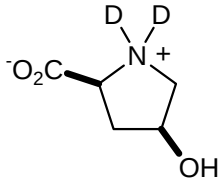
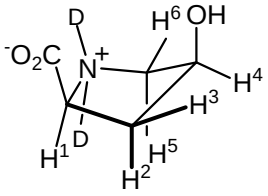
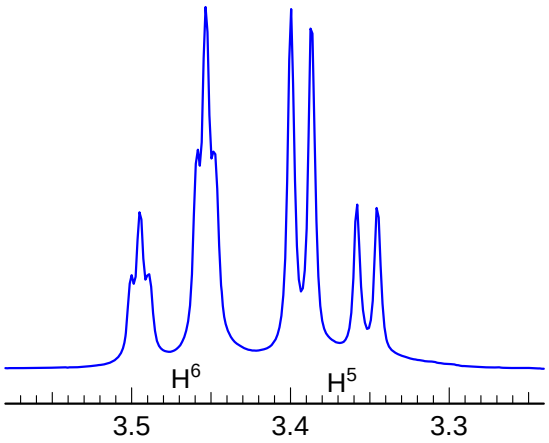
$C_8H_9NO_3$

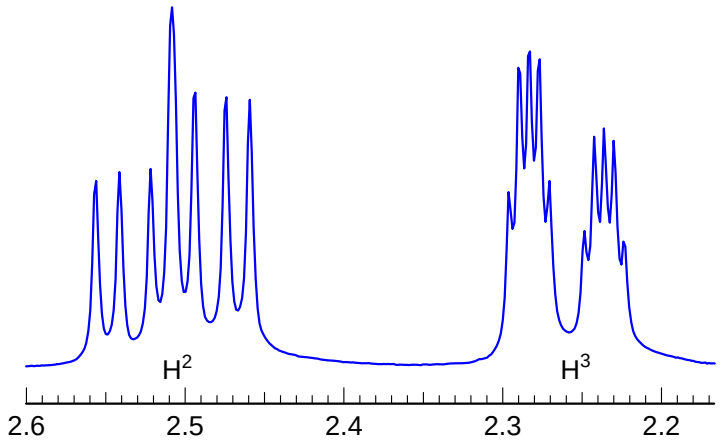
300 MHz ^{1}H NMR spectrum in D_2O

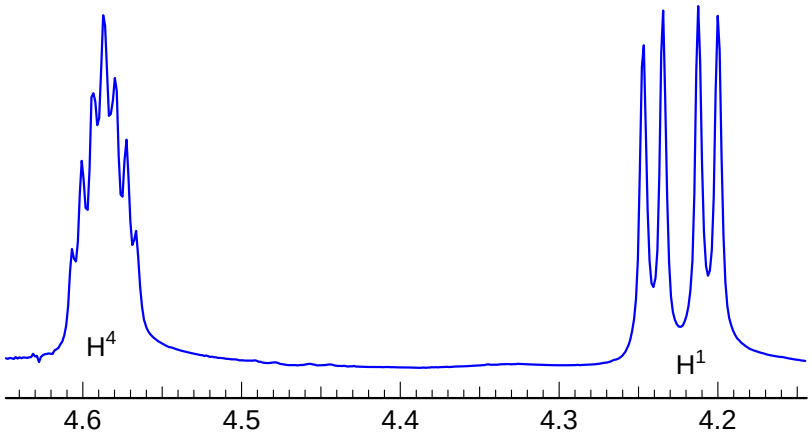
Aldrich Spectra Collection





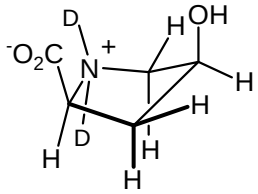


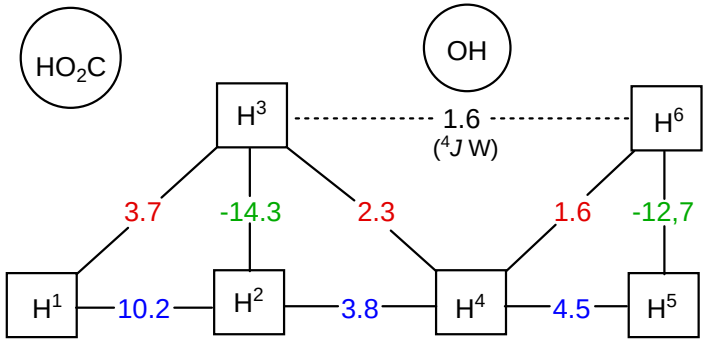


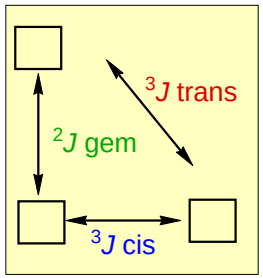


PLT NMR-proline-4-hydroxy-cis.plt

cis-4-Hydroxyproline shows somewhat surprising coupling around the ring. The NMR evidence indicates that both substituents (the OH and the CO_2H) are in pseudo-axial positions. As a result, there are an unusual number of small couplings among the ring protons, and the *cis* ^3J (3.8 to 10.3 Hz) are all larger than the *trans* ^3J (1.6 to 3.7 Hz), since there are no ax-ax relations amound vicinal protons. A ^4J W-type coupling between H^3 and H^6 is as large as one of the *trans* ^3J couplings (that between H^6 and H^4).

