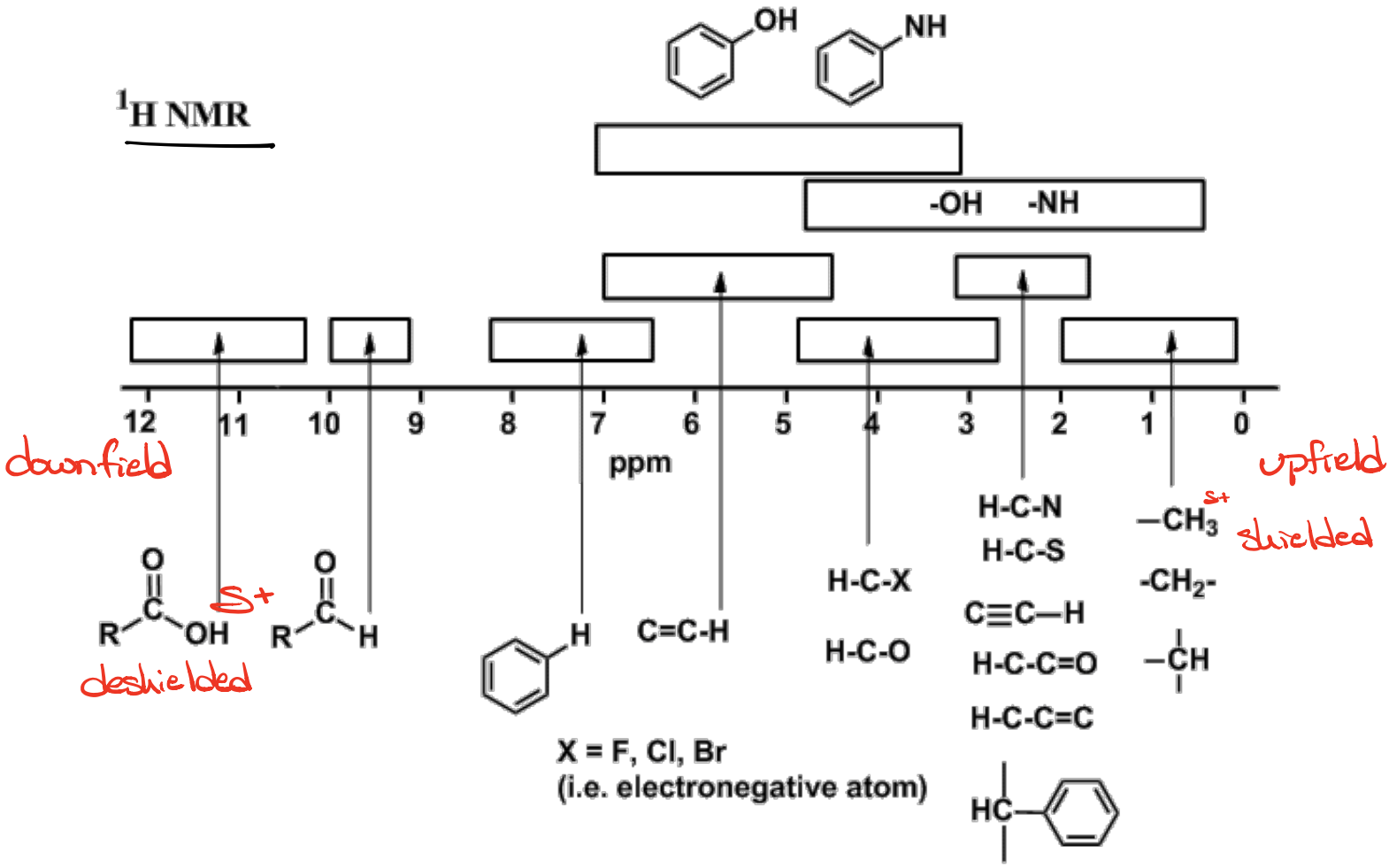
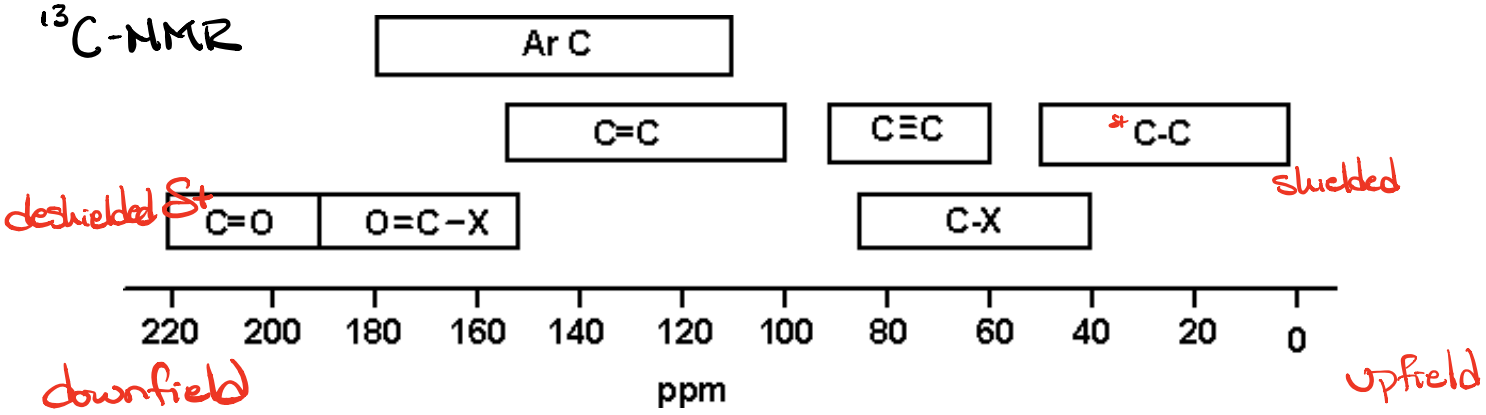
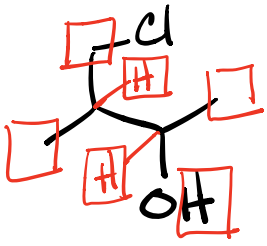
^{1}H NMR


