Supporting information for:

Resonance Raman spectra of an O_2-binding H-NOX domain reveal heme relaxation upon mutation

Rosalie Tran[‡], Elizabeth M. Boon[‡⊥], Michael A. Marletta[‡§]*, and Richard A. Mathies[‡]*

Departments of Chemistry and Molecular and Cell Biology,

University of California, Berkeley, CA 94720

* To whom correspondence should be addressed.

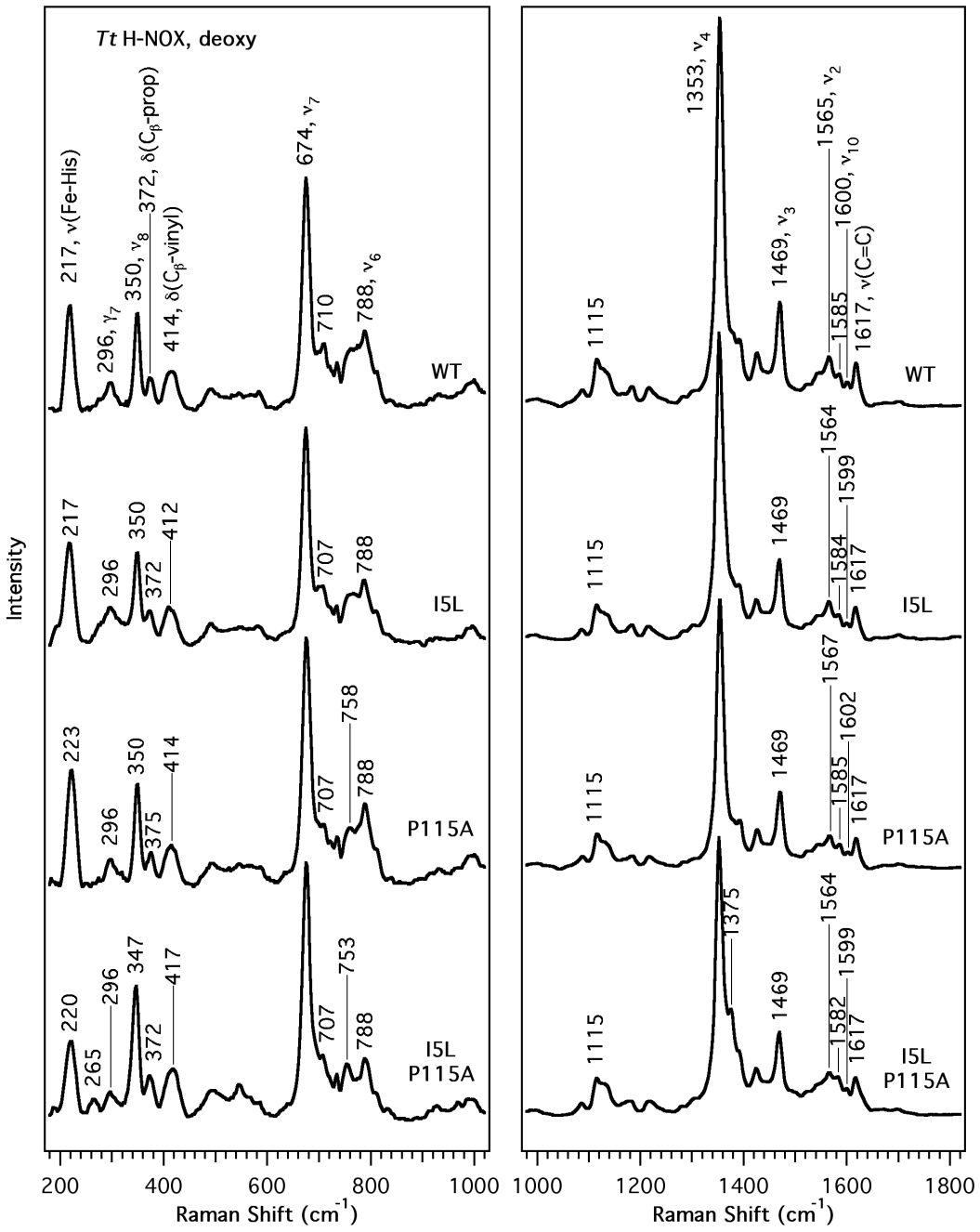

Figure 1S: Resonance Raman spectra of the Fe^{II}-unligated form of *Tt* H-NOX WT, I5L, P115A, and I5L/P115A. Spectral intensities in the low and high frequency regions were normalized to ν_7 and ν_4, respectively.