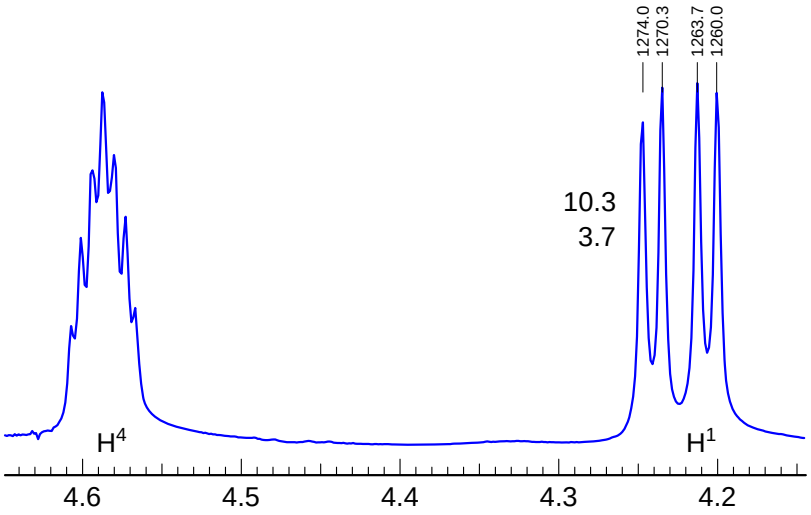


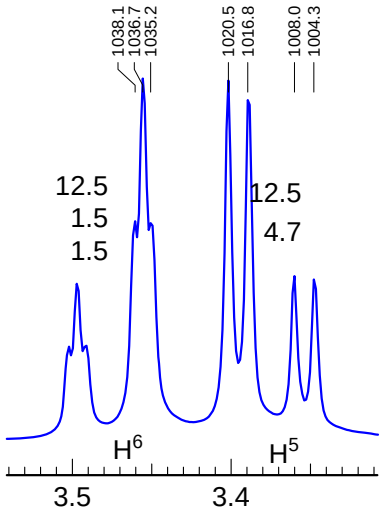


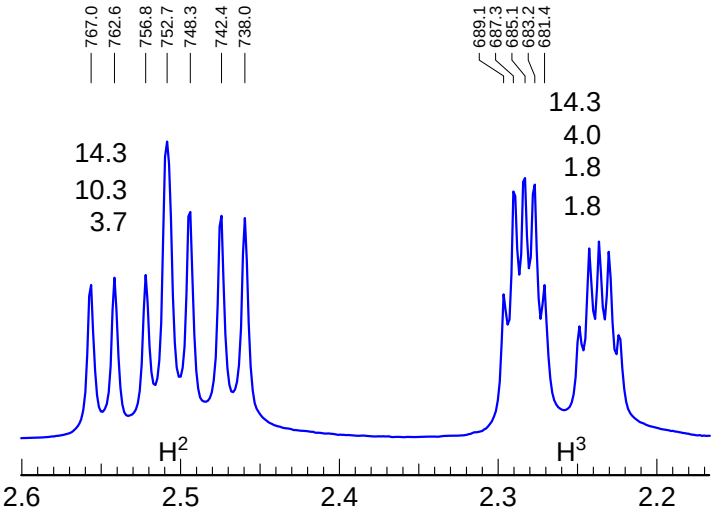


V1 = 646.78 V2 = 132.10 V3 = 58.95 V4 = 755.97 V5 = 393.18 V6 = 420.80
J12 = 10.20 J13 = 3.70 J14 = 0.00 J15 = 0.00 J16 = 0.00 J23 = -14.30 J24 = 3.80 J25 = 0.00 J26 = 0.00 J34 = 2.30 J35 = 0.00
J36 = 1.60 J45 = 4.50 J46 = 1.60 J56 = -12.70

The *J*-values over the spectrum expansions are those obtained by first order analysis of the spectra, the slightly different numbers above are from a WINDNMR simulation of the spectrum.







PLT NMR-proline-4-hydroxy-cis.plt