OH
NH
-OH -NH
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
downfield
upfield
shielded
deshielded
δ+
H-C-N
H-C-S
H-C-X
H-C-O
C≡C—H
H-C-C=O
H-C-C=C
-CH2-
C=C-H
X = F, Cl, Br
(i.e. electronegative atom)

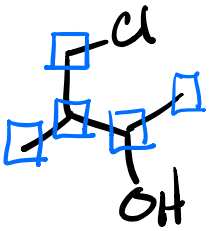
^{13}C-NMR

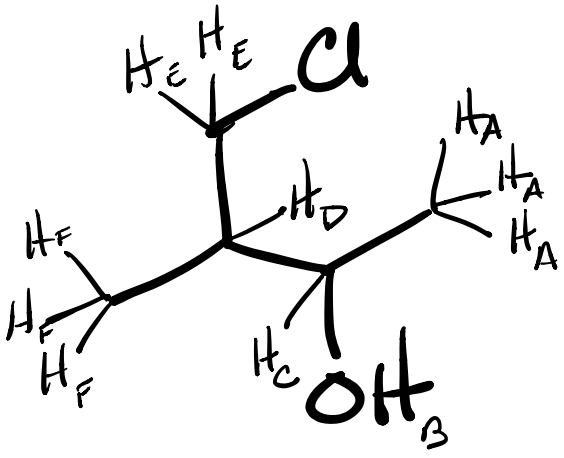


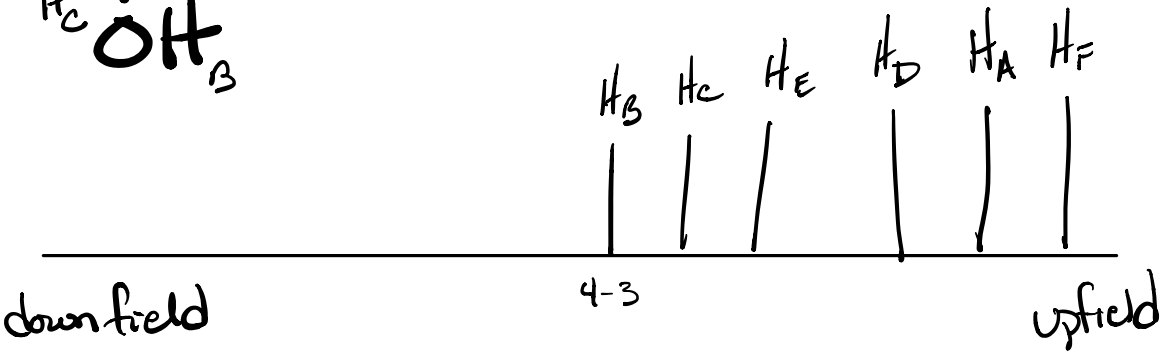


# of H Environments = 6

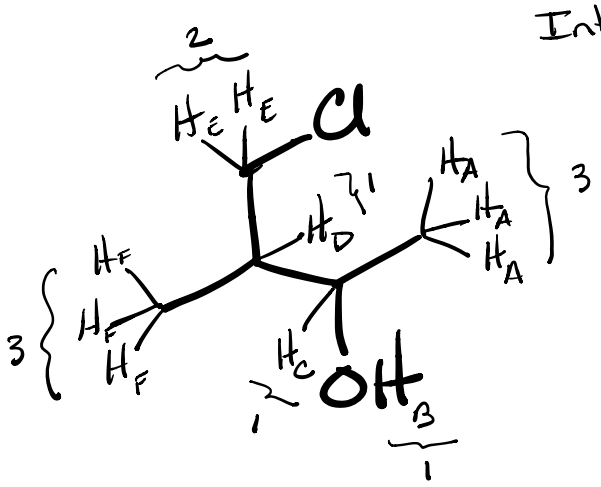
