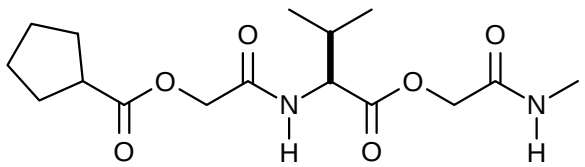
Problem R-07B ($C_{16}H_{26}N_2O_6$)
300 MHz ^{1}H NMR Spectrum in $CDCl_3$
Source: Jihong Wang/Gellman g



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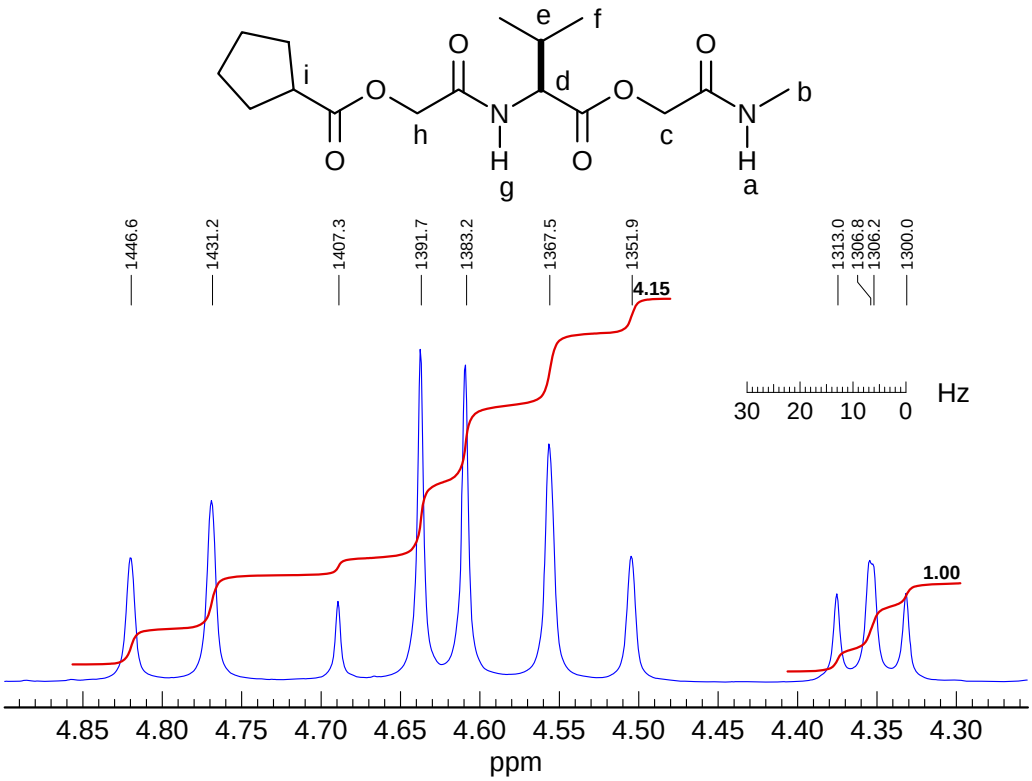
Problem R-07B. The spectrum of the depsipeptide below contains the series of peaks shown (the full spectrum is presented on the next page).