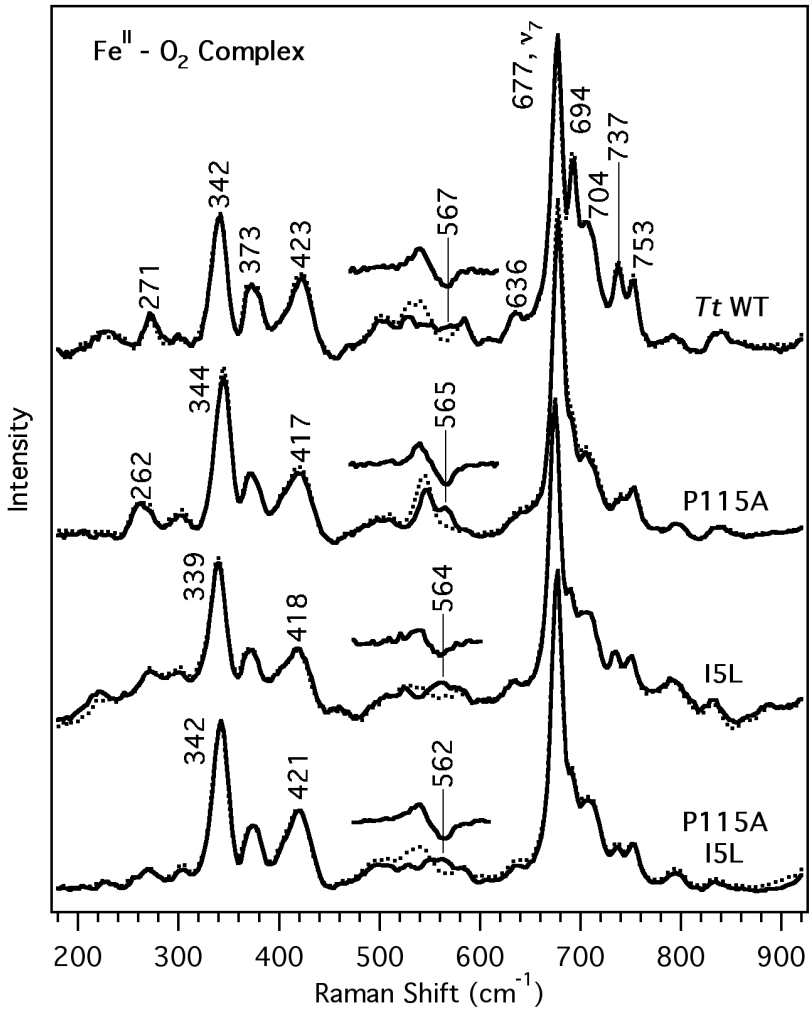

Figure 2S: Resonance Raman spectra of the O_2 complexes of *Tt* H-NOX WT, I5L, P115A, and I5L/P115A in the low frequency region. $^{18}O_2$ spectra (dotted line) are overlapped over the $^{16}O_2$ spectra to indicate the frequency shifts upon isotopic substitution, and the difference ($^{18}O_2$-$^{16}O_2$) spectra are shown above each protein for clarity in the ν(Fe-O_2) assignment. Spectral intensities were normalized to ν_7.

