CH-314 Structural Analysis
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Jigsaw 4D

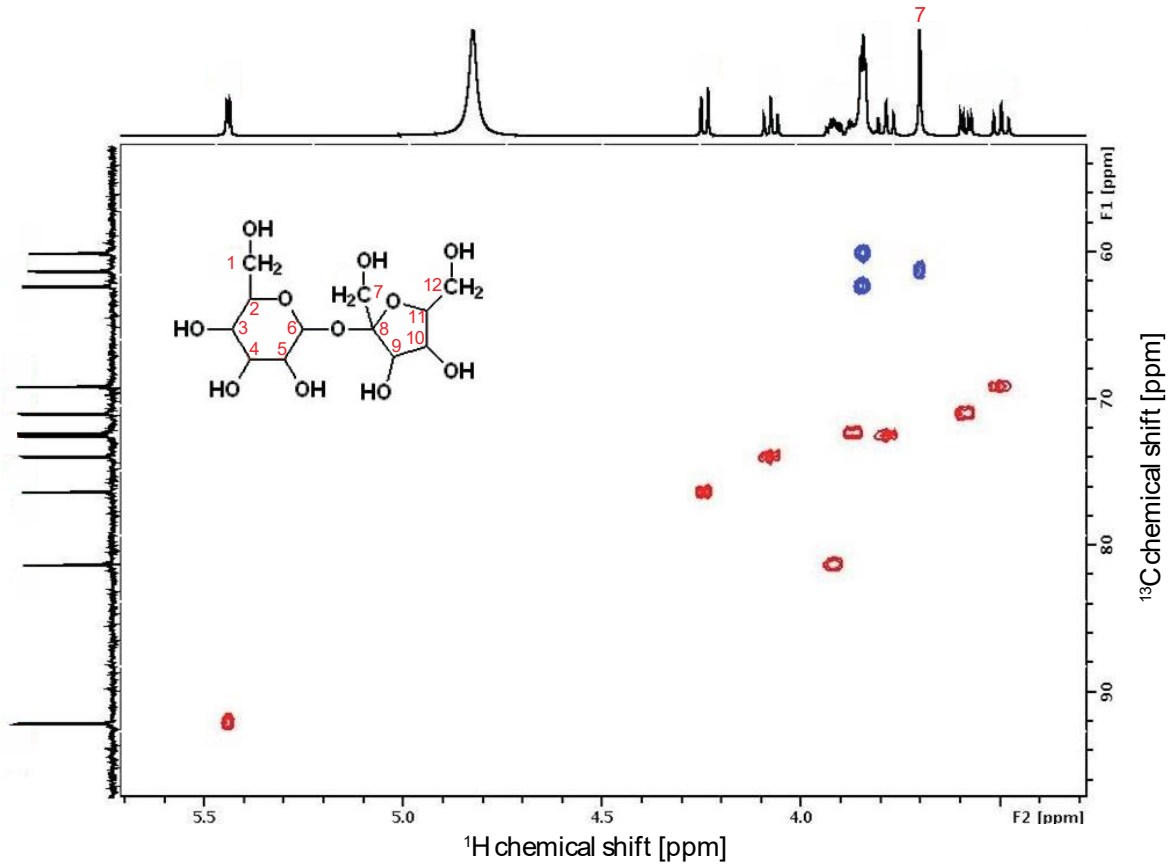
2D NMR: HSQC and HMBC

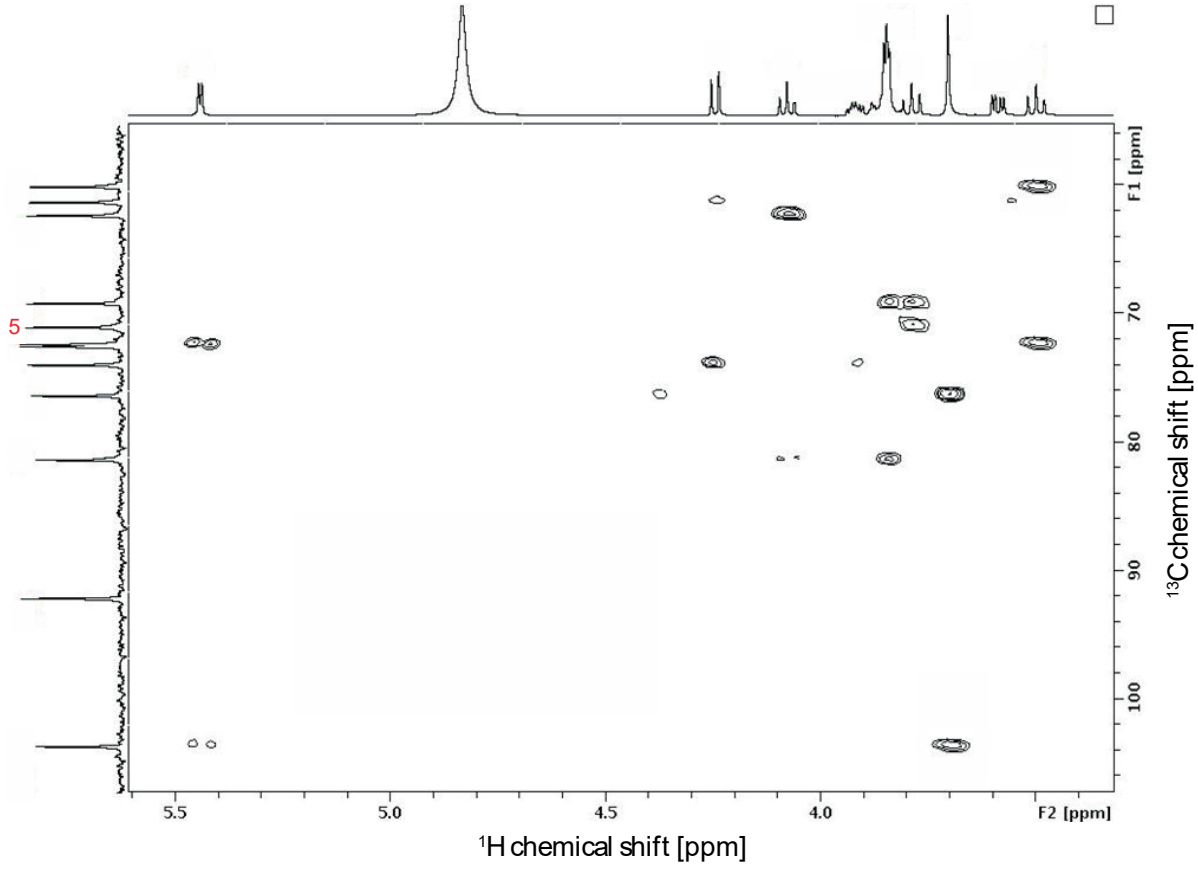
2D NMR experiments are not limited to one nucleus, but we can also perform heteronuclear 2D NMR experiments. One example is the Heteronuclear Single Quantum Coherence (HSQC) experiment, which detects ^{1}H-^{13}C single bond correlations. Another is the Heteronuclear Multiple Bond Correlation (HMBC) 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?

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?

3. Assign the ^{1}H and ^{13}C projections. Notice that the axis limits for ^{13}C vary between the experiments.


7
OH
1 CH2
2
O
HO
3
6
O
4
5
HO
OH
OH
H2C 7
8
O
11
9
10
HO
OH
OH
12 CH2
F1 [ppm]
60
70
80
90
5.5
5.0
4.5
4.0
F2 [ppm]
13C chemical shift [ppm]
1H chemical shift [ppm]


5
F1 [ppm]
70
80
90
100
5.5
5.0
4.5
4.0
F2 [ppm]
13C chemical shift [ppm]
1H chemical shift [ppm]