Supporting Information

Determination of the distance between the Mo(V) and Fe(III) heme centers of wild type human sulfite oxidase by pulsed EPR spectroscopy.

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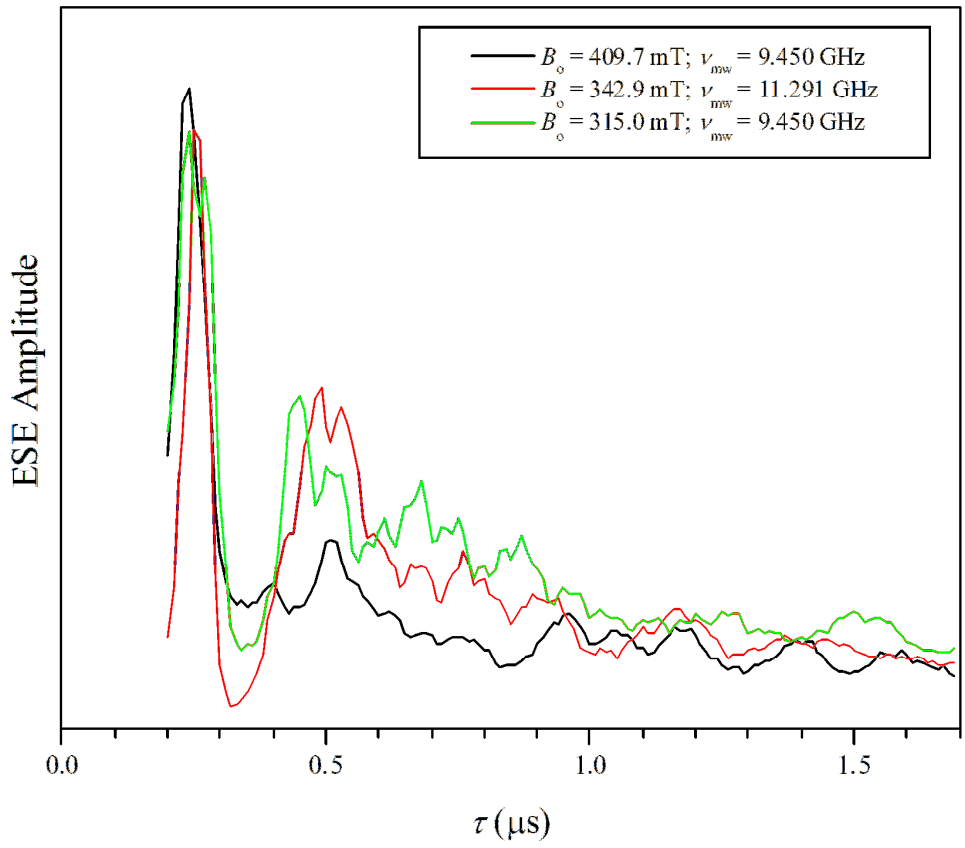

Figure S1. Examples of Fe(III) heme two-pulse ESE decays obtained at different magnetic fields and observation frequencies (as indicated in the inset), showing the strong ^{14}N ESEEM. Experimental conditions: mw pulses, 10 and 15 ns; temperature, 10 K.

