

Supplementary Information

Coordination modes of tyrosinate-ligated heme enzymes: magnetic circular dichroism studies of *Plexaura homomalla* allene oxide synthase, *Mycobacterium avium ssp. paratuberculosis* protein-2744c, and bovine liver catalase in their ferric and ferrous states

D. M. Indika Bandara^a, Masanori Sono^{a,*}, Grant S. Bruce^a, Alan R. Brash^b, and John H. Dawson^{a,c,*}

^aDepartment of Chemistry and Biochemistry and ^cSchool of Medicine, University of South Carolina, Columbia, South Carolina 29208, U.S.A. and ^bDepartment of Pharmacology, Vanderbilt University School of Medicine, Nashville, Tennessee 37232-6602, U.S.A.

*Corresponding Authors: Email: sono@mail.chem.sc.edu (M. Sono); dawson@sc.edu (J.H. Dawson)

References

- [S1] L. Vickery, T. Nozawa, K. Sauer, J. Am. Chem. Soc. 98 (1976) 343-350.
- [S2] R. Perera, M. Sono, H.L. Voegtle, Dawson, J.H. Arch. Biochem. Biophys. 507 (2011) 119-125.
- [S3] R. Perera, M. Sono, J. A. Sigman, T. D. Pfister, Y. Lu, J. H. Dawson, Proc. Nat. Acad. Sci. U.S.A. 100 (2003) 3641-3646.

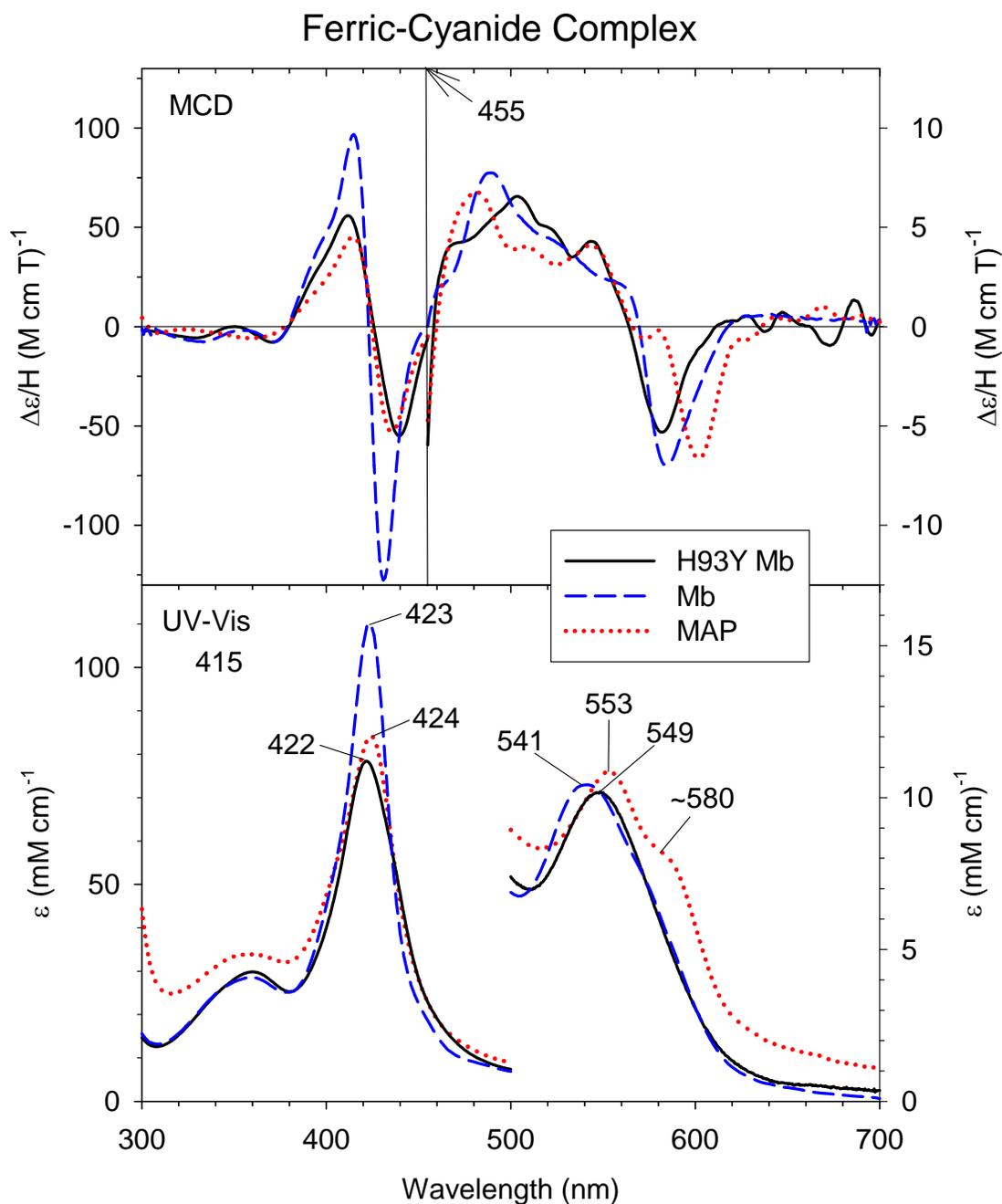


Fig. S1. MCD and UV-Vis absorption spectra of ferric cyanide complex of MAP (dotted line line), H93Y Mb (solid line line) and wt Mb (sperm whale, dashed line). The spectra of MAP and H93Y Mb were replotted from Fig. 3 and those of wt Mb were recorded in 0.1 M potassium phosphate buffer, pH 7.0 at 4 °C. The MCD spectrum of the ferric-cyanide wt Mb is essentially identical to that reported by Vickery et al. [S1] at 24 °C.

