## **Supporting Information for:**

## Cytochrome c<sub>552</sub> Mutants: Structure and Dynamics at the Active Site Probed by Multidimensional NMR and Vibration Echo Spectroscopy

Aaron M. Massari<sup>†</sup>, Brian L. McClain<sup>#</sup>, Ilya J. Finkelstein<sup>†</sup>, Andrew P. Lee<sup>‡</sup>, Heather L. Reynolds<sup>‡</sup>, Kara L. Bren<sup>‡</sup>, and Michael D. Fayer<sup>†</sup>

<sup>†</sup>Department of Chemistry, Stanford University, Stanford, CA 94305 <sup>‡</sup>Department of Chemistry, University of Rochester, Rochester, NY 14627-0216



**Figure S1.** a) Experimental vibrational echo decay data at  $T_w = a$ ) 0.5 ps, b) 2 ps, c) 4 ps, d) 8 ps, e) 16 ps, and f) linear spectrum for *Ht*-M61A (dashed lines) overlaid with the best-fit vibrational echo decay and linear spectrum calculated from nonlinear response theory (solid lines) at 1975 cm<sup>-1</sup>.



**Figure S2.** a) Experimental vibrational echo decay data at  $T_w = a$ ) 0.5 ps, b) 2 ps, c) 4 ps, d) 8 ps, e) 16 ps, and f) linear spectrum for *Ht*-M61A/Q64N (dashed lines) overlaid with the best-fit vibrational echo decay and linear spectrum calculated from nonlinear response theory (solid lines) at 1965 cm<sup>-1</sup>.