Chem 334, Exam 2 Professor Fox Spring 2009

Your Name_____

Your TA's Name_____

Question 1, 3 points each Question 2, 12 points Question 3, 12 points Question 4a, 10 points Question 4b, 10 points Question 4c, 10 points Question 4d, 10 points Question 4e, 18 points 1. Match the following compounds with their ¹³C NMR spectra. Note: only chemical shift data is given [multiplicities (s,d,t,q) are not needed to solve this problem]



2. Explain how you would use ¹H NMR spectroscopy to distinguish the following compounds. You may use chemical structures to support your answer, but <u>use no more than 30 words.</u>



3. Explain how you would use IR spectroscopy to distinguish the following compounds. You may use chemical structures to support your answer, but <u>use no more than 30 words.</u>

OH

HO

4. Elucidate the following structure

$C_{11}H_{12}N_2O_2$		
¹³ C NMR	¹ H NMR	IR (cm ⁻¹)
168.2 (s) 139.7 (s) 136.5 (s) 127.5 (d, 2 carbons) 120.5 (d, 2 carbons) 117.7 (s) 70.3 (d) 28.0 (t) 17.6 (q)	8.0 (br s, 1H) 7.57 (d, J=7.7 Hz, 2H) 7.17 (d, J=7.7 Hz, 2H) 4.50 (dd, J=7.9, 6.5 Hz, 1H) 2.89 (dd, J=7.9, 4.0 Hz, 1H) 2.78 (dd, J=6.5, 4.0 Hz, 1H) 2.02 (s, 3H) 1.98 (bs, 1H)	3600-3300 (br) 2260 1690 1530 (IR taken with dilute sample)
a) Circle the functional group that is (i) IR: 2260 cm ⁻¹ and ¹³ C NMR: 1 alkane R_O_R R_ ether alcoh	associated with 117.7 ppm (both spectral characteristics OH R NH ₂ R Cl nol amine alkyl chloride	Ar" refers to aryl, or an aromatic ring s are associated with the same functional group) $R \xrightarrow{R} \xrightarrow{R} \xrightarrow{R} \xrightarrow{R} \xrightarrow{R} \xrightarrow{R} \xrightarrow{R} R$
R HO phenyl phenol	alkyl alkyl Ar alkyl dialkylketone mono-arylketone	Ar Ar alkyl ^{CN} aryl ^{CN} alkylnitrile arylnitrile
alkyl H Ar H alkylaldehyde arylaldehyd	e secondary amide	alkyl acid chloride
O O HO alkyl HO alkyl carboxylic acid aryl carb	aryl RO alkyl boxylic acid alkyl carboxylic ester	RO aryl aryl carboxylic ester nitro aromatic

4. Elucidate the following structure



c) Identify the substructure that is associated with the following. Rationalize your answer based both on the chemical shifts and the coupling constants:

7.57 (d, J=7.7 Hz, 2H) 7.17 (d, J=7.7 Hz, 2H)

- d. Assign the following coupling constants. Your answer must clearly indicate which protons are coupled to one another.
- 4.50 (dd, J=7.9, 6.5 Hz, 1H) 2.89 (dd, J=7.9, 4.0 Hz, 1H) 2.78 (dd, J=6.5, 4.0 Hz, 1H)

e) draw the structure of the product (no partial credit)

