order analysis.



(a) For each proton give the chemical shift (δ), the multiplicity (e.g. dtq) and the coupling constants. To help you pick apart the overlapping peaks between δ 2.95 and 3.35 the signals for H^3 have been identified for you.



		δ	mult.	Coupling constants
1	H^1	2.49	dd	16.5, 6.5
1	H^2	3.01	dd	16.5, 6.0
2	H^3	3.18	dtd	13.5, 6.5, 4.5
1	H^4	2.06	tdd	13.5, 12.5, 4.5 (almost qd)
1	H^5	2.30	dtd	13.5, 4.5, 3.0
2	H^6	3.12	ddd	17.5, 4.5, 3.0
2	H^7	3.27	ddd	17.6, 12, 5.0



3 (b) A key signal is the one for H^3. Draw a stick diagram (with correct intensities) of the multiplet for H^3 above or below the appropriate peaks.

(c) **Circle** the correct conformation, and briefly explain how you made the assignment. Be specific.

5 The proton H^4 has three large couplings - one is the gem (12.5) and the other two (13.5 and 12.5) are to the axial prons H^7 and H^3. Thus the CH_2CO_2H substituent is equatorial.

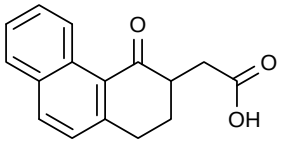
(d) Assign the proton at δ 9.3 (circle it on the structure).

2

Problem R-05F ($C_{16}H_{14}O_3$)

300 MHz ^{1}H NMR spectrum in $CDCl_3$

Source: Chris Marvin/Charlie Fry g



PLT ex-2-2005-06-gq.plt