

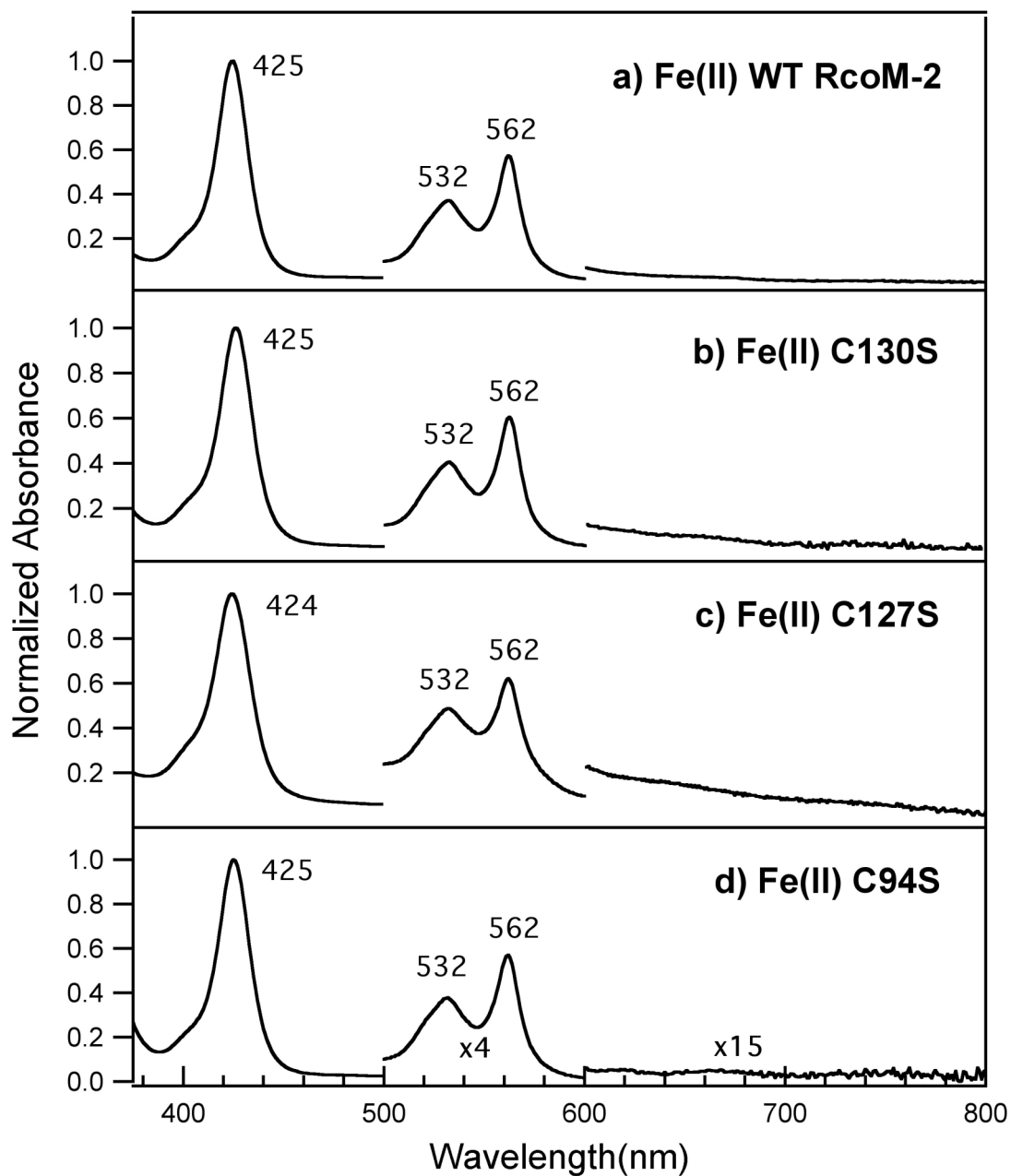
Supporting information for

Identification of Cys<sup>94</sup> as the distal ligand to the Fe(III) heme in the  
transcriptional regulator RcoM-2 from *Burkholderia xenovorans*