# of C Environments = 5

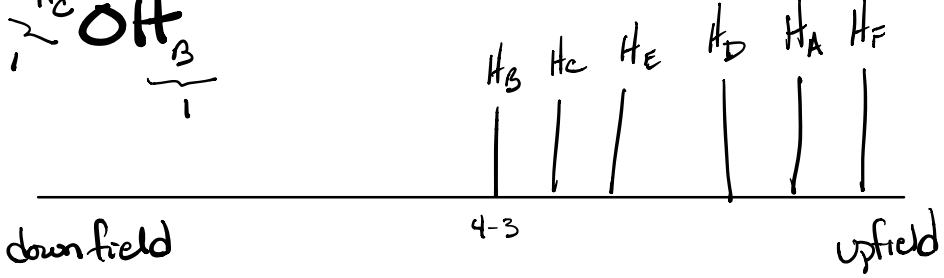


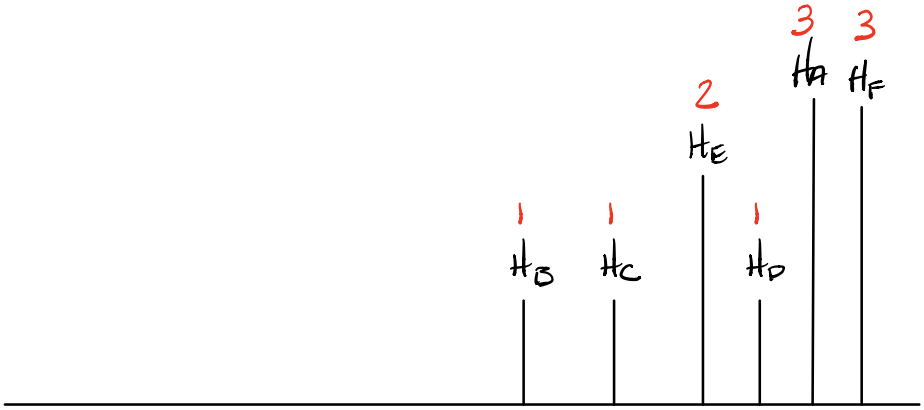




Integration - How many of each type of proton

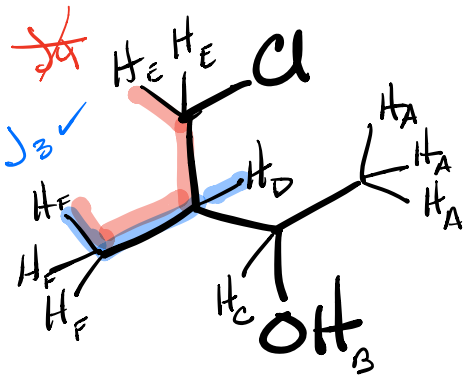


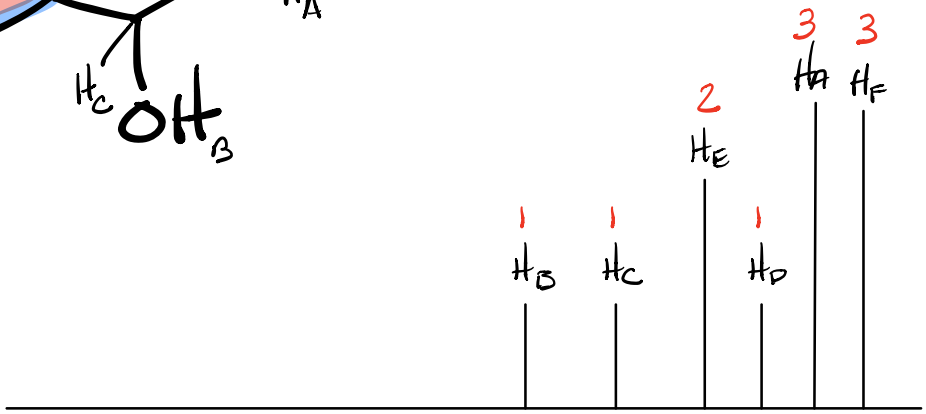




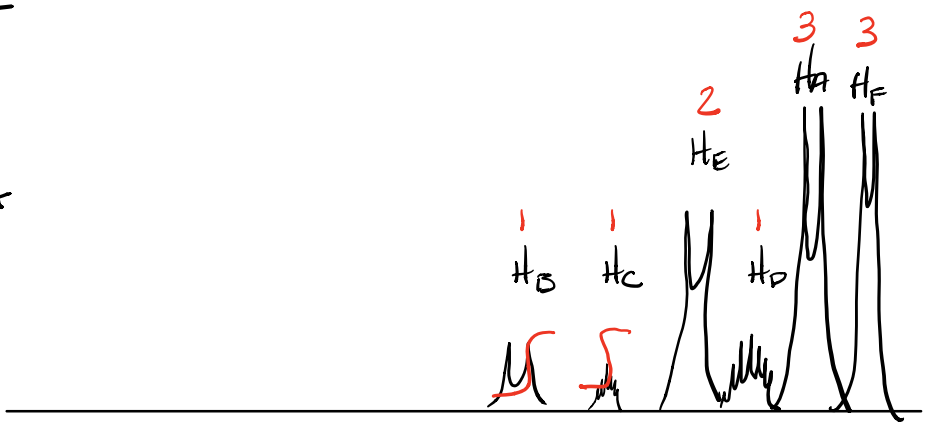
Multiplicity - Spin-Spin Coupling

n+1 rule | n = # of neighbors

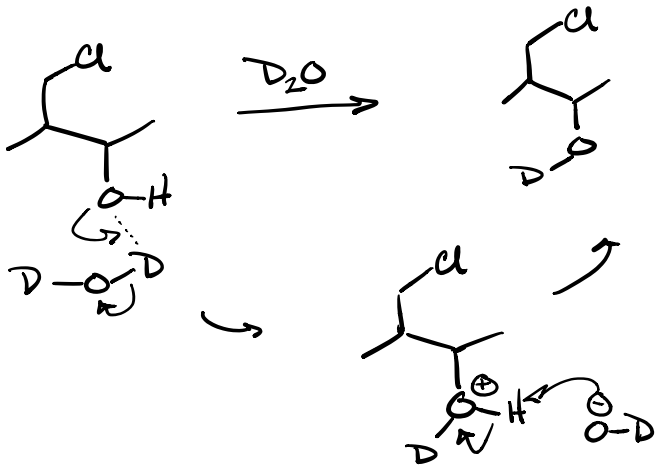




	# n	mult
