Problem R-06K. \((C_8H_{14}O_6)\)

300 MHz \(^1\)H NMR Spectrum in D\(_2\)O

Source: M. Schuster/Kiessling (Reich digitized hard copy 11/27) g
Problem R-06K. Determine the stereochemistry at the three indicated carbons from the 300 MHz $^1$H NMR spectrum presented on the next page.

(a) Analyze the individual signals and show coupling constants in the standard format. Assign them to the extent possible. Use the numbering system given on the structure in part (b).

$$\delta 1.7 - 2.1$$

$$\delta 3.4$$

$$\delta 3.9$$

$$\delta 4.0$$

(b) Determine the stereochemistry of R-06K. Place the appropriate substituents (H and OH) in each of the boxes on the structure below.

At each carbon 3, 4, and 5 there is a H and an OH group.
Problem R-06K. (C₈H₁₄O₆)
300 MHz H NMR Spectrum in D₂O
Source: M. Schuster/Kiessling (Reich digitized hard copy 11/27)
Problem R-06K. Determine the stereochemistry at the three indicated carbons from the 300 MHz $^1$H NMR spectrum presented on the next page.

(a) Analyze the individual signals and show coupling constants in the standard format. Assign them to the extent possible. Use the numbering system given on the structure in part (b).

- **δ 1.7 - 2.1**
  - $H_{2-ax}$: 1.78 dd, $J = 14$, 10.5 Hz
  - $H_{2-eq}$: 2.00 ddd, $J = 14$, 4, 2.5 Hz

  The 10.5 Hz coupling must be ax-ax, so $H_3$ must be axial

  The 2.5 Hz coupling is a "W" coupling - $H_{2-eq}$ - $H_{6-eq}$

- **δ 3.4**
  - $H_4$: 3.42, dd, $J = 9$, 3.2 Hz

  $H_4$ - only one of the downfield protons with just two couplings. It must be axial, with $H_3$ axial and $H_5$ equatorial

- **δ 3.9**
  - $H_3$: 3.90, ddd, $J = 10$, 9, 4.5 Hz

  $H_3$ - coupled twice with large couplings to axial protons at $H_2$ and $H_4$, and once to equatorial proton at $H_2$

- **δ 4.0**
  - $H_5$: 4.02, apparent quartet, $J = 3.5$ Hz (actually a ddd)

  $H_5$ - equatorial proton, coupled eq-ax to protons $H_4$ and $H_6$, and eq-eq to $H_6$

(b) Determine the stereochemistry of R-06K. Place the appropriate substituents (H and OH) in each of the boxes on the structure below.

![Structure diagram]

At each carbon 3, 4, and 5 there is a H and an OH group.
Problem R-06K. (C₈H₁₄O₆)
300 MHz ¹H NMR Spectrum in D₂O
Source: M. Schuster/Kiessling (Reich digitized hard copy 11/27)

H₅ (eq) δ 4.02, apparent quartet, J = 3.5 Hz (actually a ddd)

H₃ δ 3.90, ddd, J = 10, 9, 4.5 Hz

H₄ (ax) δ 3.42, dd, J = 9, 3.2 Hz

H₂ (eq)

2.00 ddd, J = 14, 4, 2.5 Hz

1.78 dd, J = 14, 10.5 Hz