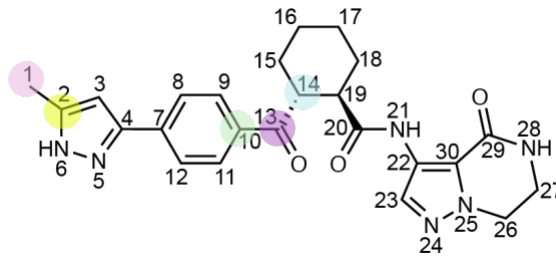
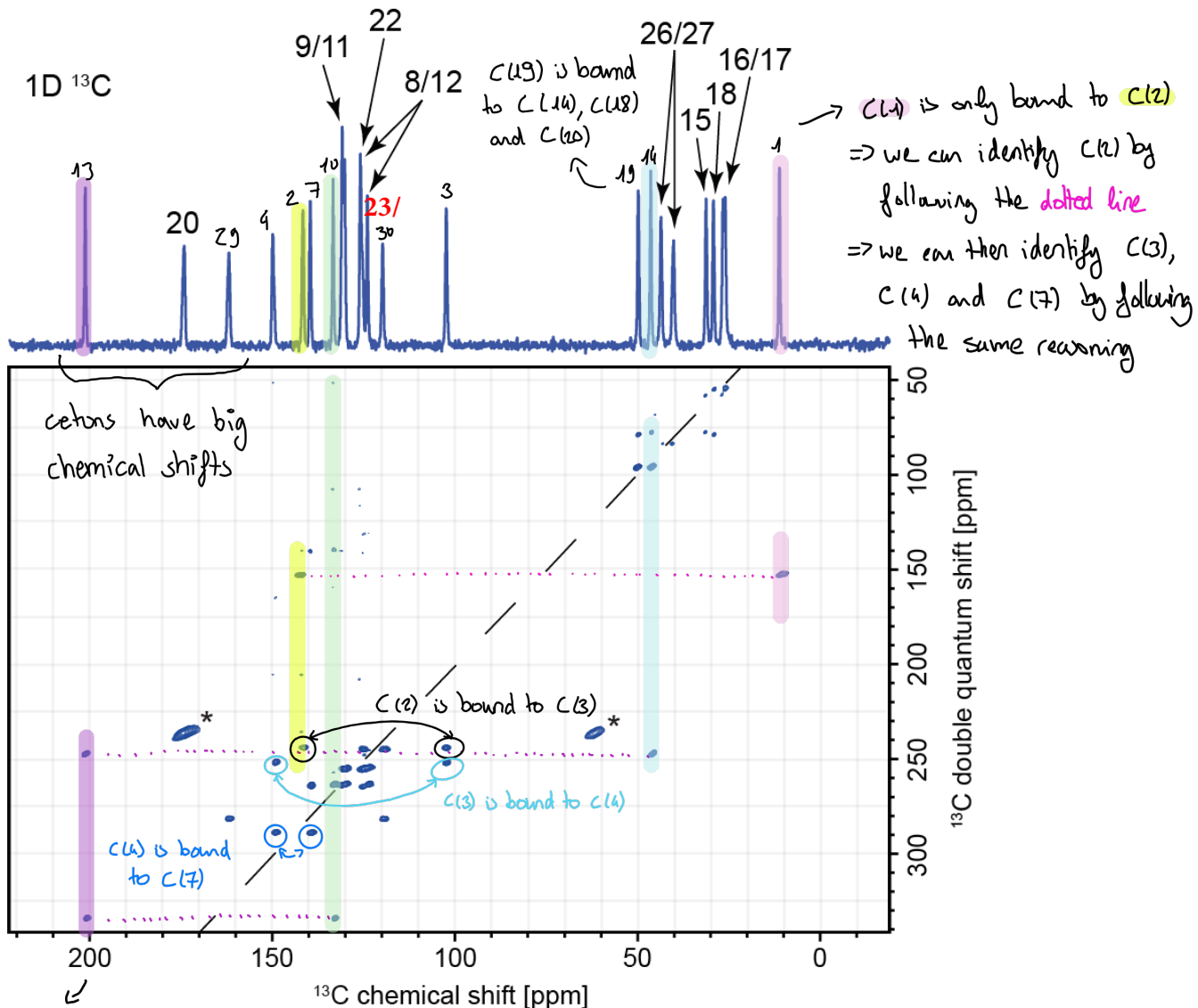