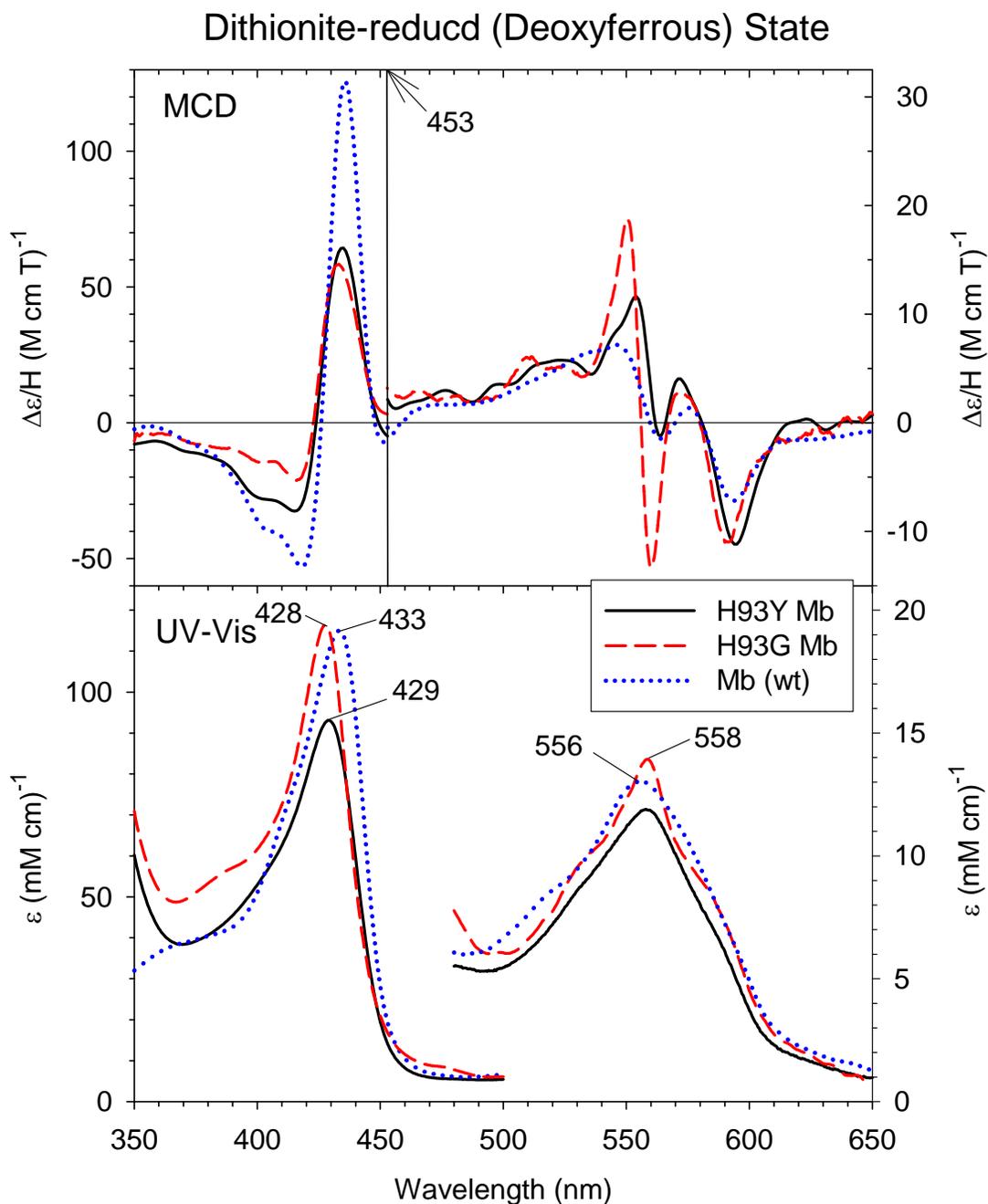


Fig. S2. MCD and UV-Vis absorption spectra of dithionite-reduced five-coordinate H93Y Mb (human), H93G Mb (sperm whale) and wt Mb (sperm whale), all recorded in 0.1 M potassium phosphate buffer, pH 7.0 at 4 °C. These spectra were replotted from refs. [S2] (H93Y Mb and wt Mb) and [S3] (H93G Mb). Note that the spectra of the three proteins are overall similar in band position and shape except that the ferrous H93G Mb mutant has an additional sharp derivative-shaped MCD feature and a corresponding absorption band centered around 560 nm that originate from a minor six-coordinate species.