2/2 Nice job!

CH-314 Structural Analysis
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Jigsaw 4D

2D NMR: HSQC and HMBC

2D NMR experiments are not limited to one nucleus, but we can also perform heteronuclear 2D NMR experiments. One example is the Heteronuclear Single Quantum Coherence (HSQC) experiment, which detects ^{1}H-^{13}C single bond correlations. Another is the Heteronuclear Multiple Bond Correlation (HMBC) experiment, which gives correlations between carbons and protons that are separated by two or three bonds. Direct one-bond correlations are suppressed. The intensity of cross peaks depends on the coupling constant. Thus, the absence of a cross peak doesn't confirm that carbon-proton pairs are many bonds apart.

1. Two spectra for sucrose are shown below. Which spectrum corresponds to HSQC and which corresponds to HMBC? How do you know?

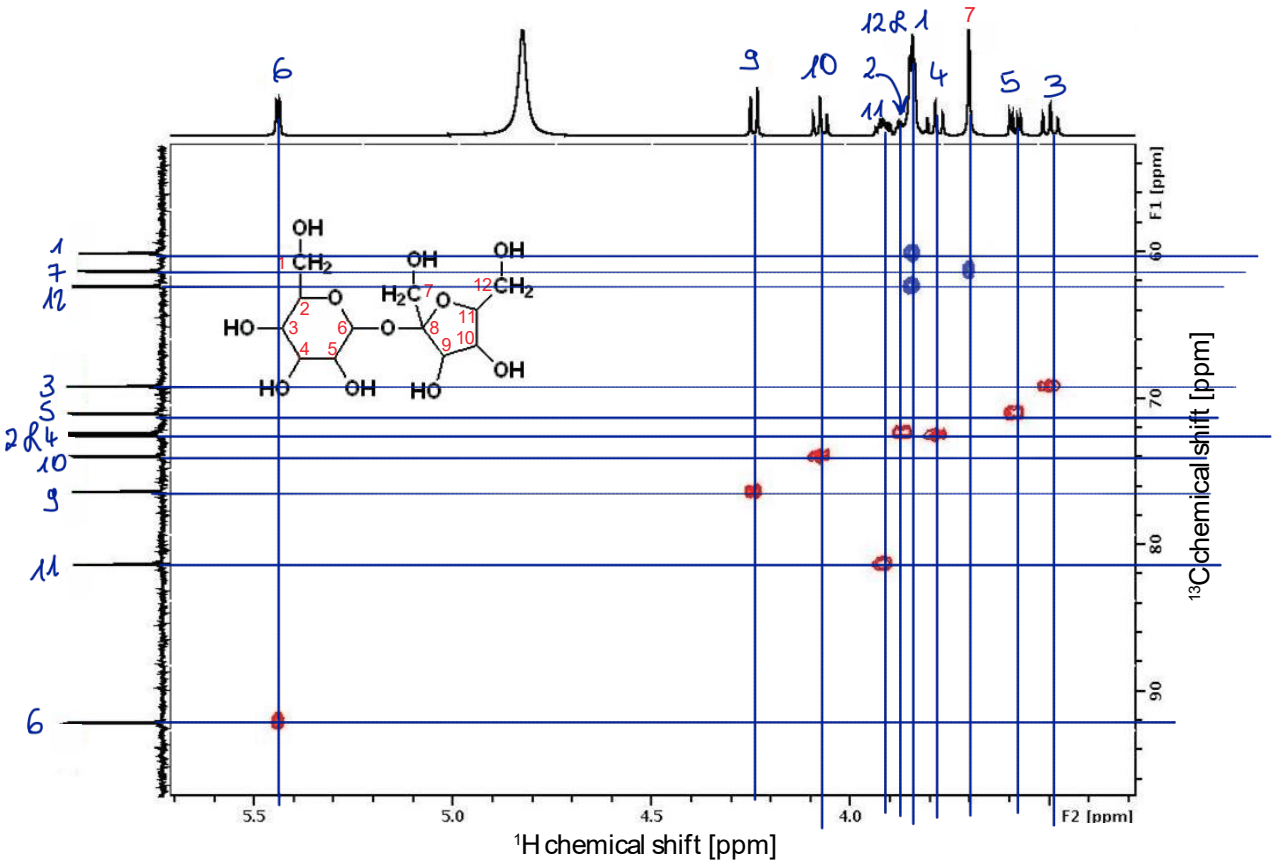
The first spectrum corresponds to HSQC because each carbon is attached to one hydrogen
The second one corresponds to HMBC because there are multiple hydrogens for each carbon.