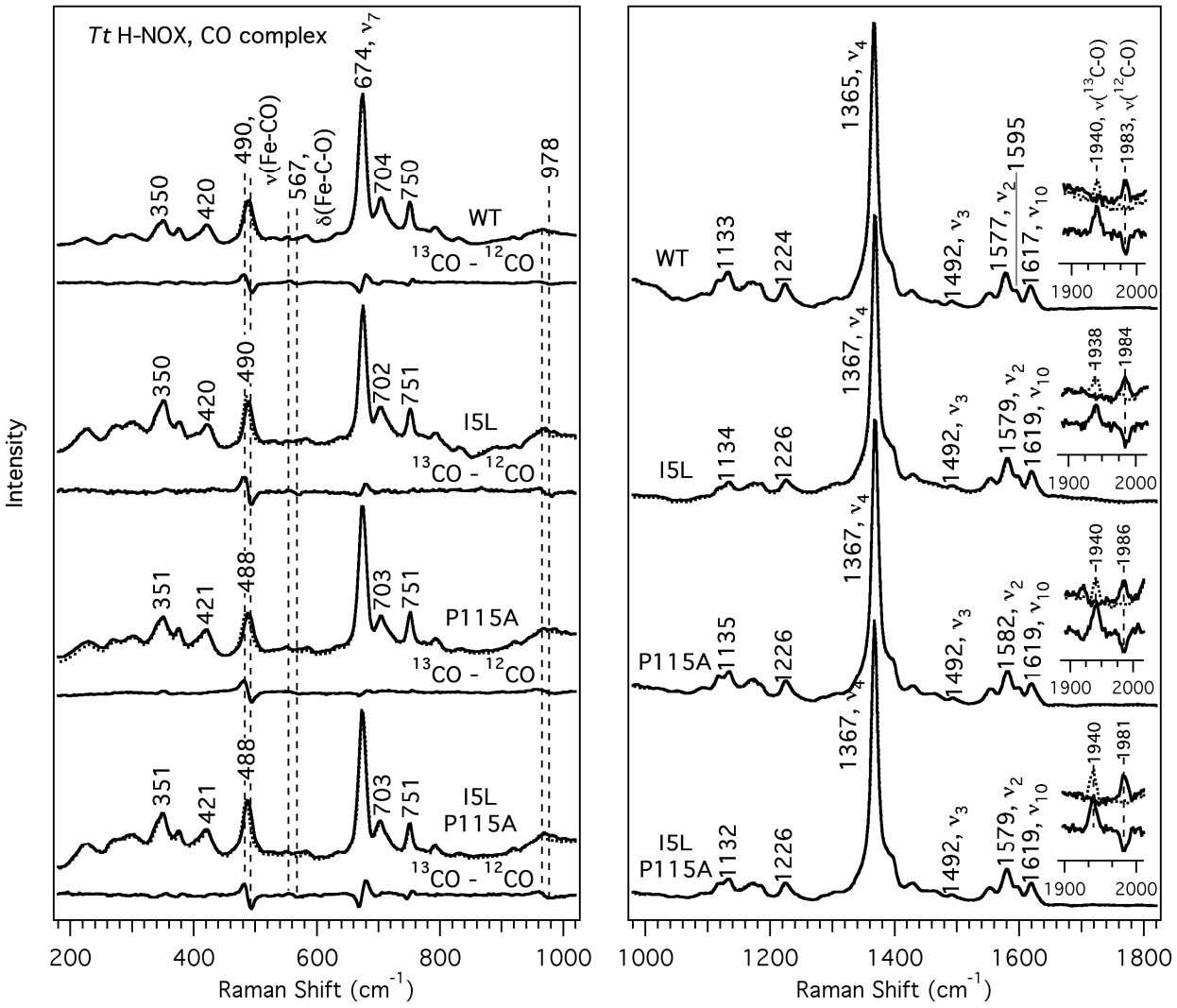

Figure 3S: Resonance Raman spectra of the CO complexes of *Tt* H-NOX WT, I5L, P115A, and I5L/P115A. ^{13}CO spectra (dotted line) are overlapped over the ^{12}CO spectra to indicate the frequency shifts upon isotopic substitution, and the difference (^{13}CO-^{12}CO) spectra are shown below each protein for clarity. Spectral intensities were normalized to ν_7 and ν_4 for the low and high frequency regions, respectively.

