Supporting Information:

Specific Zinc Binding to Heliorhodopsin

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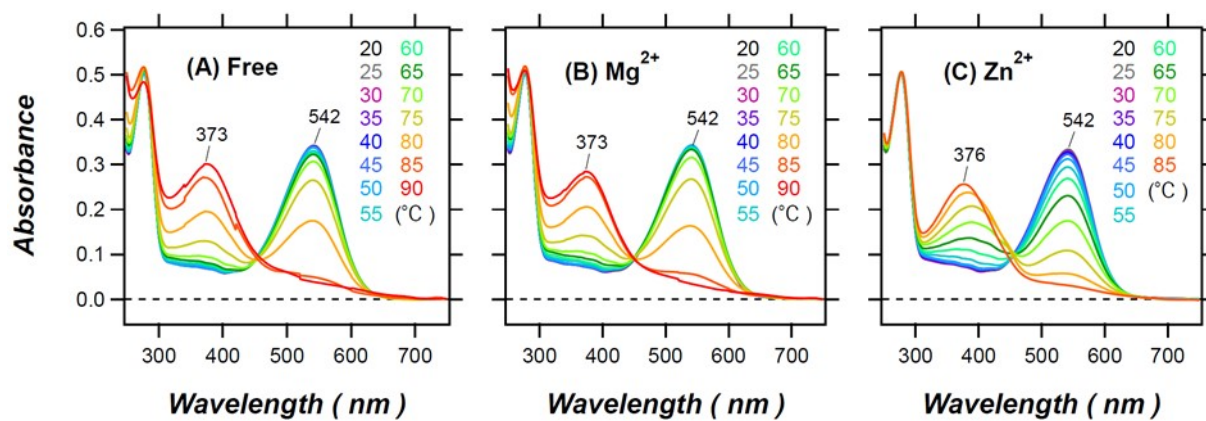
Figure S1.   UV-visible absorption spectra of TaHeR at various temperatures (20 to 90 ºC) in the absence of divalent cations (A), presence of 0.5 mM Mg²⁺ (B), and 0.5 mM Zn²⁺ (C).
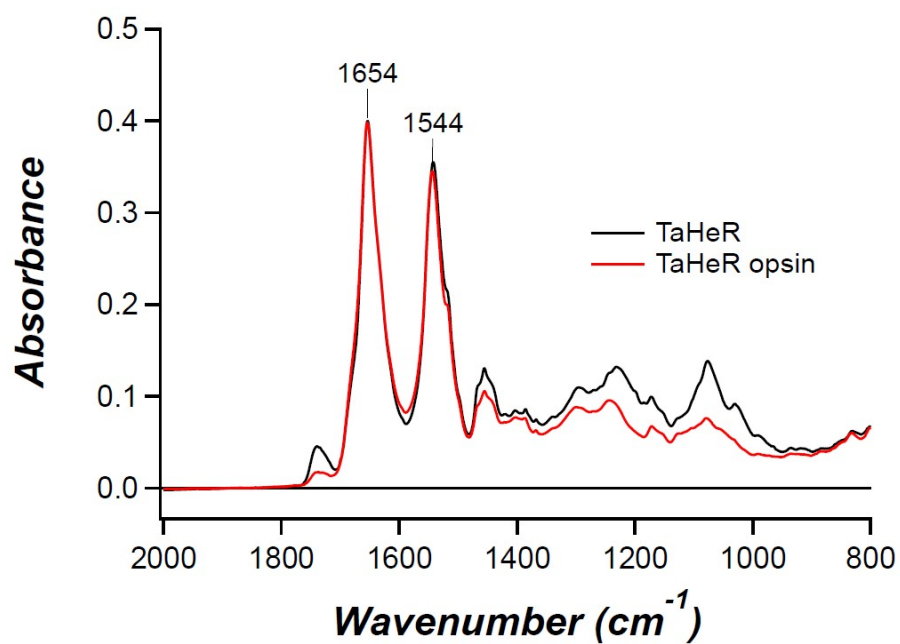
Figure S2. Comparison of apparent absolute absorption spectra of proteins between TaHeR (black line) and TaHeR opsin (red line) in the 2000-800 cm^{-1} region. Each sample is naturally dried on the surface of a silicon ATR crystal after removal of detergent.