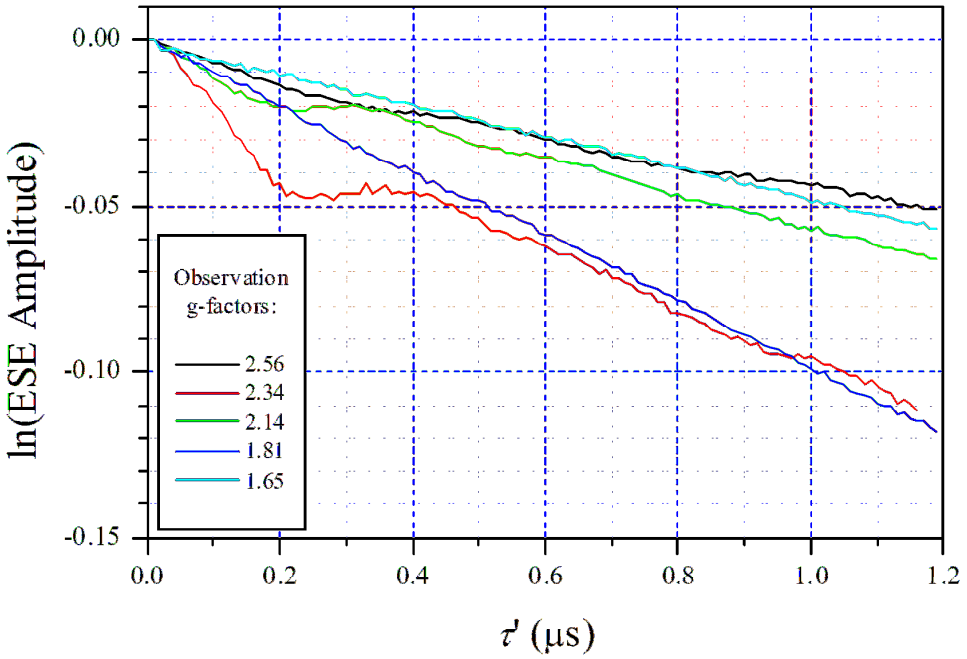

Figure S2. Natural logarithms of the ELDOR traces obtained at various EPR positions across the Fe(III) EPR spectrum (as indicated by the observation g-values, g_{obs}). Each trace was normalized by the corresponding g_{obs} to account for the effect of g-dependent rescaling of the dipole interaction on k_{mat}. The ELDOR pulse sequence is shown in Figure 3a of the manuscript. The Mo(V) signal was used for pumping, and Fe(III) for observation. The experimental conditions are listed in the legend of Figure 6 of the manuscript.

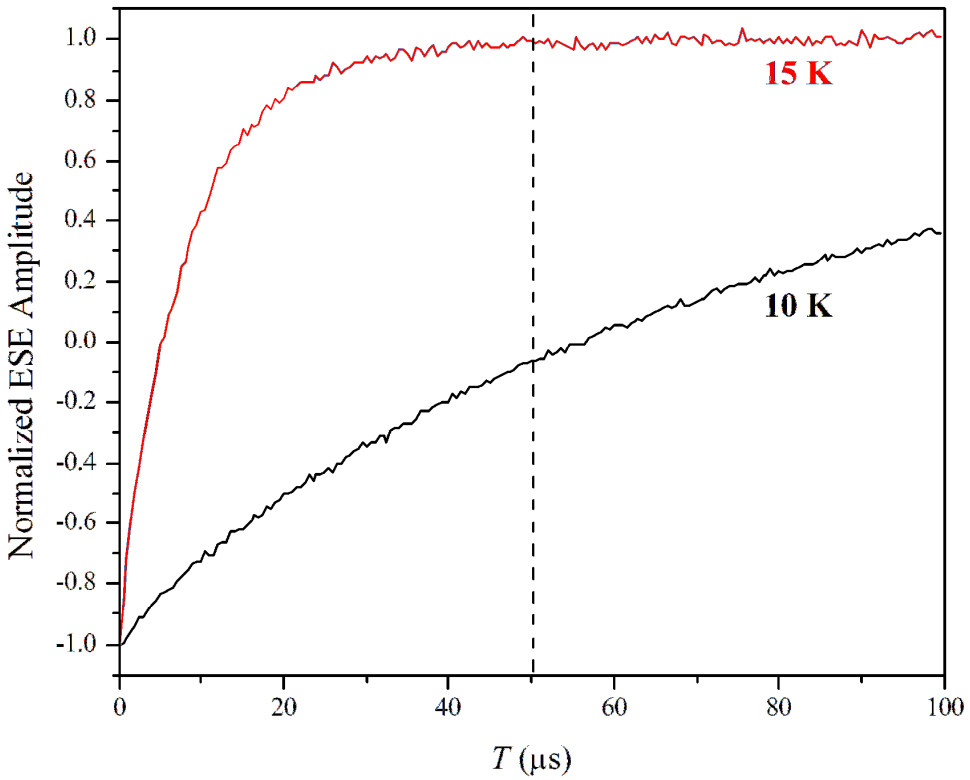

Figure S3. Inversion recovery of the Fe(III) heme center of hSO at different temperatures (as indicated in the Figure). Experimental conditions: mw frequency, 9.444 GHz; B_o = 300 mT (near g_Y); mw pulses, inversion: 10 ns (π), observation: 20 and 40 ns; time interval between the observation pulses, τ = 250 ns.

