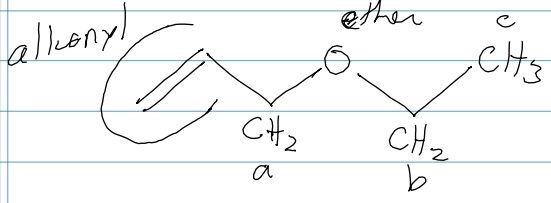
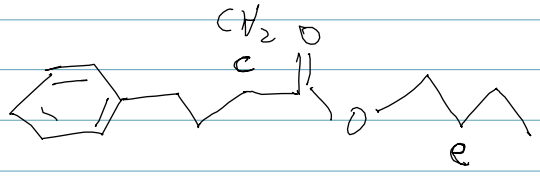
Using NMR Chemical Shift Prediction Tables

Predicting shifts for H on sp^3 carbons

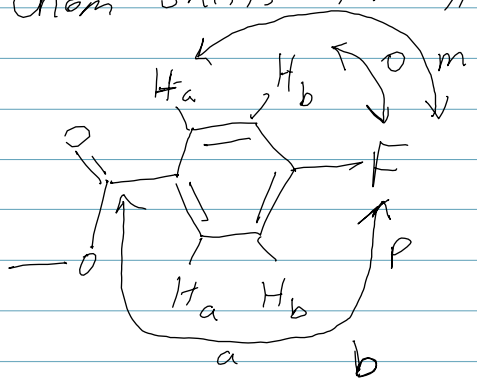




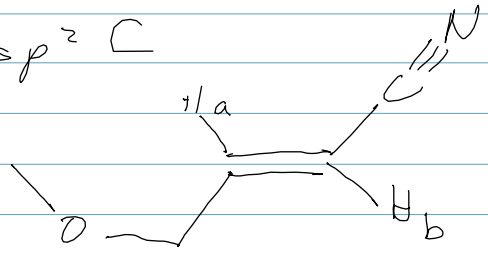
	a	b	c
start	1.2	1.2	0.9
$-CR=CR_2$	0.8 (α)	—	—
$-OR$	2.1 (α)	2.1 (α)	0.3 (β)
	4.1	3.3	1.2

	c	e
start	1.2	1.2
Ar −	0.1 (γ)	—
Ester (C)	1.1 (α)	
Ester (O)		0.5 (β)
	2.4	1.7
obs	(2.3)	(1.6)

Chem shifts for H on sp^2 C



	a	b
start	7.27	7.27
−C(O)OR	+0.9	+0.2
−F	−0.2	−0.3
	7.97	7.17



	a	b
start (C_2H_4)	5.25	5.25
$-CH_2$ O(H or R)	0.67 (gem)	−0.02 (cis)
$-C\equiv N$	+0.78 (cis)	+0.23 (gem)
	6.70	5.46

Expect agreement within 0.2 ppm

(Also ChemDraw)