CH-314 Structural Analysis
ruben.rodriguezmadrid@epfl.ch
ray.cowen@epfl.ch

Jigsaw 2C

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1. [From Past Exams] Determine if each statement is true or false. If false, correct the statement to make it true.

a. NMR spectroscopy uses infrared pulses to flip nuclear spins.

FALSE = NMR uses radio frequency (Rf) pulse.

b. A more shielded proton will resonate at a higher ppm value.

FALSE = "The greater the smaller the chemical shift"

c. 13C spectra with 1H decoupling are more sensitive than without decoupling.

Good thinking! And remember that the sensitivity is proportional to the S/N (the second part of your options)

TRUE and FALSE

This affirmation can be both true or false depending on our interpretation of "more sensitive". For example, one can consider that the coupled spectra is more sensitive because it gather more informations since it shows more peaks. Therefore, the affirmation would be false. On the other side, one can consider the decoupled spectra as more sensitive because it significantly reduces the noise increasing the data interpretability. Therefore the information would be true.

d. Fourier transformation converts the time domain into the frequency% domain.

TRUE

e. Multiplet splitting patterns are caused by scalar couplings.

TRUE

f. Increasing the magnetic field will result in a larger separation of peaks within multiplets in ppm.

FALSE = The reference frequency ν_{ref} is proportional to the magnetic field $\vec{B}$. The chemical shift is $\tau = \left(\frac{\nu - \nu_{ref}}{\nu_{ref}}\right) 10^6$ [ppm]. Therefore, if $\vec{B}$ increases, ν_{ref} will increase resulting in a smaller separation of peaks in ppm.

Good!!

2. [Hore Section 2.2] How many different signals will you see in a 1H spectrum in the following molecules? See also: Jigsaws 2A.1, 2B.3, 2D.1, and 2E.1.

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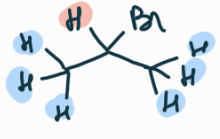
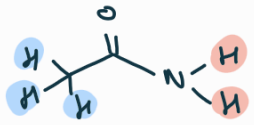
Every peak of the spectrum corresponds to a different type of proton. Therefore, the number of signals in a 1H spectrum of a molecule is equal to the number of different H in that molecule.

a. CH3CBrHCH



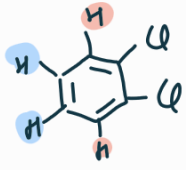
- 2 types of H
- 2 peaks

b. CH3C(O)NH2



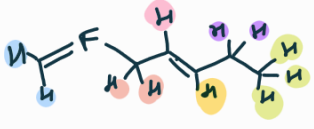
- 2 types of H
- 2 peaks

c. 1,2-dichlorobenzene



- 2 types of H
- 2 peaks

d. CH2FCH2CHCHCH2CH3



- 6 types of H
- 6 peaks

3. [Hore Section 2.3] Two students prepared each an NMR tube of ethanol in deuterated chloroform. The first one used 1 mM of ethanol, the second student used 100 times that concentration. Apart from the difference in intensity, will they obtain the same proton spectrum? Why or why not?

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No, the two students will likely not obtain identical proton spectra due to a phenomenon known as "concentration-dependent effects". When the concentration of ethanol increases significantly, as in the second student's sample (100 mM), interactions between ethanol molecules, such as hydrogen bonding, becomes stronger. These intermolecular interactions can slightly shift the chemical environment of protons (more positive ppm) because gen-bonded proton will be deshielded, especially for the hydroxyl (-OH) proto im ethanol, which is particularly sensitive to hydrogen bonding.

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Jigsaw 2C

1. [From Past Exams] Determine if each statement is true or false. If false, correct the statement to make it true. **1.75/2**

   a. NMR spectroscopy uses ~~infrared~~ radio pulses to flip nuclear spins. F

   b. A more shielded proton will resonate at a ~~higher~~ lower ppm value. F

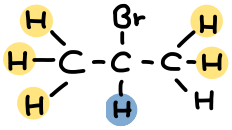
   c. ^{13}C spectra with ^{1}H decoupling are more sensitive than without decoupling. T

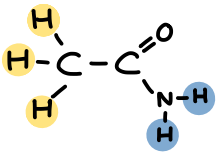
   d. Fourier transformation converts the time domain into the frequency domain. T

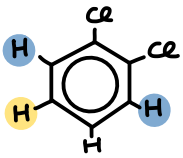
   e. Multiplet splitting patterns are caused by scalar couplings. T

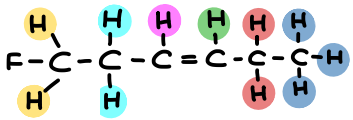
   f. Increasing the magnetic field will result in a larger separation of peaks within multiplets in ~~ppm~~ Hz. F … will result in a smaller separation of peaks within multiplets in ppm

2. [Hore Section 2.2] How many different signals will you see in a ^{1}H spectrum in the following molecules? *See also: Jigsaws 2A.1, 2B.3, 2D.1, and 2E.1.* **2/2**

   a. $CH_3CBrHCH_3$  2 signals

   b. $CH_3C(O)NH_2$  2 signals

   c. 1,2-dichlorobenzene  2 signals

   d. $CH_2FCH_2CHCHCH_2CH_3$  6 signals

3. [Hore Section 2.3] Two students prepared each an NMR tube of ethanol in deuterated chloroform. The first one used 1 mM of ethanol, the second student used 100 times that concentration. Apart from the difference in intensity, will they obtain the same proton spectrum? Why or why not? **1/2**

   The higher sample concentration increases the number of H-bonds, causing the spectrum to shift to a higher frequency. **Why? See Hore Section 2.3**