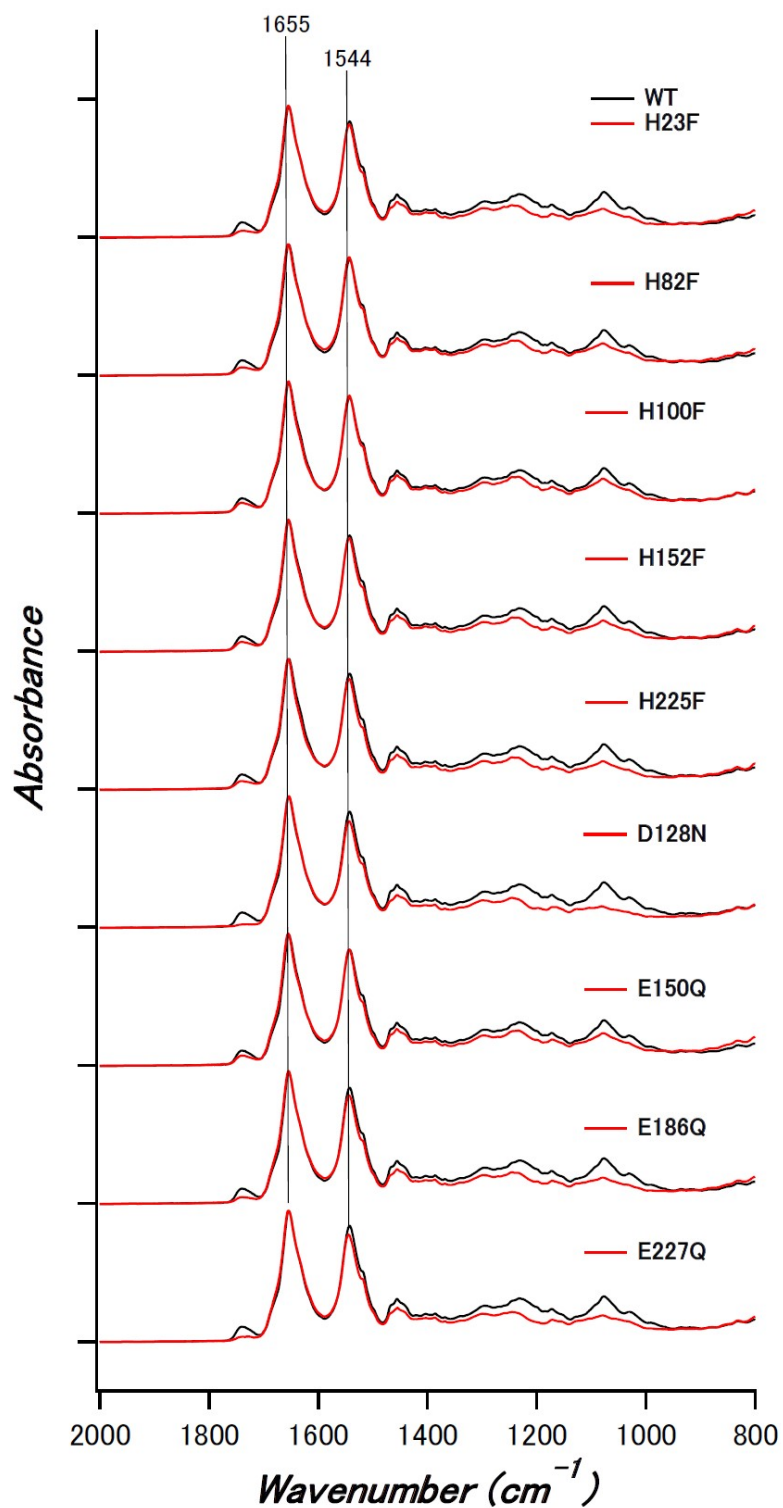
Figure S3. Comparison of apparent absolute absorption spectra of proteins between TaHeR (black line) and TaHeR mutants (red line) in the 2000-800 cm^{-1} region. One division of the y-axis corresponds to 0.3 absorbance units. Each sample is naturally dried on the surface of a silicon ATR crystal after removal of detergent.
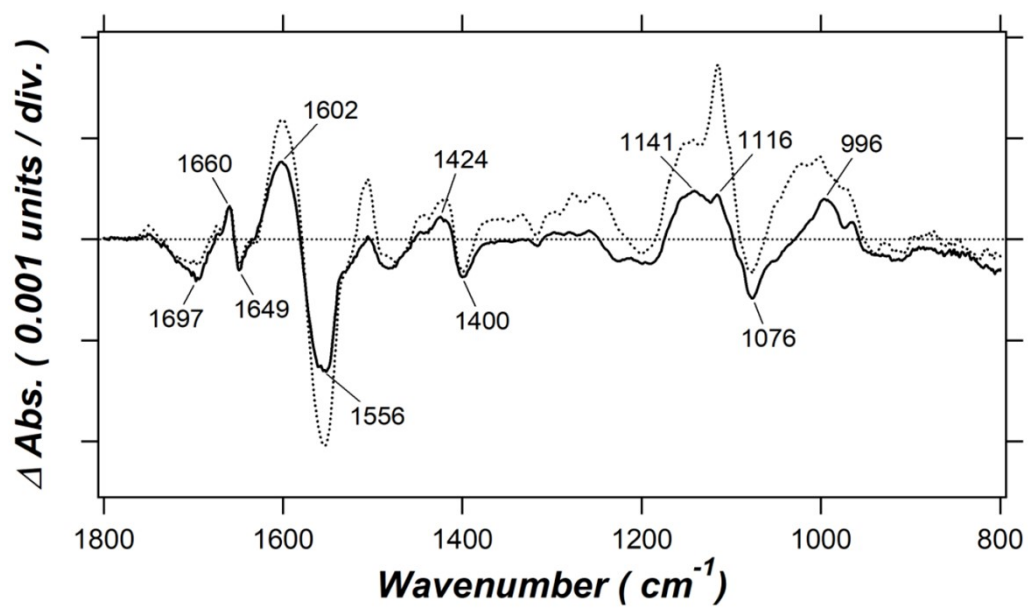
Figure S4. Difference ATR-FTIR spectra of TaHeR with (black dotted line) and without His-tag (black solid line). These spectra are reproduced from ref. (1).
