Electronic Supplementary Material (ESI) for Dalton Transactions

Changes in the Heme Ligation during Folding of a *Geobacter sulfurreducens* Sensor GSU0935

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Supporting Information

Submitted to *Dalton Transactions*

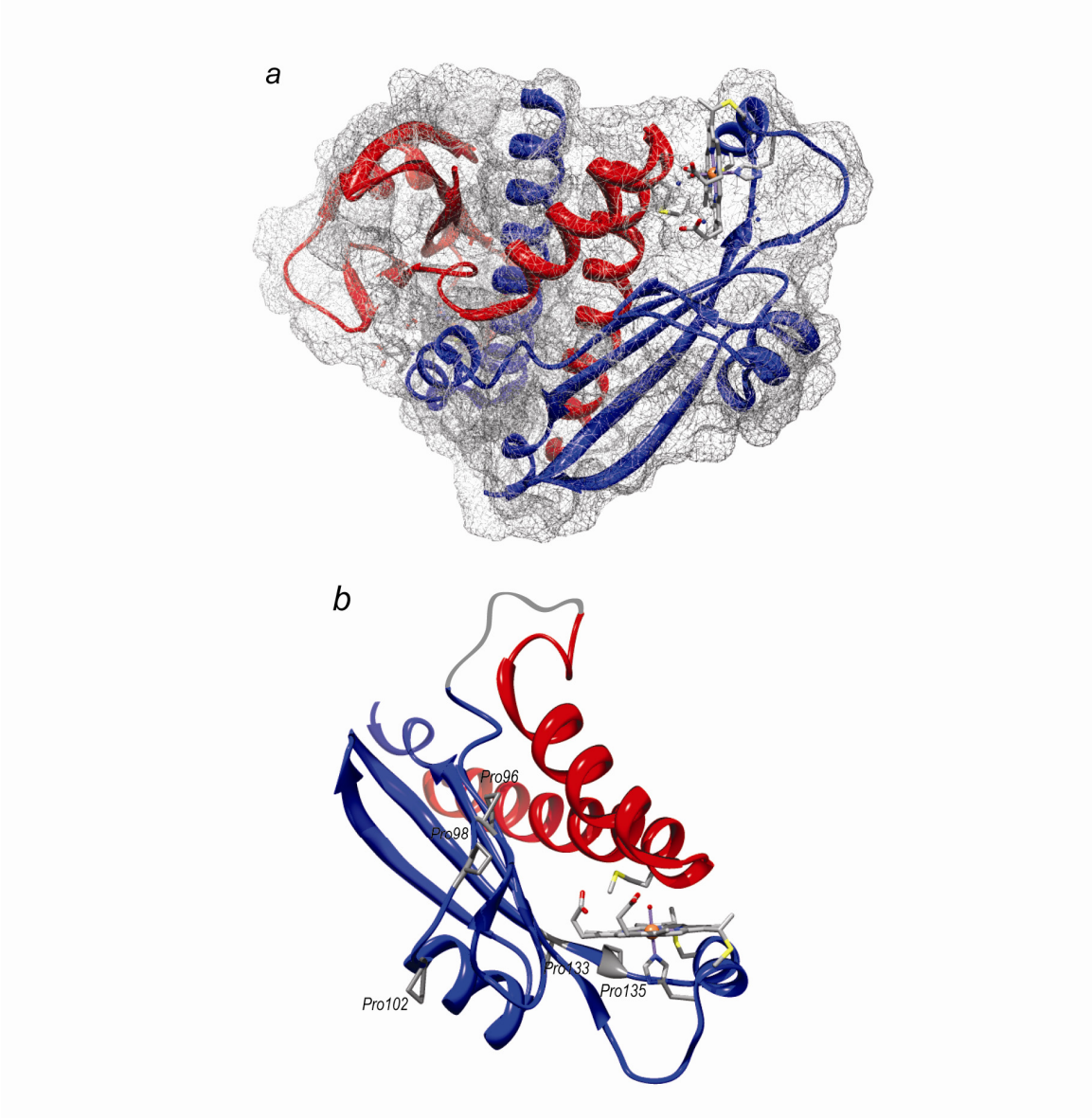

Figure S1. (*a*) A helix-swapped dimer of the GSU0935 heme domain (one monomer is shown in *red*, the other one is in *blue*) from the crystal structure 3B42.[1] (*b*) A model of the monomer with the H_2O-Fe-His ligation constructed from the segments of the swapped dimer. Positions of the Pro residues are shown.

