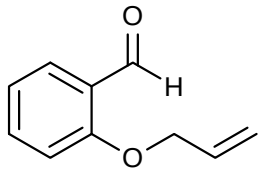
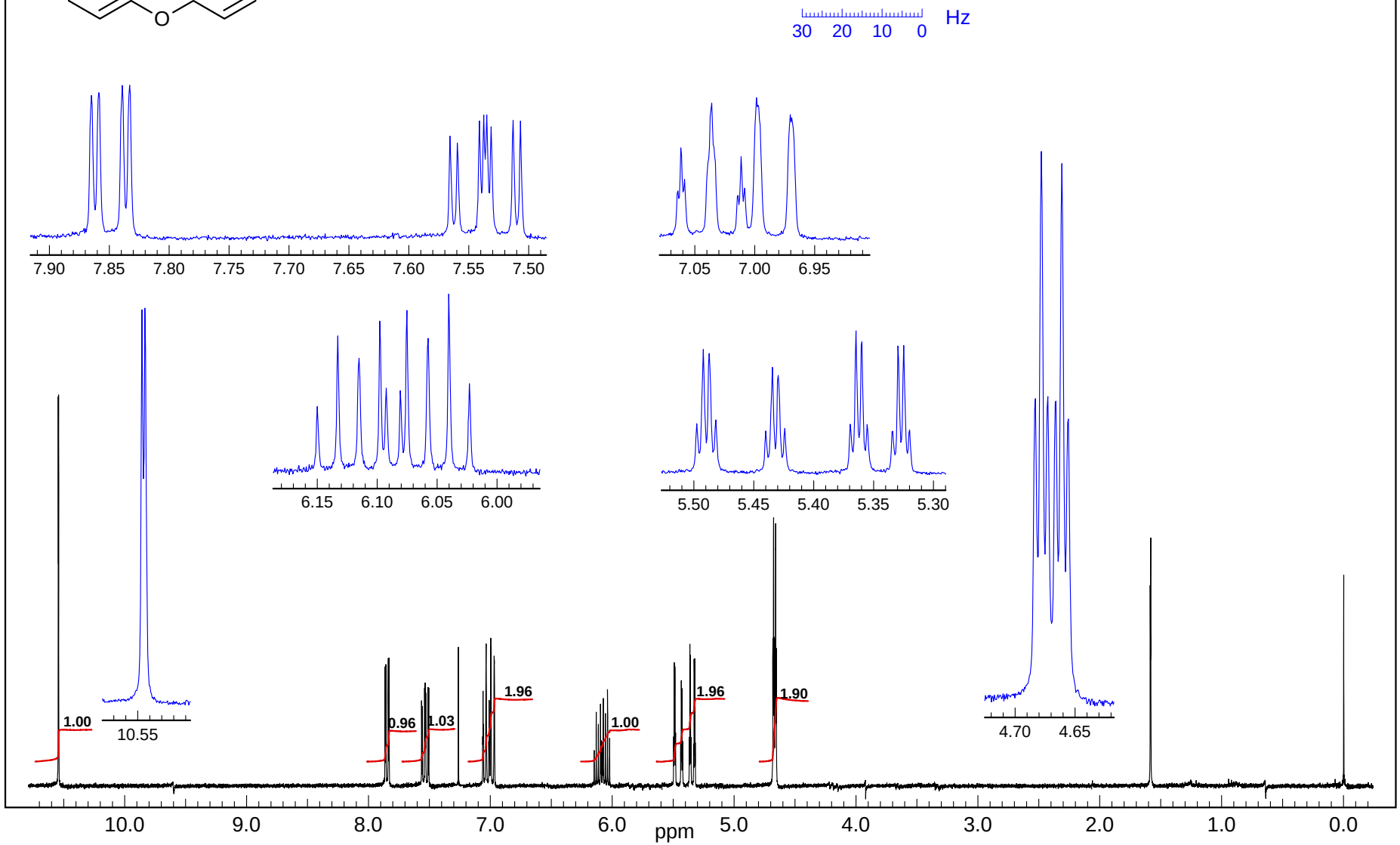
Problem R-13J ($C_{10}H_{10}O_2$)

