Supporting Information

For

Modeling the Active Site of Nitrile Hydratase:
Synthetic Strategies to Ensure Simultaneous Coordination of
Carboxamido-N and Thiolato-S to Fe(III) Centers

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Figure S1. $^1$H NMR spectrum of (Et$_4$N)[Co(PiPepS)$_2$] (2) in dmsø-$d_6$. The peaks at 2.5 and 3.3 ppm arise from the solvent (dmsø and water respectively).
Figure S2. IR spectrum of the disulfide (PiPepS)_2 isolated from the reaction mixture of Fe(III) and PiPepSH₂ (KBr matrix). The peaks at 3310 and 1628 cm⁻¹ represent the \( \nu_{\text{NH}} \) and \( \nu_{\text{CO}} \) stretches, respectively.

Figure S3. \(^1\)H NMR spectrum (500 MHz) of the disulfide (PiPepS)_2 isolated from the reaction mixture of Fe(III) and PiPepSH₂ in CDCl₃.