2. Why are some peaks in the first spectrum blue and others are red? What additional information does this provide/how does it aid in the assignment?

The blue peaks represents CH_2 groups and the red peaks represents the CH groups.
The blue points are less shielded than the red ones.

Good! Note that in 2D NMR spectra, different colors usually represent different signs. The HSQC experiment (and sometimes other experiments) usually has a portion included that makes all the signals with an even number of protons (C, -CH2) negative and those with an odd number (-CH, -CH3) positive

3. Assign the ^{1}H and ^{13}C projections. Notice that the axis limits for ^{13}C vary between the experiments.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9
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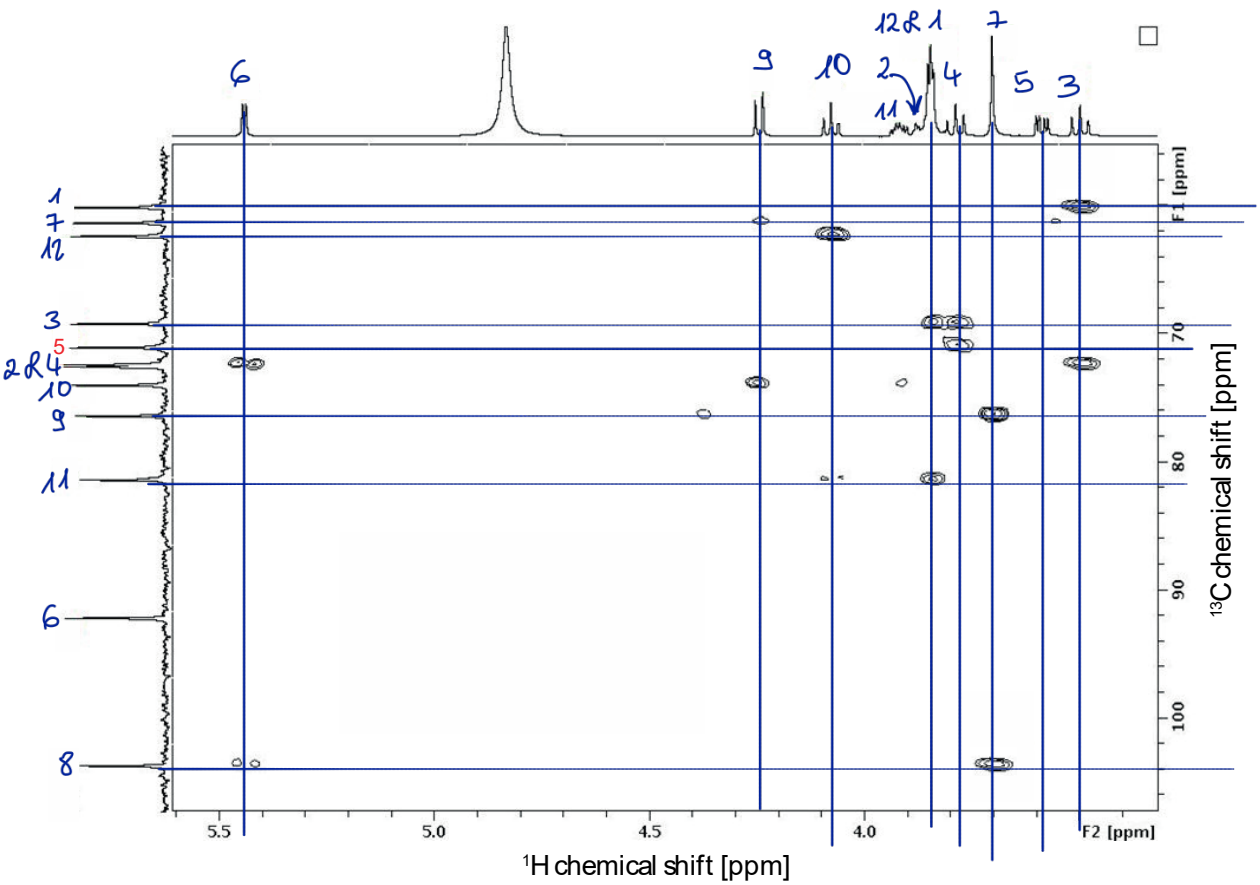
12&1
2
11
4
7
5
3
1
7
12
3
5
2&4
10
9
11
6
OH
CH2
HO
O
H2C
12CH2
F1 [ppm]
60
70
80
90
13C chemical shift [ppm]
5.5
5.0
4.5
4.0
F2 [ppm]
1H chemical shift [ppm]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10
9
11
6
8
F1 [ppm]
70
80
90
100
13C chemical shift [ppm]
5.5
5.0
4.5
4.0
F2 [ppm]
1H chemical shift [ppm]

2/2 Good work!