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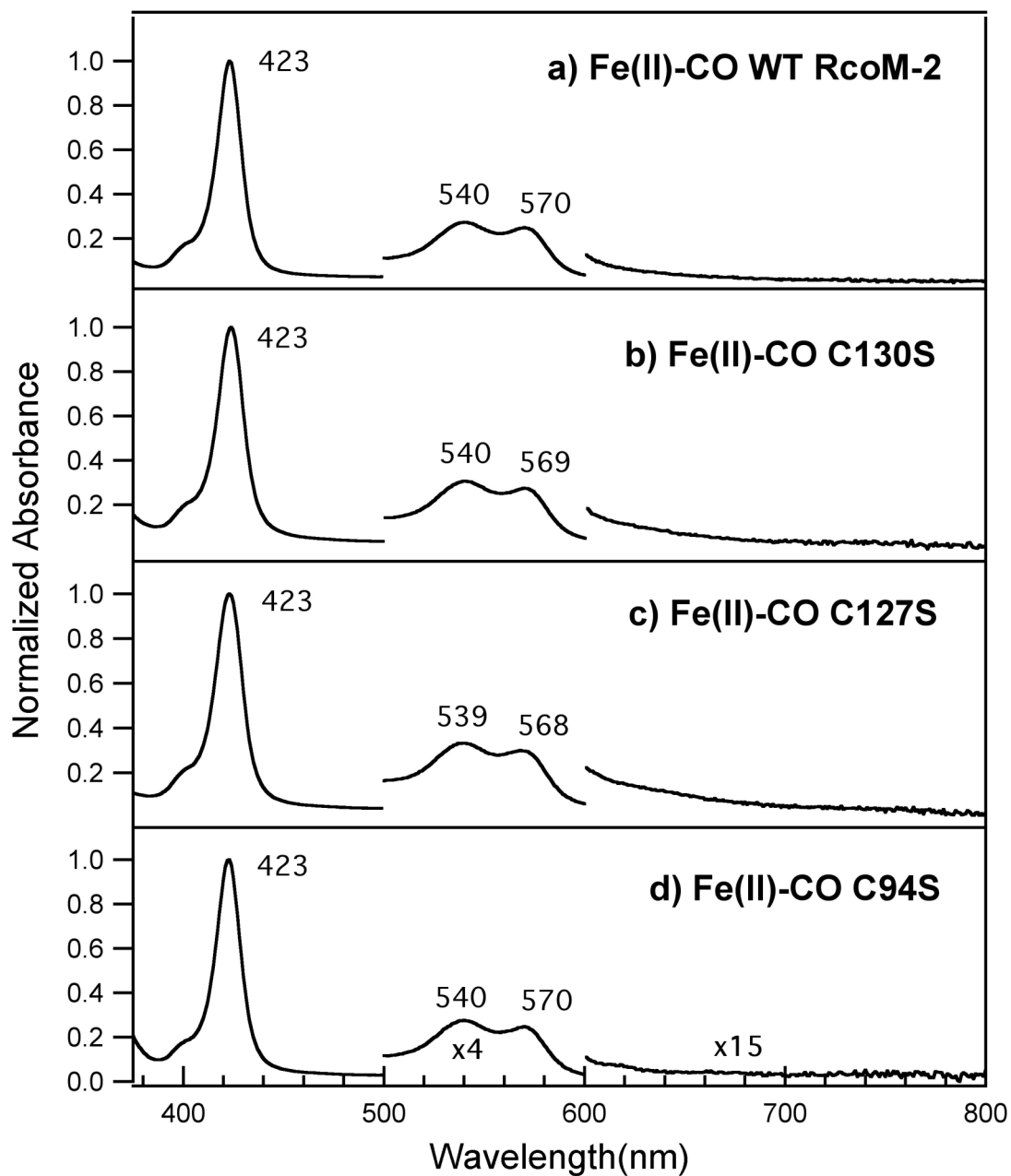
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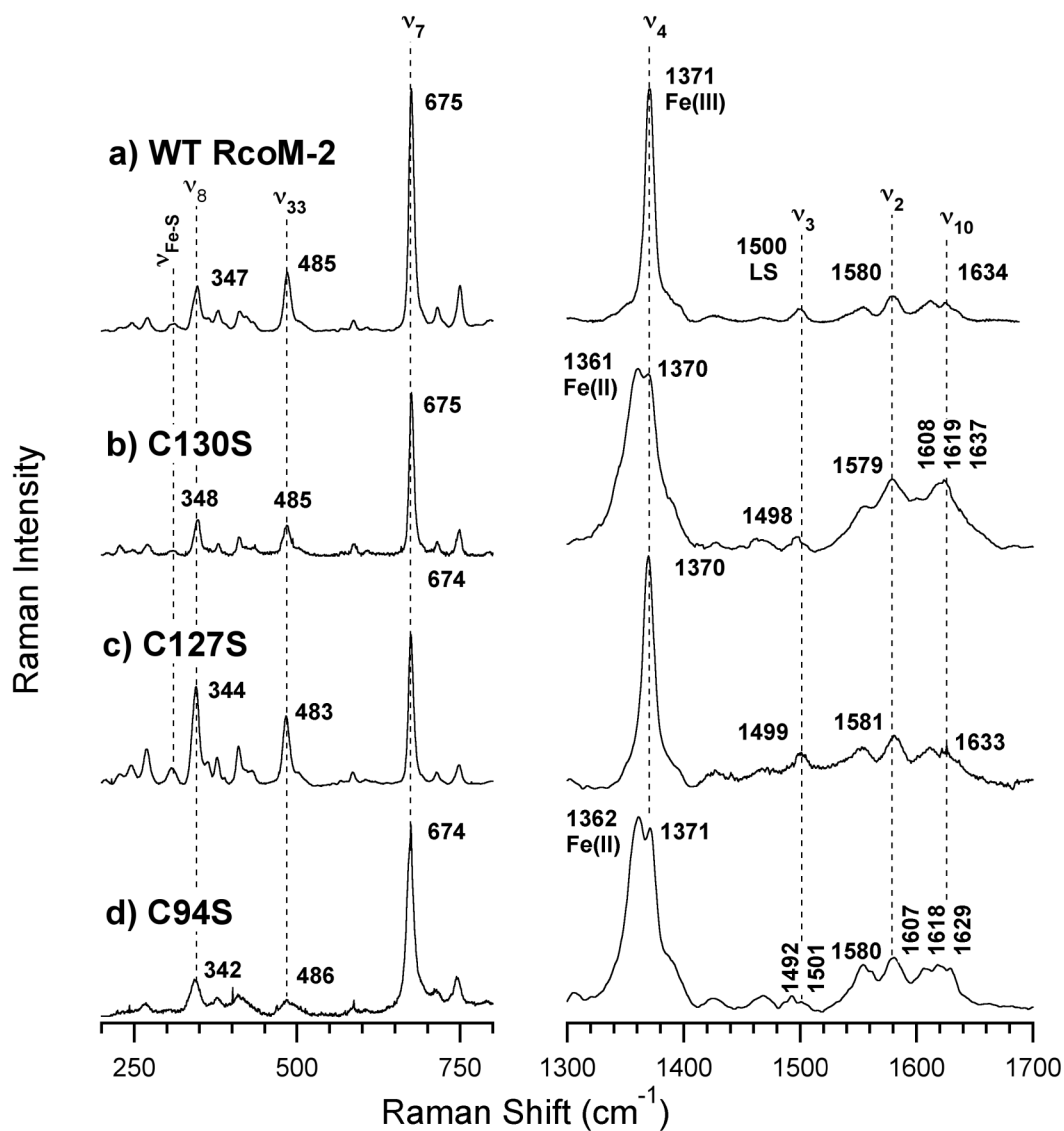