300 MHz ^{1}H NMR spectrum in $CDCl_3$

Source: Rui Tang/Reich g





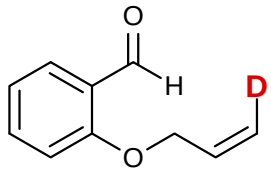
PLT ex-3-2013-14-gq.plt

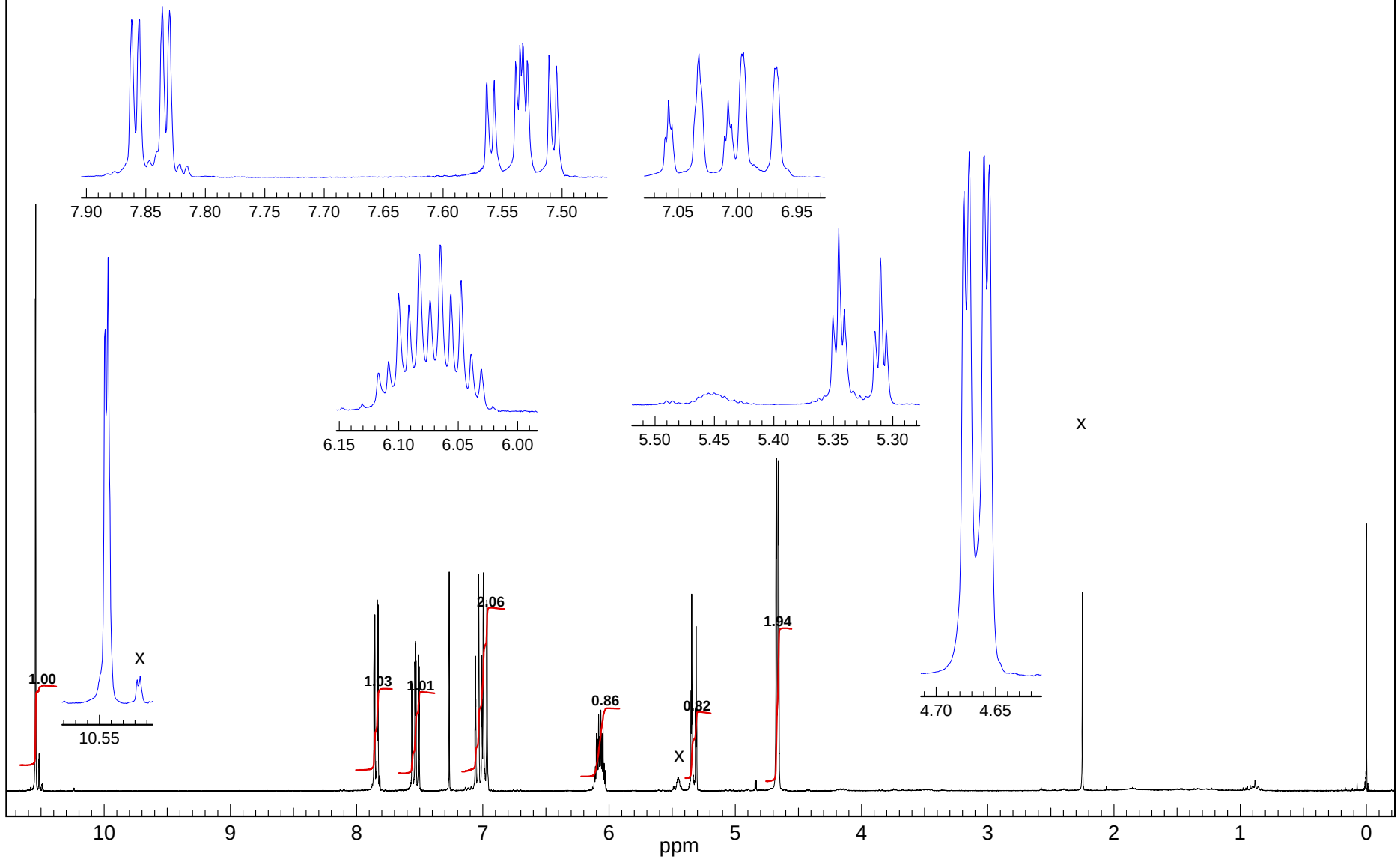
Problem R-13J ($C_{10}H_9DO_2$)

300 MHz ^{1}H NMR spectrum in $CDCl_3$

Source: Rui Tang/Reich

x = solvent/impurity peaks

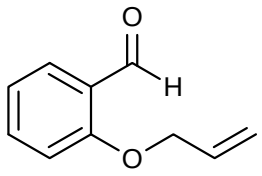




PLT ex-3-2013-14-gq.plt

Problem R-13J. In this problem you are required to interpret the NMR spectrum of a mono-deuterated compound, and identify the position of the deuterium.