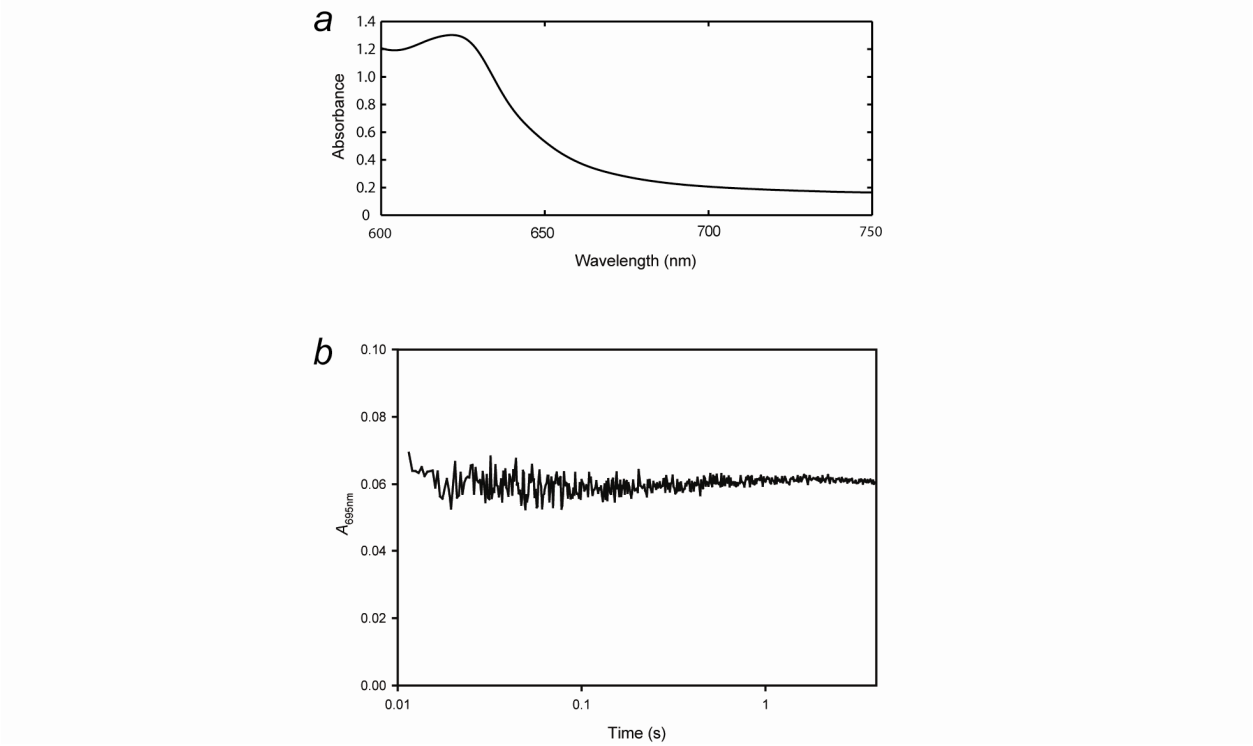

Figure S2. (*a*) Absorption spectrum of the GSU0935 heme domain. The protein concentration was 120 μM. (*b*) Lack of the absorption changes at 695 nm during refolding of the GSU0935 heme domain at pH 5.0. The protein concentration was 47 μM. Refolding of horse heart cytochrome *c* at similar protein concentrations yielded well-developed spectral changes at this wavelength.

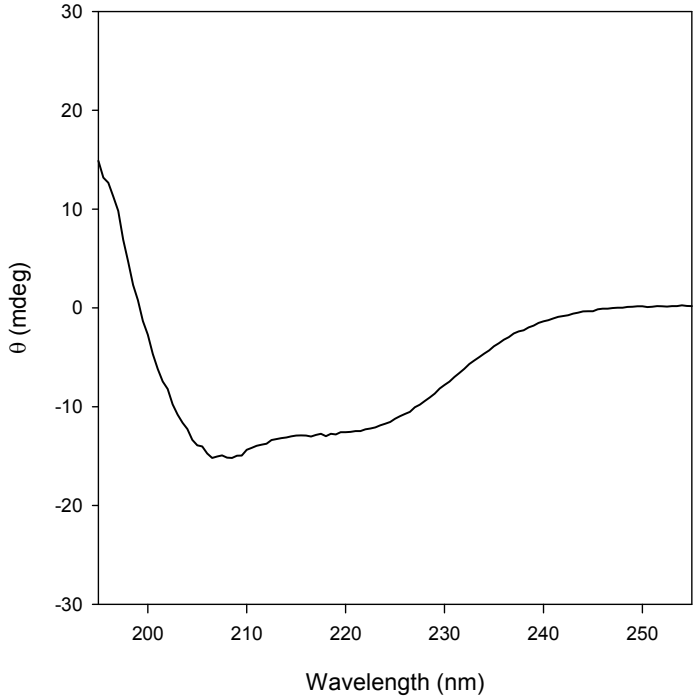

Figure S3. A far-UV CD spectrum of the wild-type GSU0935 in a 100 mM sodium phosphate buffer at pH 7.4 and 22 °C: [GSU0935]=5.7 μM, *l*=0.1 cm.