**Figure S1.** Electronic absorption spectra of a) Fe(II) WT *BxRcoM-2*, b) Fe(II) C130S *BxRcoM-2*, c) Fe(II) C127S *BxRcoM-2* and d) Fe(II) C94S *BxRcoM-2* as isolated.

Sample a) contained 12  $\mu\text{M}$  heme in 25 mM EPPS pH 8.0 with 500 mM KCl; samples b-d) contained 8-10  $\mu\text{M}$  heme in 25 mM MOPS pH 7.4 with 500 mM KCl.



**Figure S2.** Electronic absorption spectra of a) Fe(II)-CO WT *BxRcoM-2*, b) Fe(II)-CO C130S *BxRcoM-2*, c) Fe(II)-CO C127S *BxRcoM-2* and d) Fe(II)-CO C94S *BxRcoM-2* as isolated. Sample a) contained 12  $\mu$ M heme in 25 mM EPPS pH 8.0 with 500 mM KCl; samples b-d) contained 8-10  $\mu$ M heme in 25 mM MOPS pH 7.4 with 500 mM KCl.



**Figure S3.** Resonance Raman spectra of a) WT Fe(III) *BxRcoM-2* compared to b) C130S *BxRcoM-2*, c) C127S *BxRcoM-2* and d) C94S *BxRcoM-2* as isolated. Sample a) contained 250  $\mu\text{M}$  heme in 50 mM borate pH 8.0 with 500 mM KCl; samples b-d) contained 80-170  $\mu\text{M}$  heme in 25 mM MOPS pH 7.4 with 500 mM KCl. Spectra were acquired with 8-15 mW of power at the frozen (77 K) sample using the 413.1 nm  $\text{Kr}^+$  laser line. Key porphyrin stretching modes are noted, including major oxidation and spin state marker bands ( $\nu_2$ ,  $\nu_3$ ,  $\nu_4$  and  $\nu_{10}$ ) and the putative Fe-S stretch band ( $\nu_{\text{Fe-S}}$ ).