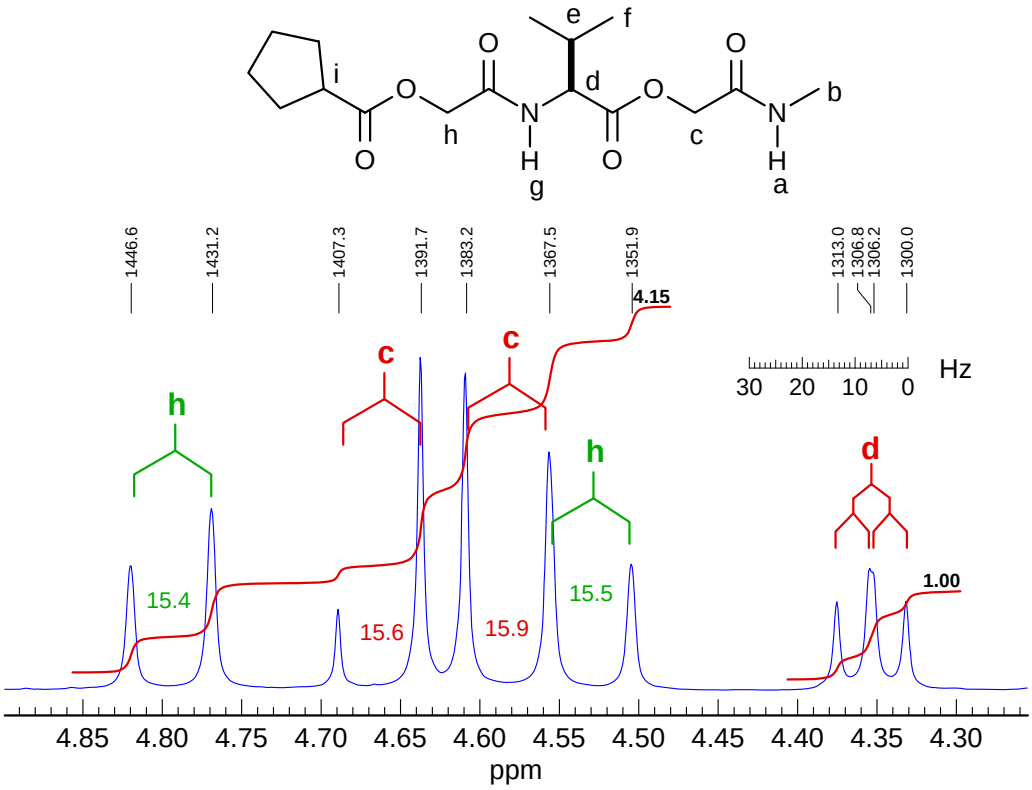
(a) Identify the patterns and assign the peaks in this part of the spectrum to the structure. Use the letters a-i to identify the protons, and mark the spectrum appropriately.

(b) Using the frequencies given, do an exact calculation of the chemical shifts and couplings of each of the 5 protons in this part of the spectrum. Point out any ambiguities in the peak assignments.

(c) Explain and assign the pattern at δ 2.8-3.0 .

(d) Explain and assign the signals at δ 6.5-7.0 .

Problem R-07B ($C_{16}H_{26}N_2O_6$). The spectrum of the depsipeptide below contains the series of peaks shown (the full spectrum is presented on the next page).



(a) Identify the patterns and assign the peaks in this part of the spectrum to the structure. Use the letters a-i to identify the protons, and mark the spectrum appropriately.

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The peaks marked c and those marked h each form an AB quartet. Their assignments can be reversed.

The signals marked d are a dd from coupling to e and g

(b) Using the frequencies given, do an exact calculation of the chemical shifts and couplings of each of the 5 protons in this part of the spectrum. Point out any ambiguities in the peak assignments.

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h AB quartet: J_{AB} = 15.4, δ 4.53, 4.79

c AB quartet: J_{AB} = 15.7, δ 4.66, 4.59

d: δ 4.35, dd, J = 6.8, 6.2 (coupling to g and e)

Assignments of h and c could be reversed

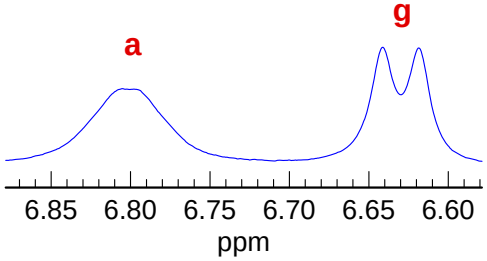
(c) Explain and assign the pattern at δ 2.8-3.0 .

3

This is the superposition of a methyl doublet (b) on top of peaks for i (tt?)

(d) Explain and assign the signals at δ 6.5-7.0 .

3



These are the two NH protons a and g (a is an unresolved quartet from coupling to b, g is a doublet from coupling to d, J_{gd} = 7 Hz). The extra broadening is probably mostly unresolved H-^{14}N coupling, but there could also be a contribution from dynamic exchange between the N-H protons, and exchange with other labile Hs (e.g. water)

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