H_F	1	d
H_A	1	d
H_D	6	mult
H_E	1	d
H_C	5	mult
H_B	1	d



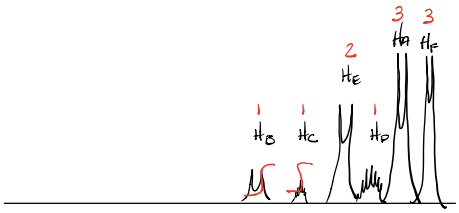
Exchange Experiment with D_2O (Heavy Water)

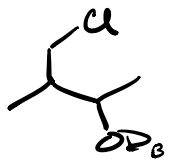


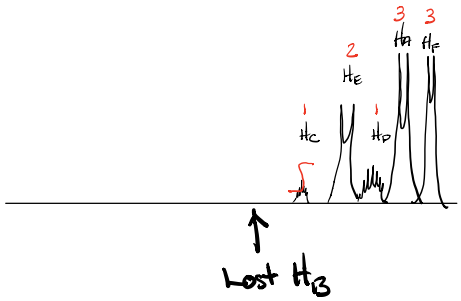
^1H NMR Active

$^2H = D$

non-NMR Active

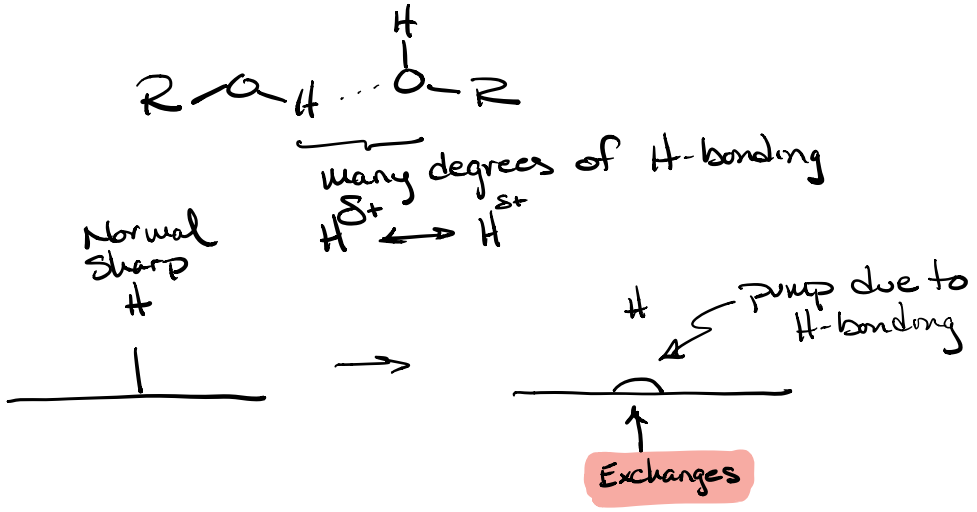




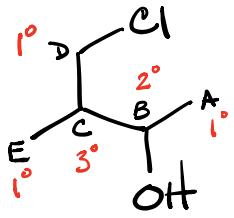


H_B exchanges w/ D_2O & it's NMR signal goes away.

