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EPR and Semi-Empirical Studies as Tools to Assign the Geometric Structures of Fe^{III} Isomer Models for Transferrins

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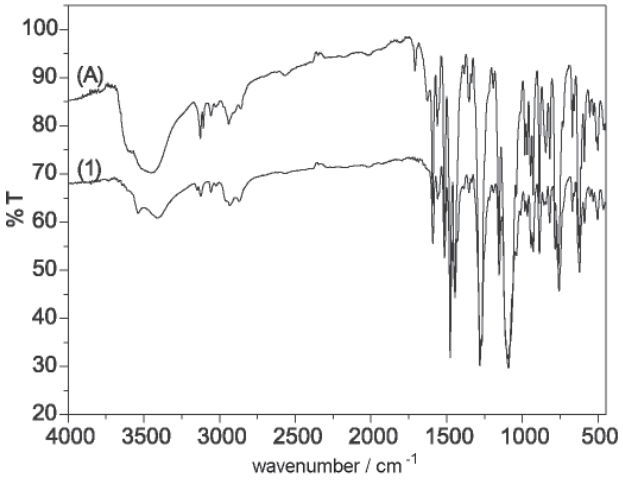

Figure S1. IR spectra of **1** and **A** recorded as KBr pellets.

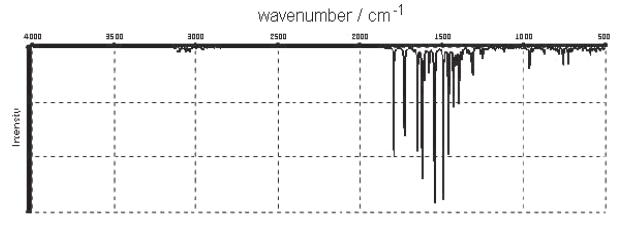

Figure S2. Theoretical IR spectrum of **A**.

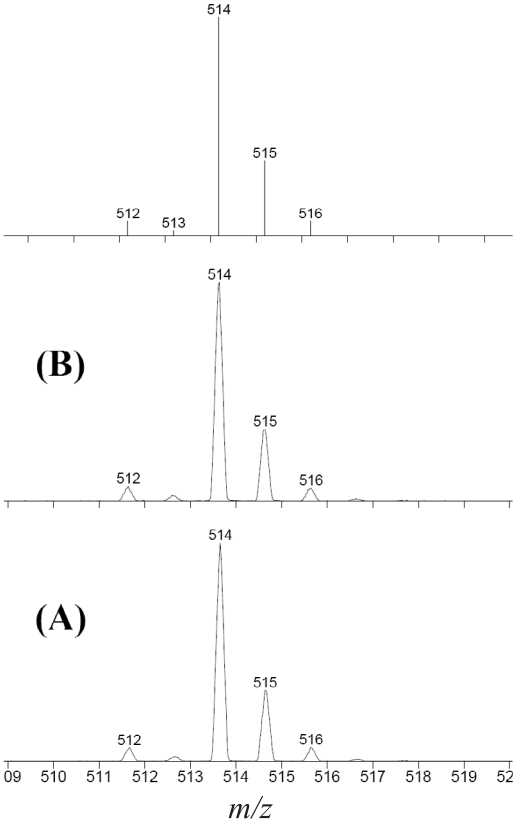

Figure S3. ESI-MS (positive mode) of **A** (bottom) and **B** (middle) recorded in acetonitrile solution, and predicted isotopic distribution (top).

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Dedicated to Prof. Vincent Louis Pecoraro on the occasion of his 50th birthday.

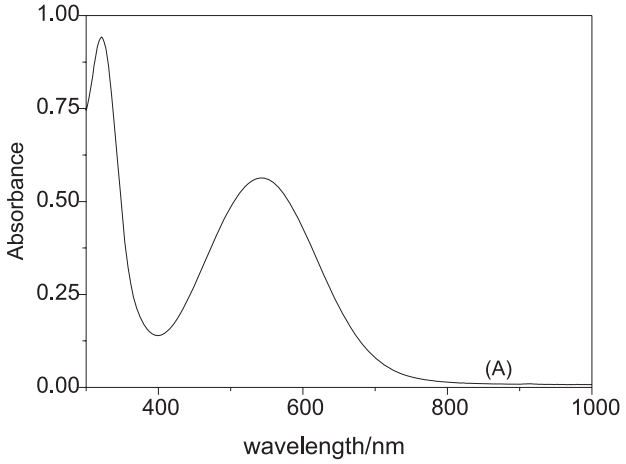

Figure S4. UV-visible spectrum of **A** in acetonitrile solution.

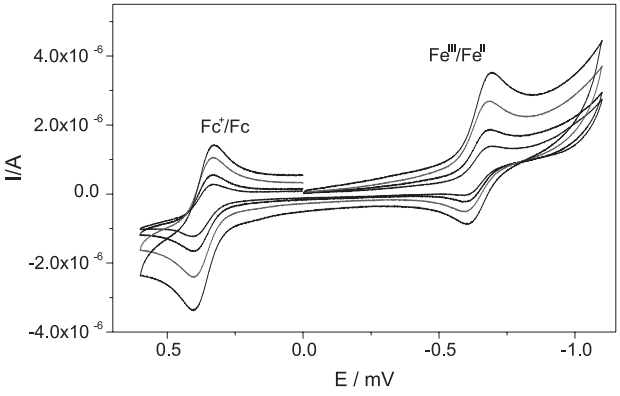

Figure S5. Cyclic voltammograms of **A** in CH_3CN, $TBAPF_6$ (0.1 mol L^{-1}) at 50 (internal), 100, 150, 200 and 250 mV s^{-1} scan rates, Fc^+/Fc internal standard (left) and Fe^{III}/Fe^{II} (right).