1) Draw the $^1$H-NMR spectrum of a 2:3:2 mixture of 1,4-dimethoxybenzene, 2-propanone, and diethyl ether.

Clearly show the multiplicity, the relative peak heights, and integration value of each signal in the $^1$H-NMR spectrum of this mixture. You do not need to show signals from the solvent or reference compound.

1,4-Dimethoxybenzene (CDCl$_3$): δ 3.80 (CH$_3$), 6.80 ppm (Ph-H).

2-Propanone (CDCl$_3$): 2.10 ppm (CH$_3$)

Diethyl ether (CDCl$_3$): δ 1.20 ppm (CH$_3$), 3.40 ppm (CH$_2$)

10 pts total
Questions 2 - 4 require you to use a combination of molecular formula, NMR and MS data in order to identify each unknown compound. Spectroscopic data are given on the following pages.

- show clearly your calculation of the IHD value for each compound.
- show all lone pairs and charges for each structure, partial structure, or fragment.
- label each set of equivalent protons using the H_a, H_b, H_c etc. labeling system shown in the NMR lectures and practice problem sets.
- assign each ¹H-NMR signal to a particular set of equivalent protons and write your assignments directly onto the spectrum.
- draw the molecule directly onto the ¹H-NMR spectrum.
- identify each ¹³C-NMR signal as either alkyl, vinyl, alkynyl, aryl, nitrile, imine, or carbonyl (you do not need to assign individual carbon atoms to each signal).
- identify each IR absorption band as due to a specific functional group.
- draw MS fragments for all labeled peaks in the EI-MS directly onto the spectrum (you do not need to show the fragmentation mechanism).
- use all data supplied and hand in all spectra for each question.
- write and sketch clearly! Your TA cannot grade what he/she cannot read.
- points will be deducted for illegible writing, unclear/ambiguous drawings, etc.

2) Use the supplied ¹H-NMR, ¹³C-NMR, and IR data to identify Compound A, C₈H₅NO₅ (10 pts).

3) Use the supplied ¹H- NMR, ¹³C-NMR, IR, and EI-MS data to identify Compound B, C₅H₇NO₂ (14 pts).

4) Use the supplied ¹H- NMR, ¹³C-NMR, and EI-MS data to identify Compound C, C₁₃H₂₀N₂O₂ (16 pts).
Q2) Compound A C₈H₅NO₅

¹H-NMR Spectrum 6 – 10.5 ppm (no signals 0-6 ppm)
Q2) Compound A $\text{C}_8\text{H}_5\text{NO}_5$ $^{13}\text{C}$-NMR Spectrum
Q2) Compound A $C_8H_5NO_5$  IR Spectrum

1722 cm$^{-1}$
Q3) Compound B  C$_5$H$_7$NO$_2$  $^1$H-NMR Spectrum

300 MHz $^1$H NMR
In CDCl$_3$
Q3) Compound B  C$_5$H$_7$NO$_2$  $^{13}$C-NMR Spectrum
Q3) Compound B \( \text{C}_5\text{H}_7\text{NO}_2 \) IR Spectrum

2266 cm\(^{-1}\)

1751 cm\(^{-1}\)
Q3) Compound B  $\text{C}_5\text{H}_7\text{NO}_2$  EI-MS
Q4) Compound C  \( \text{C}_{13}\text{H}_{20}\text{N}_{2}\text{O}_{2} \)

\(^1\text{H}-\text{NMR} \text{ Spectrum} 0-8 \text{ ppm} \)
Q4) Compound C  $\text{C}_{13}\text{H}_{20}\text{N}_{2}\text{O}_{2}$

$^1\text{H}$-NMR Spectrum 1.0 – 4.5 ppm

300 MHz $^1\text{H}$ NMR
In CDC$_{13}$
Q4) Compound C $\text{C}_{13}\text{H}_{20}\text{N}_2\text{O}_2$

$^1\text{H}$-NMR Spectrum 6.5 – 8.0 ppm
Q4) Compound C \( \text{C}_{13}\text{H}_{20}\text{N}_2\text{O}_2 \) \(^{13}\text{C}\)-NMR Spectrum
Q4) Compound C \( C_{13}H_{20}N_2O_2 \)  EI-MS