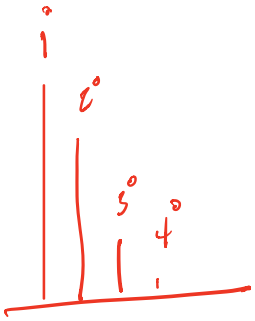
- –OH
- –NH
- –SH



"Exchanges" → means they did the D_2O experiment & proton was found to dissapear from spectrum



^{13}C-NMR



Solving an NMR Problem

① Start w/ Formula

$C_7H_8O_2$

② units of unsaturation

$C_nH_{2n+2+N-X}$

$2(7)+2+0-0$ = 16 Hydrogens for Saturated
-8 hydrogens in molecule
2 | 8 hydrogens missing
4 units of unsaturation

4 units =  3 double bonds + ring = 4 units

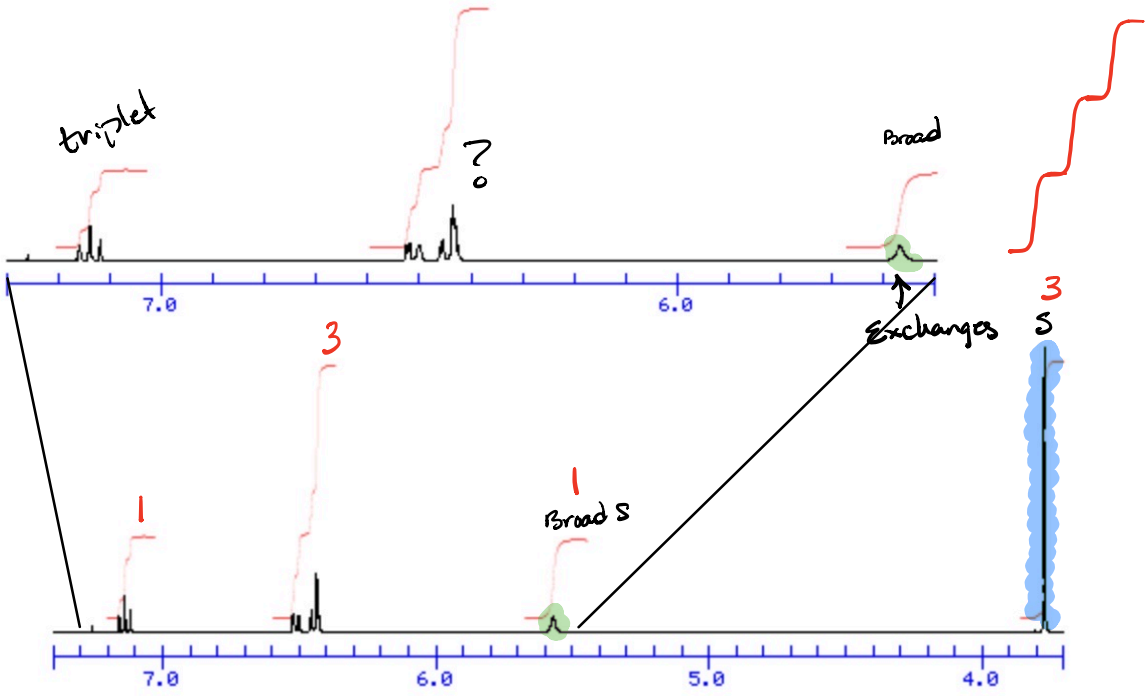
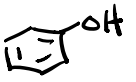
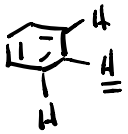


Table of Data

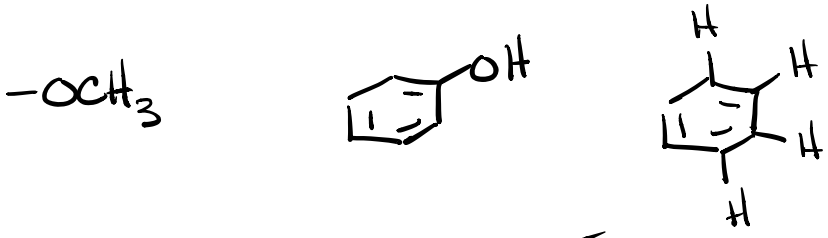
ppm	Int	mult	# of neighbors	assignment
3.8 ppm	3	S	0	EWG-CH_3 ($-O-CH_3$)
5.6 ppm	1	S (Broad) Exchanges	0	
6.5 ppm	3	mult ?	?	Ar-H
7.2 ppm	1	3	2	