Jigsaw 4C

1. [From Past Exam] Below is a ^{13}C - ^{13}C INADEQUATE spectrum of the molecule shown. The INADEQUATE experiment correlates the shifts of bonded ^{13}C , such that the chemical shift on the y-axis corresponds to the sum of the two chemical shifts of the two correlated carbons. Peaks indicated with a (*) are artifacts and should not be considered in the analysis. Assign the unlabeled ^{13}C peaks using the INADEQUATE experiment.



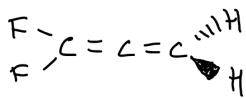
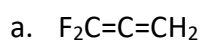
(C13) could not be assigned to a peak
 → this is probably due to some overlapping between the peaks



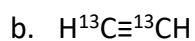
C(14) & C(10) are bound to C(13)

$\text{C}(14) = \text{sp}^3$ hybridized
 => smaller shift than C(10)

2. [Keeler Section 12.2 and Hore Section 3.3] For each of the following compounds determine whether the protons are magnetically or chemically equivalent. Explain why.



The two protons have the same chemical shift and each has identical couplings to each of the fluorines
 \rightarrow they are magnetically equivalent



The ^{13}C nuclei couple with the hydrogens in a way that causes different coupling constants for each hydrogen

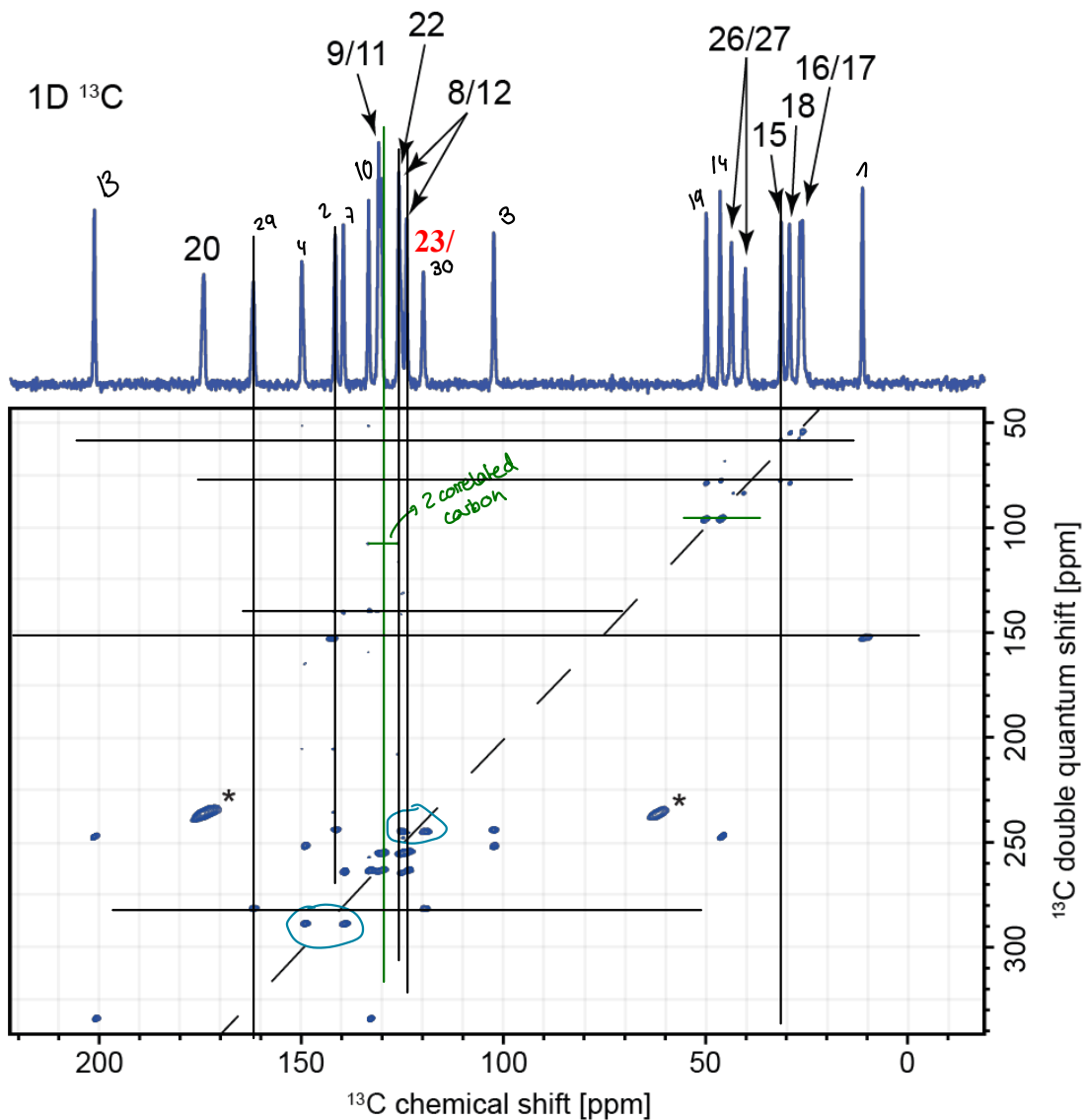
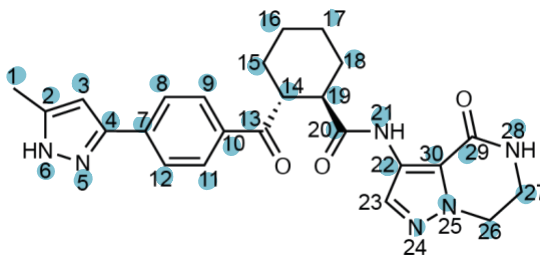
\rightarrow they are only chemically equivalent