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1. Two spectra for sucrose are shown below. Which spectrum corresponds to HSQC and which corresponds to HMBC? How do you know?

(A) corresponds to HSQC because each carbon is associated to one proton.

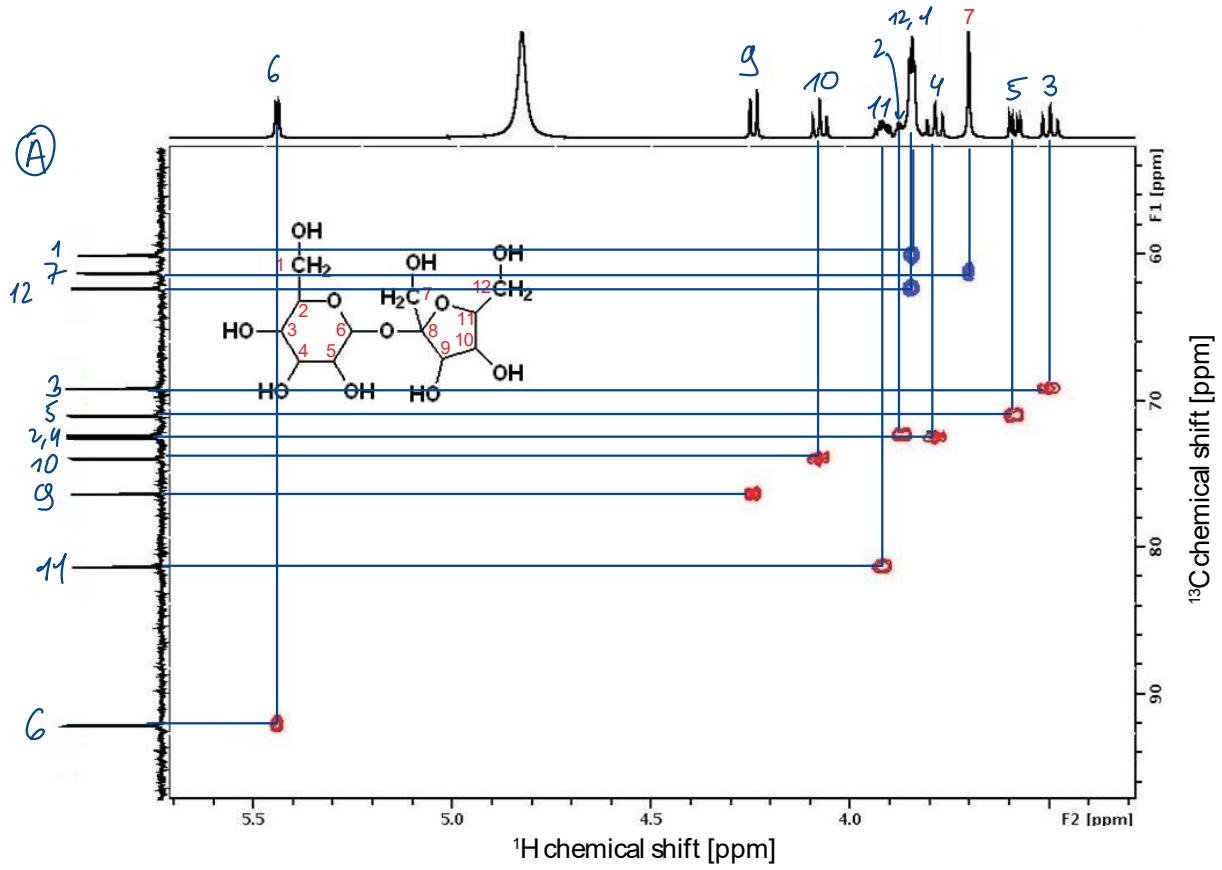
(B) corresponds to HMBC because there are multiple protons per carbon.

2. Why are some peaks in the first spectrum blue and others are red? What additional information does this provide/how does it aid in the assignment?

