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Figure S1. The electronic absorption spectrum of Fe(III)CooA showing the thiolate sulfur-to-Fe(III) charge-transfer bands (inset). Fe(III)CooA samples contained 10.2 μ M heme or 102 μ M heme (inset) and 25 mM MOPS, 1 mM DTT, 0.1 M NaCl at pH 7.4. The spectra were recorded at 25°C on a Varian Cary 4 Bio spectrophotometer.

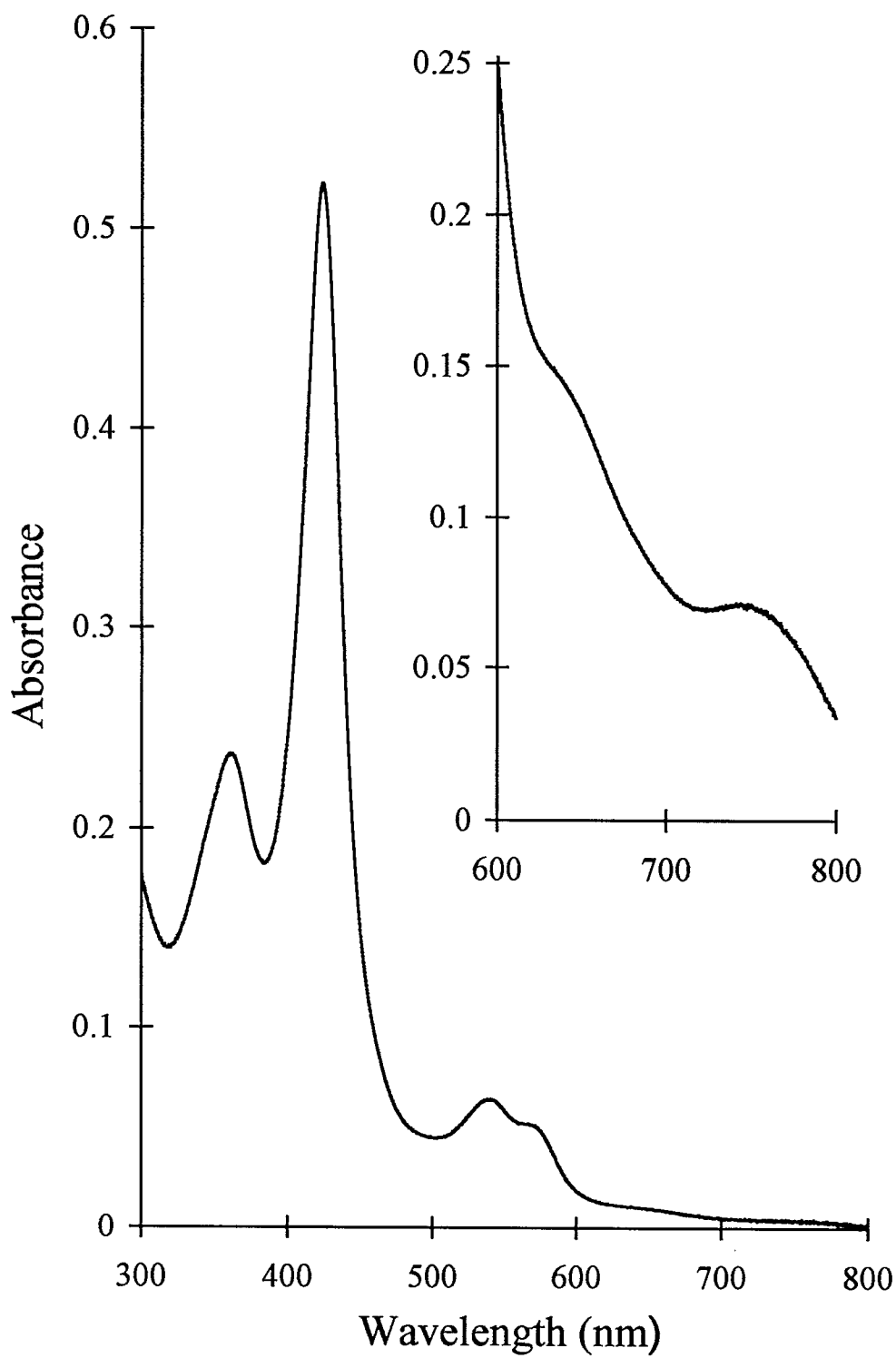


Table S2. Comparison of the electronic absorption spectral parameters of CooA derivatives with those of thiolate-ligated heme proteins and model complexes.

Protein	Iron Ligands	δ (nm)	Soret (nm)	β (nm)	α (nm)	LMCT (nm)	Ref.
Fe(III) derivatives							
Fe(III)CooA, pH 7.4		362	424	540	574	649, 750	a
Fe(III)P450 + ImH	ImH/Cys	358	425	542	574	638, 753	20
Fe(III)cyt c-M80C ^b	His/Cys ^b	355	416	540	570	635, 734	20
Fe(III)cyt c(M80A) + CH ₃ S ⁻	His/RS ⁻	355	416	535	566	648, 763	20
Fe(III)H450 ^c	His/Cys ^c	360	428	550	NR ^f	NR ^f	16
Fe(III)Mb + H ₂ S	His/SH ⁻		425	545	570	625	13
Fe(III)P420 ^d	d	367	422	541	566	651	27
Fe(II) derivatives							
Fe(II)CooA, pH 7.4			425	529	559		a
Fe(II)P450 + py	Cys/py		444	538	566		21
Fe(II) cyt c-M80C ^b	b		416	520	550		22
Fe(II)H450 ^c , pH 6.0	His/Cys ^c		425	530	558		16
Fe(II)H450 ^c , pH 8.0	His/Cys ^c		448	540	571		16
Fe(II)P420 ^d	d		424	530	558		27
Fe(II)Mb-H93C ^e	e		429	NR ^f	558		28
Fe(II) + CO							
Fe(II)CooA, pH 7.0			422	540	569		a
Fe(II)Mb	His	346	423	540	579		20
Fe(II)H450 ^c	His ^c		420	540	570		16
Fe(II)P420 ^d	d		420	540	570		27
Fe(II)Mb-H93C ^e	e		422	541	571		28
Fe(II)P450	Cys	366	446	551			21

^aThis work. The protein samples⁹ were in 25 mM MOPS buffer, 1 mM DTT, 0.1 M NaCl and the spectra were recorded at 25°C on a Varian Cary 4 Bio spectrophotometer.

^bcyt c-M80C contains a His/Cys ligated heme in the ferric form but the ligation state of the reduced and CO bound states is not known.^{20,22,24}

^cH450 is proposed to contain a His/Cys ligated heme iron.¹⁶

^dP420 is an inactive form of P450; the ligation state of the heme in the oxidized, reduced and CO-bound states is not known.²⁷

^eMb-H93C contains a cysteine that has been substituted for the histidine bound to the heme iron; the ligation state of the heme in the reduced and CO-bound states is not known.^{28,29}

^fNot reported