**Fall 2020 Chem 222-234: Homework Assignment 2 – Week 4 (50 marks)**

1. (10 marks) Provide brief explanations for each statement below – can be point form (please type out answers if possible, if handwriting is necessary, be sure to be legible and use pen):
   1. Coupling constants are reported in Hz rather than ppm
   2. Enantiotopic hydrogens appear as one 1H signal
   3. Diastereotopic hydrogens appear as two 1H signals
   4. Hydrogens on isolated alkenes show less deshielding than those on aromatic rings
   5. S shows a different molecular ion pattern than Cl
2. (6 marks) Describe two distinguishing features between the following pair of molecules, one using 1H NMR Spectroscopy and one using mass spectrometry (MS).
   1. 

Technique 2: MS

Distinguishing Feature between A and B:

Technique: 1H NMR Spectroscopy

Distinguishing Feature between A and B:

1. (10 marks) **Sketch the 1H NMR spectrum** that you would expect from the given molecule. In addition to positioning the signals in the appropriate chemical shift regions, include peak labels (starting with most deshielded as “A”), integration values, and splitting patterns (ignoring long range, 4J, splitting) for each signal. See example below.

Example: Bromoethane

CH3 **B**

3 H, triplet

CH2 **A**

2 H, quartet

δ (ppm)

2

4

6

8

10

0

2

4

6

8

10

0

δ (ppm)



1. (4 marks) Determine the relationship (homotopic, enantiotopic, diastereotopic, heterotopic) between the indicated hydrogens in each structure below. How many total 1H signals would you expect for each structure?

Relationship:

# 1H signals:

Relationship:

# 1H signals:



1. (10 marks) An unknown compound produces an 1H NMR spectrum with only three signals: 1.8, 2.8, and 7.5 (broad) ppm, all singlets that integrate in a 6:3:1 ratio, respectively. The 13C NMR spectrum shows 4 signals. Both spectra are provided below. The mass spectrum shows a molecular ion region with the following peaks: *m/z* 135 (100%), 136 (5.9 %), 137 (33%). **Determine the number of carbons, molecular formula, and propose a structure**. **Assign all 1H and 13C NMR signals to specific chemical environments or specific hydrogens in your structure.**

Number of carbons:

Structure of Unknown:

Formula:

**1H NMR Spectrum of Unknown**



**13C NMR Spectrum of Unknown**

1. (10 marks) **Lacosamide** (Vimpat) is an anticonvulsant drug used for the prevention and control of seizures. Using SciFinder, find a primary source (i.e. an academic journal article) that contains a 1H NMR spectrum of lacosamide. Assign the 1H signals in your spectrum that match hydrogens A, B, and C on the structure provided (full assignment is not needed). Include your annotated spectrum in your answer. Draw a clearly labelled tree diagram to describe the expected splitting pattern for signal A or B (include all J relationships). Provide the reference you used to obtain the spectrum, formatted using ACS style. **HINT: For information on using SciFinder to find spectra, refer to the “Searching the Literature” document on myCourses.**

**Annotated 1H NMR spectrum:**



**Tree diagram of A or B:**

**Reference in ACS Style:**