Supporting Information for

X-ray Structural Characterization of Imidazolylcobalamin and Histidinylcobalamin: Cobalamin Models for Aquacobalamin bound to the B_{12} Transporter Protein Transcobalamin

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Figure S1. ^{1}H NMR spectrum of $ImCbl^{+}$ in TAPS buffer (0.10 M, pD 8.80). Chemical shifts (δ, ppm): 7.27, 7.08, 6.93, 6.80, 6.72, 6.35(d), 6.20 and 5.95. Minor peaks (~5%) are attributable to HOCbl (7.19, 6.67, 6.50, 6.27(d) and 6.16 ppm) and an unknown impurity/impurities present in the starting material at 7.12, 7.11, 6.84, 6.74, 6.44 and 6.08 ppm.

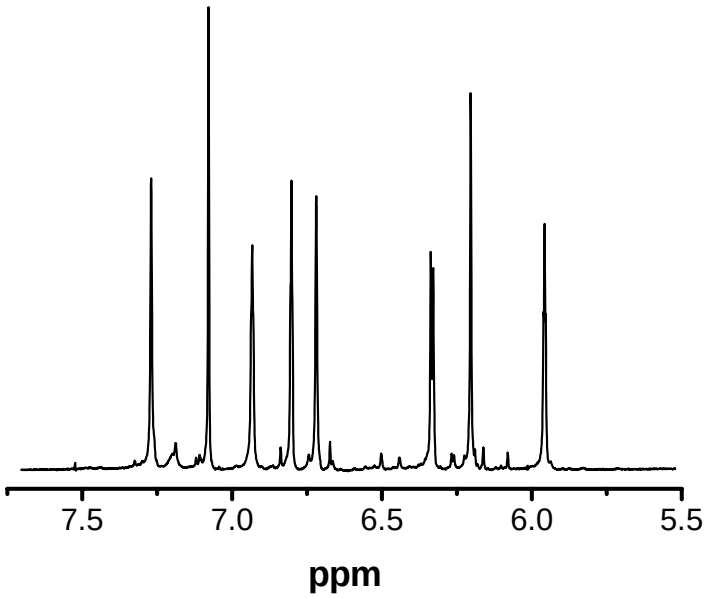

Figure S2. ^{1}H NMR spectrum of HisCbl^{+} in TES buffer (0.10 M, pD 7.80). Chemical shifts (δ, ppm): 7.28, 7.10, 6.81, 6.72, 6.32(d), 6.20, and 5.75. Chemical shifts of free histidine (labeled L) at 7.95 and 7.17 ppm. Other minor peaks are attributable to HOCbl/H_2OCbl^{+} and an unknown impurity/impurities from the starting material.

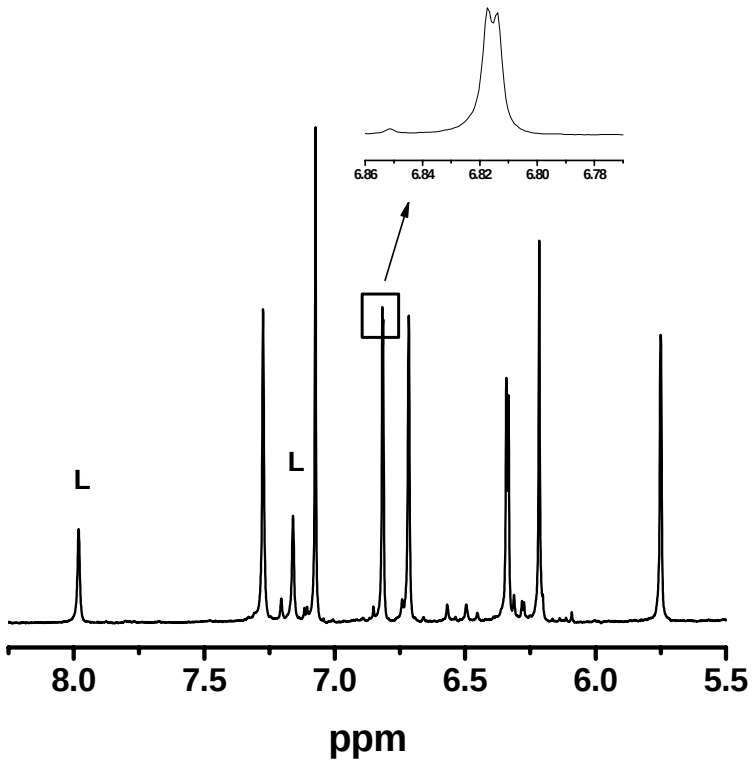

Figure S3. UV-visible spectra of HOCbl•HCl, [ImCbl]Cl and [HisCbl]Cl in H_2O at 25 °C. Absorption maxima occur at 357, 413, and 536 nm for $ImCbl^+$ and 358, 414, and 538 nm for $HisCbl^+$.