Jigsaw 4C

1. [From Past Exam] Below is a ^{13}C - ^{13}C INADEQUATE spectrum of the molecule shown. The INADEQUATE experiment correlates the shifts of bonded ^{13}C , such that the chemical shift on the y-axis corresponds to the sum of the two chemical shifts of the two correlated carbons. Peaks indicated with a (*) are artifacts and should not be considered in the analysis. Assign the unlabeled ^{13}C peaks using the INADEQUATE experiment.

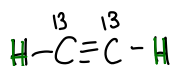
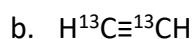
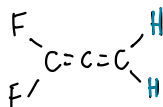
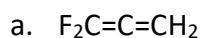
2/2

correlated means bonded
 2 signals on the same horizontal row means both carbons are correlated.



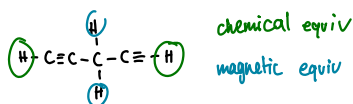
• We haven't put 23, which should be correlated to 22.

2. [Keeler Section 12.2 and Hore Section 3.3] For each of the following compounds determine whether the protons are magnetically or chemically equivalent. Explain why.



magnetic equivalent means identical configuration
chemical equivalent means identical linkage

Example :



$F_2C=CH_2$ are linked to the same C and are not magnetically equivalent...

Answer : Hydrogens from a) are magnetic equivalent (linked on the same C)

Hydrogen from b) are chemically equivalent (have the same configuration)

Two nuclei are:

CHEMICALLY EQUIVALENT:

if

1) The spins are of the same isotropic species.

AND

2) There exists a molecular symmetry operation which exchanges the two spins.

MAGNETICALLY EQUIVALENT (implies chemically equivalent, but not the opposite)

if

1) The spins have the same chemical shift

AND

2a) The spins have identical coupling to all other spins in the molecule. (eg. molecule a from the exercise)

OR

2b) There are no other spins in the molecule (e.g. benzene)