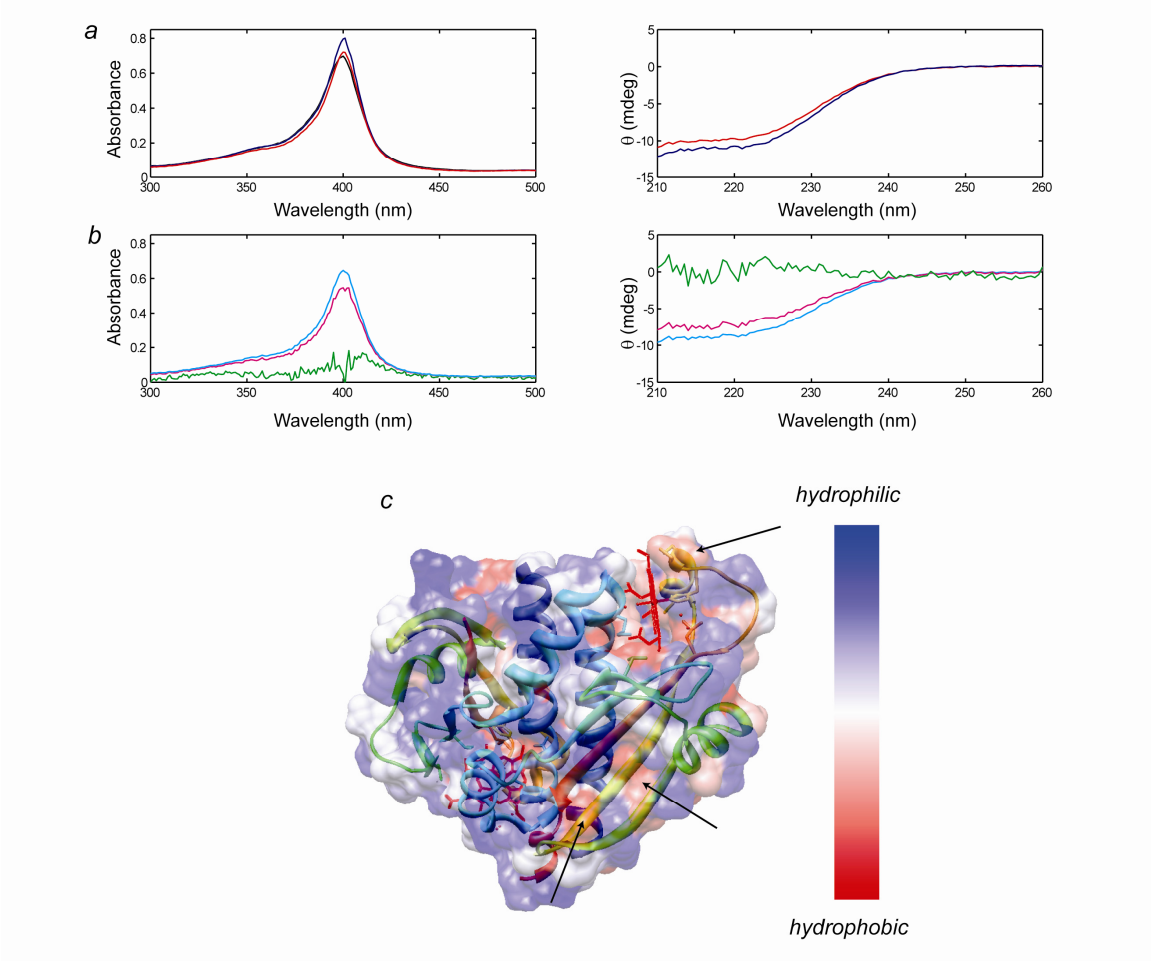

Figure S4. (*a*) Absorption (*left*) and CD (*right*) spectra of the unfolded (*black*), folded (*blue*), and refolded (*red*) heme domain of GSU0935. (*b*) Absorption (*left*) and CD*(right*) spectra of the misfolded species calculated assuming the refolded sample contains 50% (*cyan*), 70% (*magenta*), and 90% (*green*) of the native protein conformations. At high projected populations of the native conformations, absorption spectra of the misfolded species show very small signals in the visible region, inconsistent with the heme species. These results suggest that the misfolded protein posesses some secondary structure. (*c*) Hydrophobic (the Kyte-Doolittle scale) surface plot of the GSU0935 dimer. Arrows indicate exposed hydrophobic regions in the folded protein. Images created with Chimera 1.5.3.

References

1. P. R. Pokkuluri, M. Pessanha, Y. Y. Londer, S. J. Wood, N. E. Duke, R. Wilton, T. Catarino, C. A. Salgueiro and M. Schiffer, *J. Mol. Biol.*, 2008, **377**, 1498-1517.