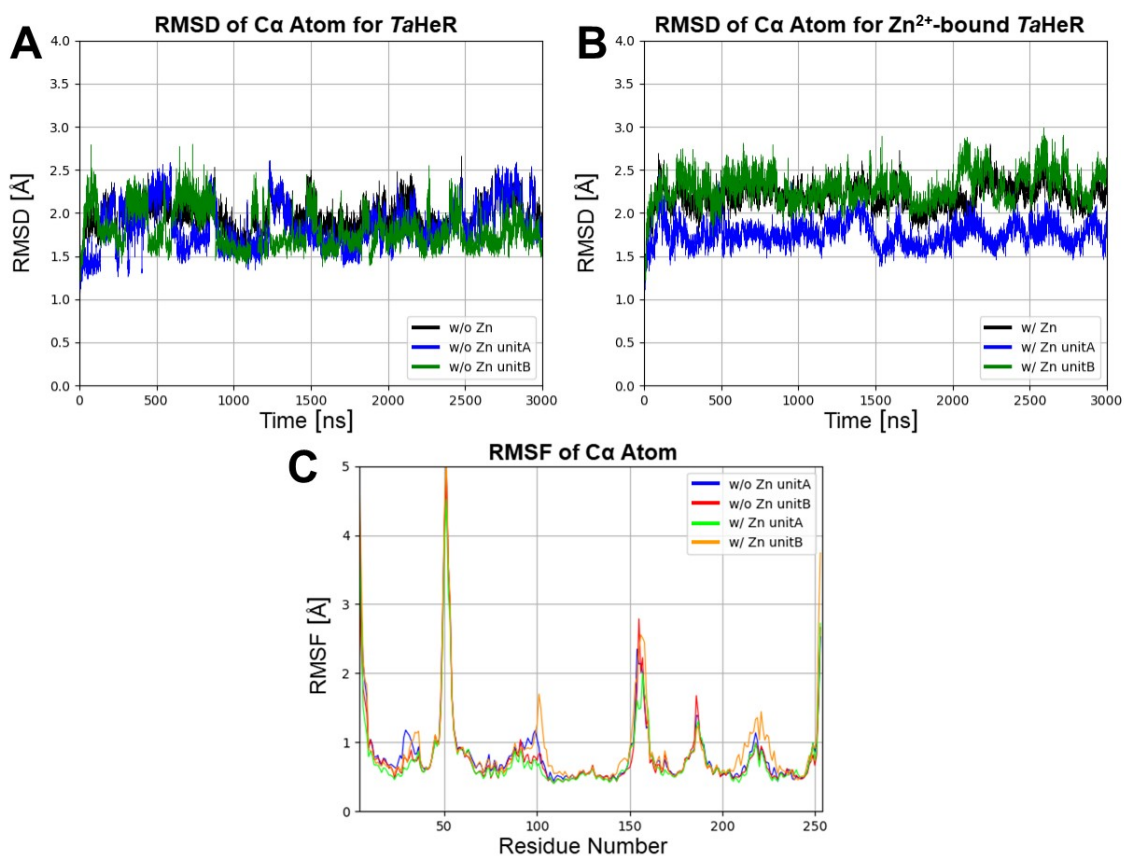
Figure S5. C$_\alpha$ Root-mean-square deviation (RMSD) of (A) *Ta*HeR and (B) Zn^{2+}-bound *Ta*HeR for 3μs. (C) C$_\alpha$ Root-mean-square fluctuation (RMSF) of trajectories obtained by 3μs MD simulations. In these figures, w/o Zn means *Ta*HeR, while w/ Zn does Zn^{2+}-bound *Ta*HeR.

References

(1) Hashimoto, M.; Katayama, K.; Furutani, Y.; Kandori, H. Zinc Binding to Heliorhodopsin. *J. Phys. Chem. Lett.* **2020**, *11*, 8604-8609.