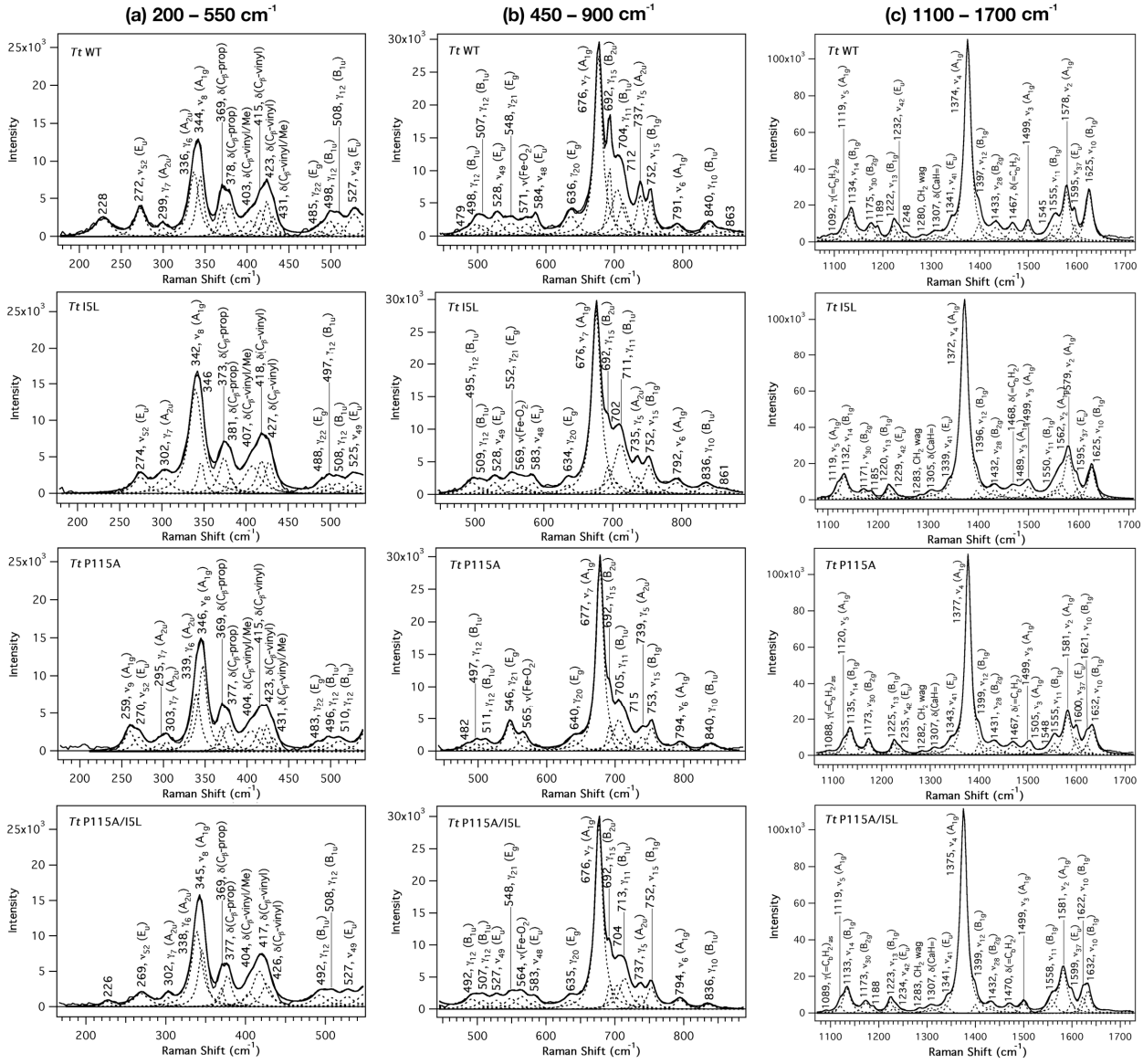

Figure 4S: Spectral decomposition of resonance Raman spectra for *Tt* H-NOX WT, I5L, P115A, and I5L/P115A in different frequency regions: (a) 200 – 550 cm^{-1}, (b) 450 – 900 cm^{-1}, (c) 1100 – 1700 cm^{-1}.