The blue ones are CH and the red ones are CH_2.

This provides the numbers of CH and CH_2. And, it helps to find the structure of the molecule. Also, it gives which CH and CH_2 are more or less shielded, therefore knowing the structure we can attribute the carbons and protons.

3. Assign the ^{1}H and ^{13}C projections. Notice that the axis limits for ^{13}C vary between the experiments.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2, 4
10
9
11
6
OH
CH2
HO
O
OH
H2C
CH2
OH
HO
OH
HO
F1 [ppm]
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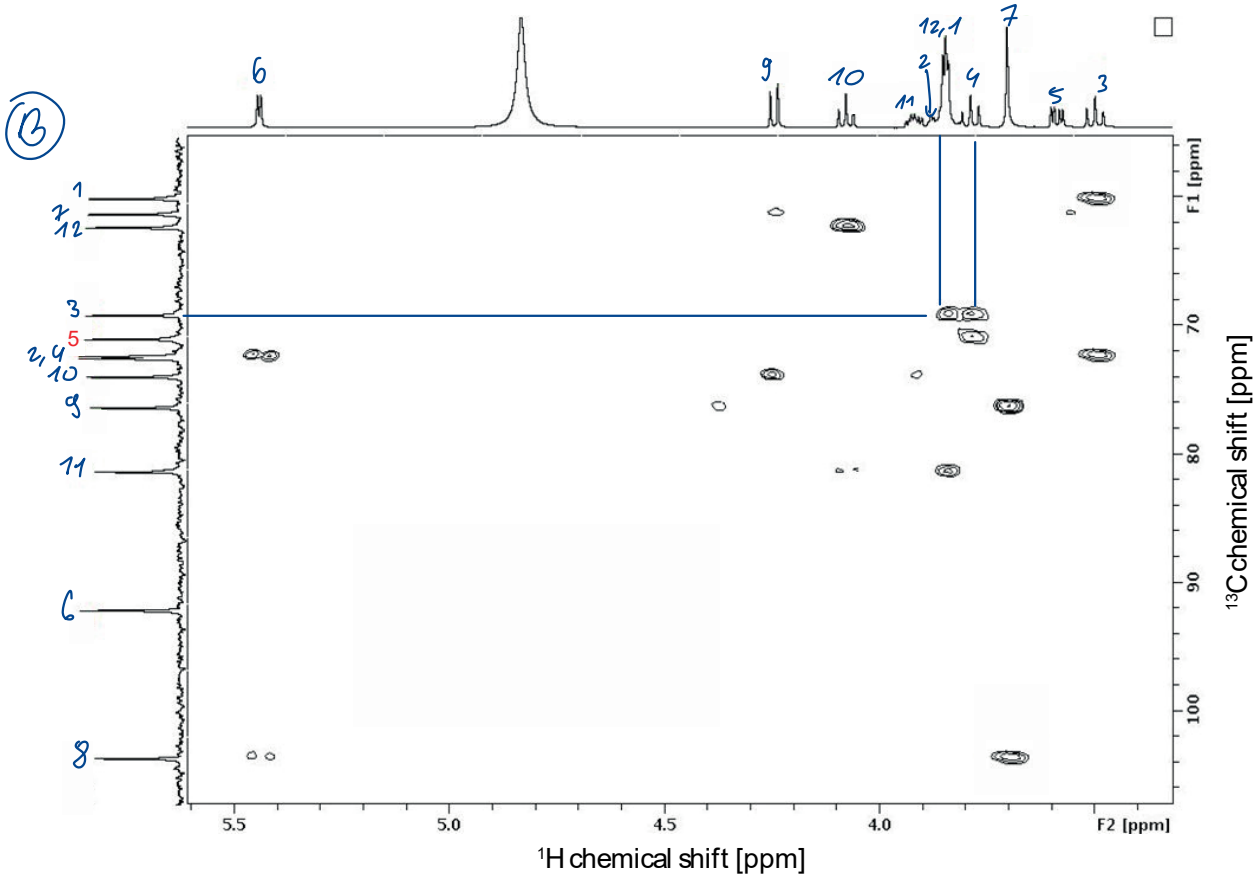
80
90
13C chemical shift [ppm]
5.5
5.0
4.5
4.0
F2 [ppm]
1H chemical shift [ppm]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F1 [ppm]
70
80
90
100
13C chemical shift [ppm]
5.5
5.0
4.5
4.0
F2 [ppm]
1H chemical shift [ppm]