Integration Values

3, 6, 9 ⟹ CH_3 (methyl) × 2 or × 3

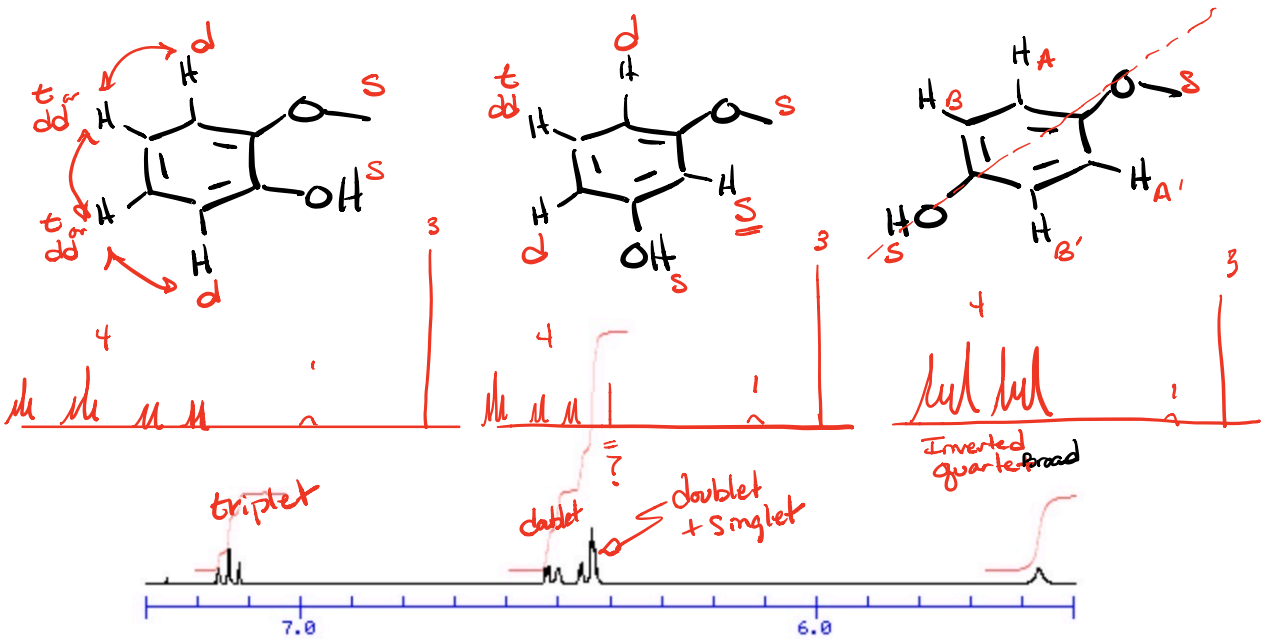
2, 4, 6 ⟹ $-CH_2-$ (methylene) × 2 × 3

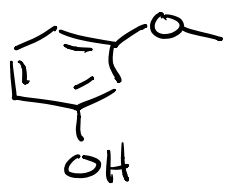
1 ⟹ $-\overset{|}{C}H$, $\overset{O}{\|}-H$, Ar-H, $-\overset{|}{C}-H$, R-OH



$C_7H_8O_2$ ✓

3 possible Structures



Propose  as best match

① Formula
② Units of unsaturation ⇒ Sets limits
③ Made table & analyzed Signals
ppm Int mult # of neighbors assignment
④ Account for all the parts
⑤ Assembled parts into molecules
⑥ Analyze each proposed molecule
⇒ Look for things in Spectrum to throw out Candidates
⑦ Propose single molecule that fits data