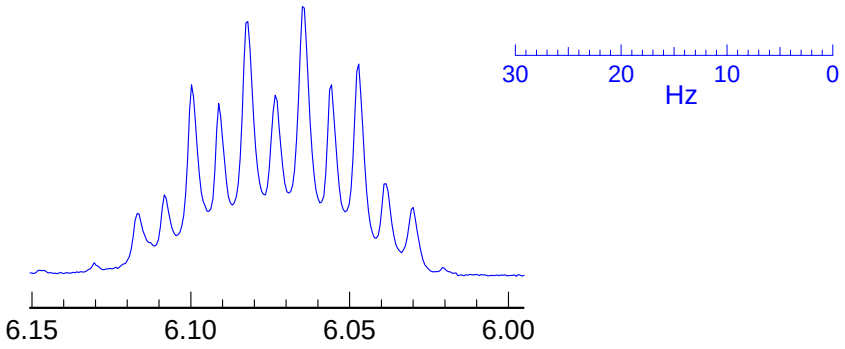
NOTE: the spectrum of the undeuterated compound was not provided for this question



(a) Assign the protons between δ 6.9 and 8.0 and write the δ values on the structure above. Don't report all of the couplings, but do specifically explain the multiplicity of the signal at δ 7.03.

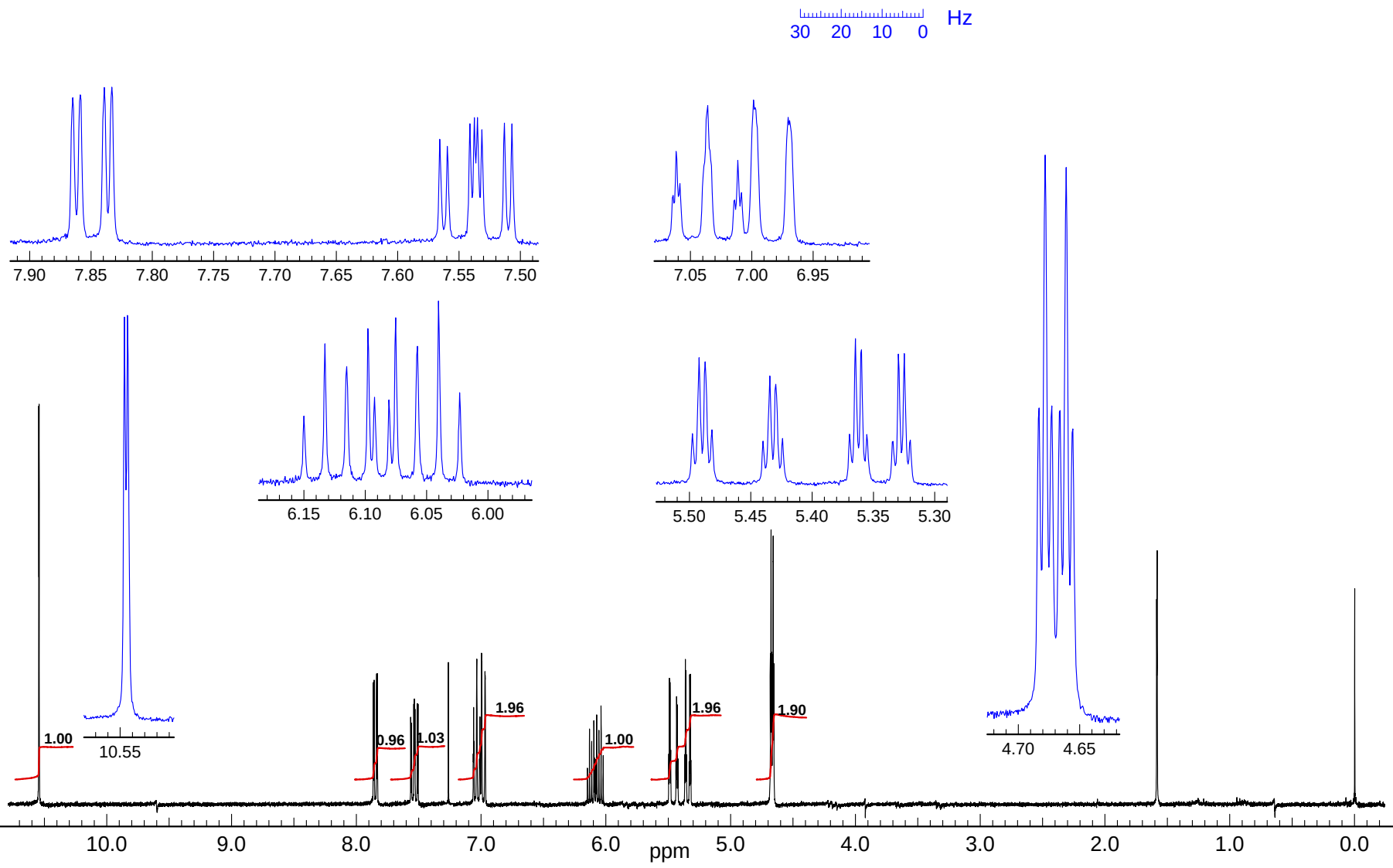
(b) Analyze and assign the protons between δ 4.5 and 5.5 (put the chemical shifts on the structure). Report all couplings.