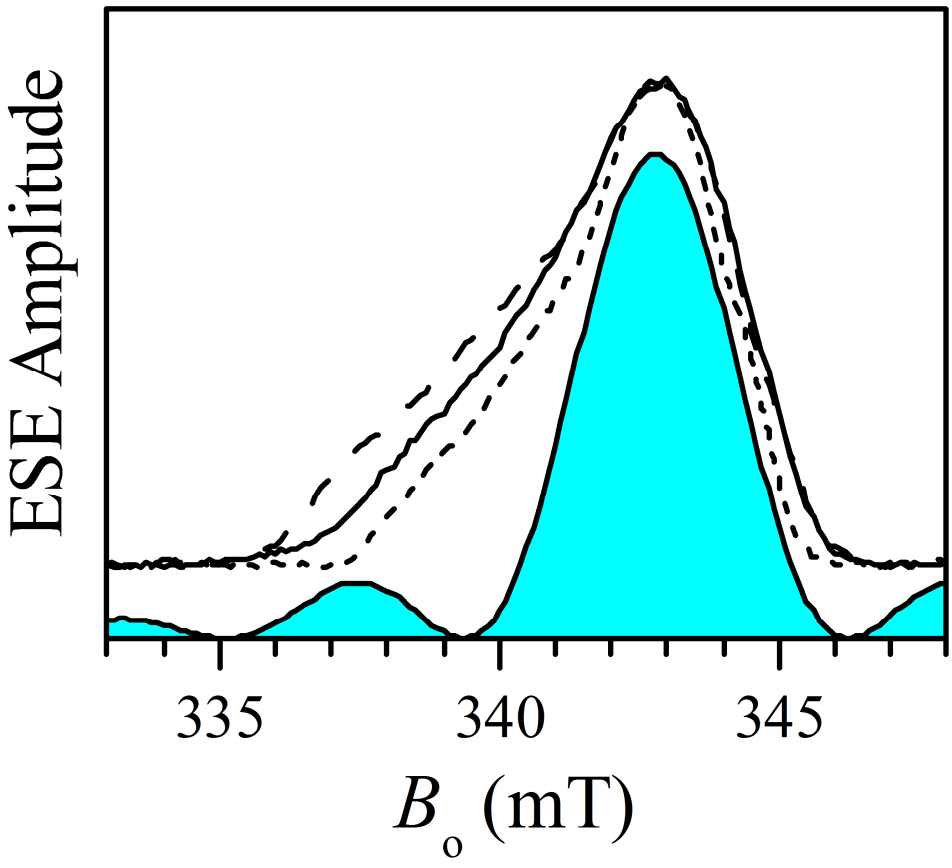

Figure S4. The top three traces are the two-pulse field sweep ESE spectra of the Mo(V) center obtained at the mw frequencies of 9.450 GHz (solid line), 11.291 GHz (long-dashed line), and 8.681 GHz (short-dashed line). These traces are reproduced from Figure 5 of the manuscript. The bottom trace represents the calculated excitation profile of the 9 ns π-pulse.

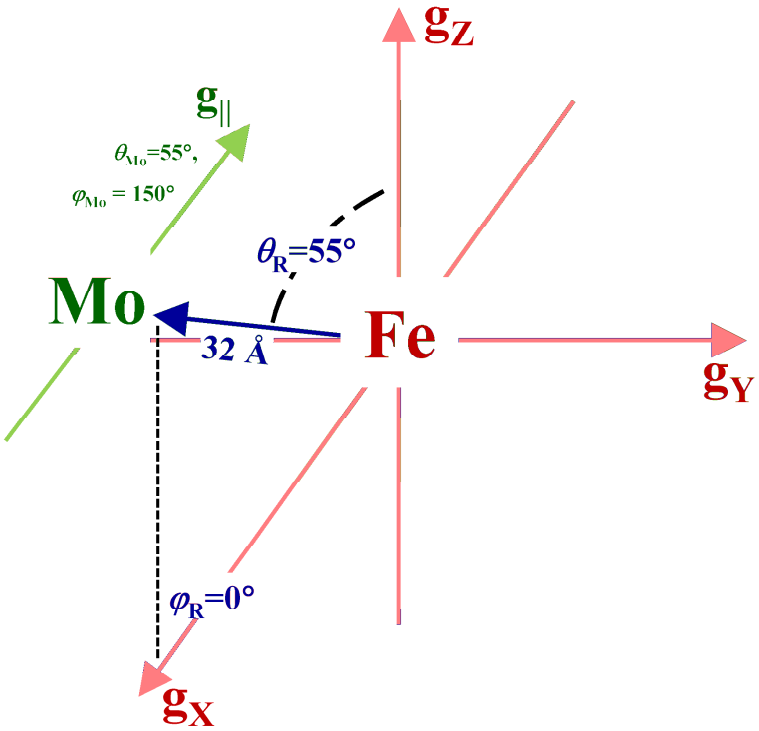

Figure S5. Summary of structural information regarding the relative arrangement of the Mo(V) and Fe(III) heme centers of Ti(III)-reduced *wt* hSO in frozen glassy solution as obtained by pulsed EPR in this work.