(c) Analyze the multiplet at δ 6.1, draw a coupling tree, report all couplings



(d) Where is the deuterium? Show it on the structure, and explain briefly.

Problem R-13J ($C_{10}H_{10}O_2$)
300 MHz ^{1}H NMR spectrum in $CDCl_3$
Source: Rui Tang/Reich g



PLT ex-3-2013-14-gq.plt

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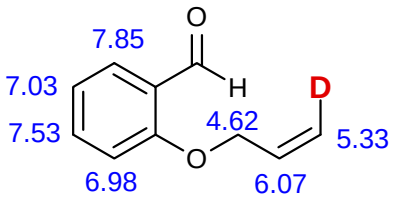
Problem R-13J. In this problem you are required to interpret the NMR spectrum of a mono-deuterated compound, and identify the position of the deuterium.



(a) Assign the protons between δ 6.9 and 8.0 and write the δ values on the structure above. Don't report all of the couplings, but do specifically explain the multiplicity of the signal at δ 7.03.

δ 7.03, tt, J = 8, 1 Hz
The large triplet splitting is from two ortho protons
The small triplet splitting is from a meta proton and a long-range coupling to the aldehyde proton

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The protons o and p to the OR are upfield, those o and p to C=O are downfield

(b) Analyze and assign the protons between δ 4.5 and 5.5 (put the chemical shifts on the structure). Report all couplings.

δ 4.62, dd, J = 5, 1.5 Hz, OCH_2, coupling to middle vinyl proton and one of the terminal vinyl protons, the other terminal vinyl position is deuterated, and C-D coupling is too small to observe

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δ 5.33, dt, J = 10.5, 1.5 Hz
The 10 Hz coupling is Cis, the triplet is coupling to the two allylic protons. The coupling to D is too small to observe.

(c) Analyze the multiplet at δ 6.1, draw a coupling tree, report all couplings

δ 6.07, dt(1:1:1)t, J = 10, 5, 2.5
the 1:1:1 triplet splitting is $^3J_{H\text{-}D}$-trans, the 10 Hz coupling is $^3J_{H\text{-}H}$ - cis
Equivalent H-H coupling: 6.51 x 2.5 = 16.3, appropriate for trans coupling (i.e. D is trans to H)

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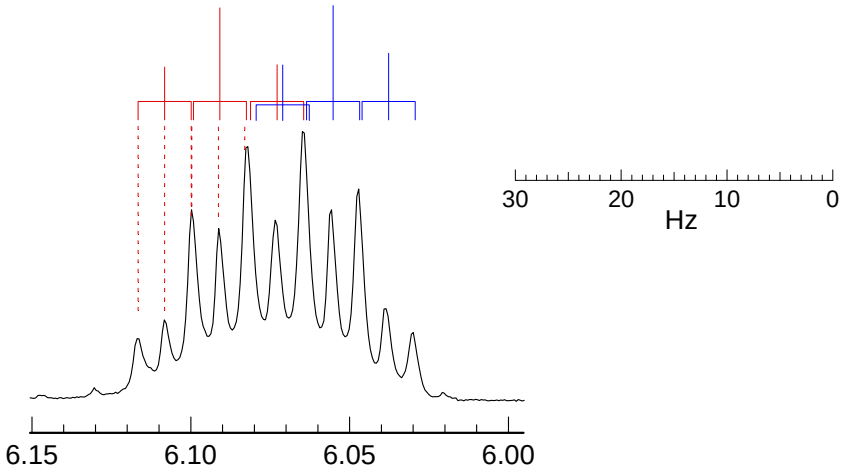

(d) Where is the deuterium? Show it on the structure, and explain briefly.

5

2007 - Biggest problem was with parsing the multiplet

Problem R-13J ($C_{10}H_9DO_2$)

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Source: Rui Tang/Reich

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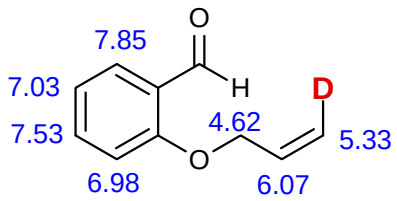

PLT ex-3-2013-14-gq.plt