

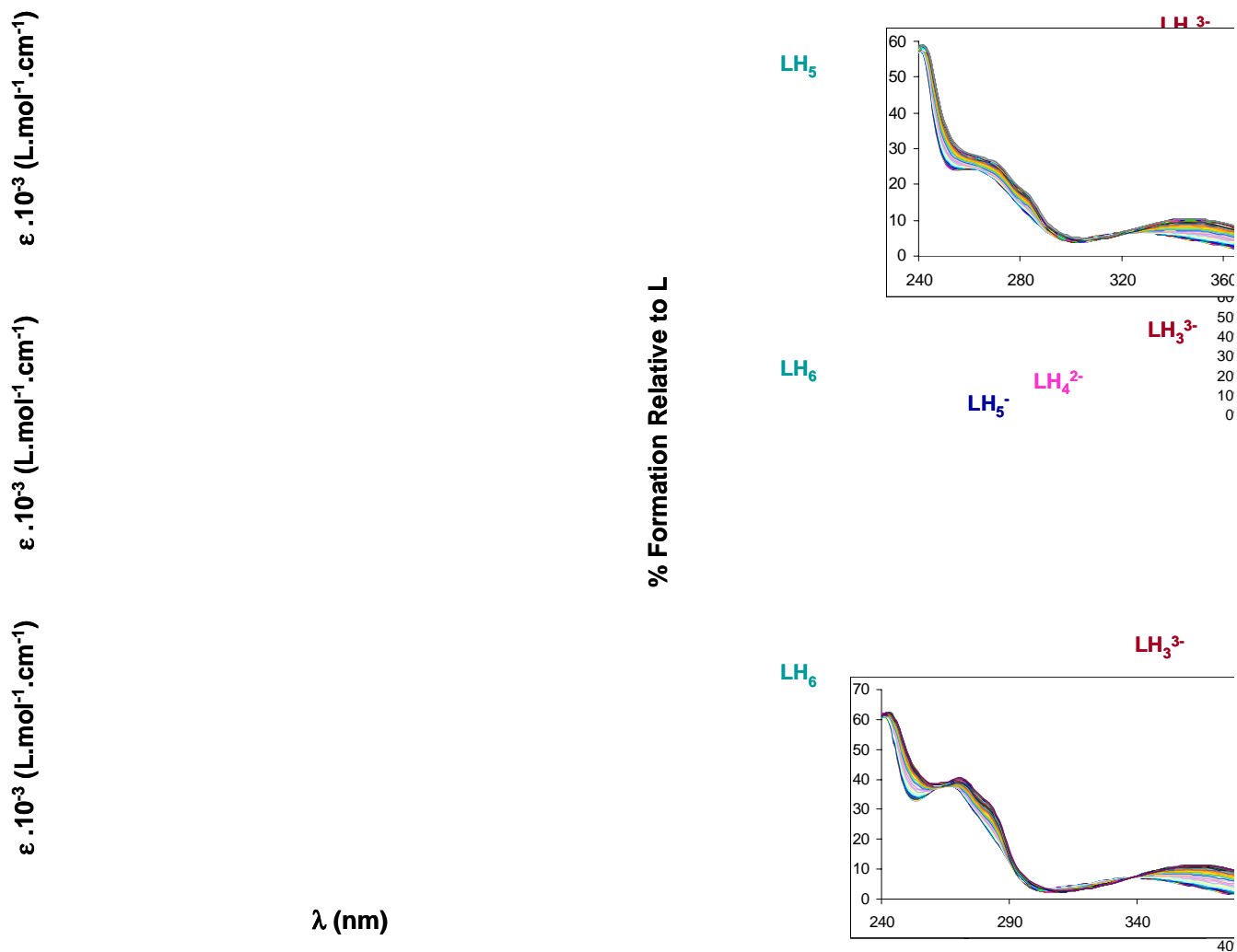
# Synthesis and Thermodynamic Evaluation of Mixed Hexadentate Linear Iron Chelators Containing Hydroxypyridinone and Terephthalamide Units

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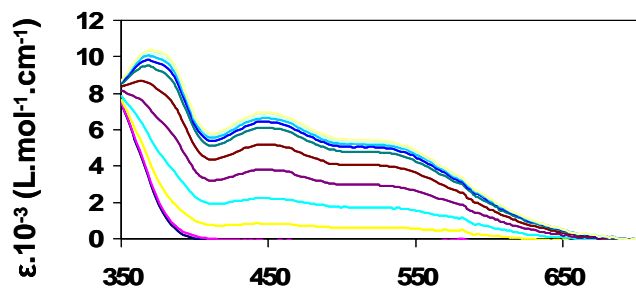
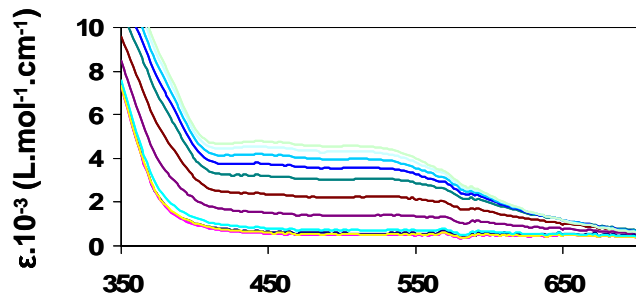
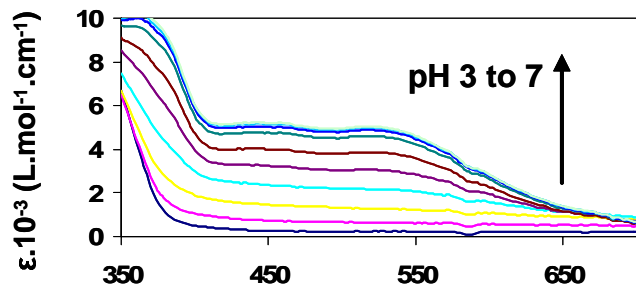
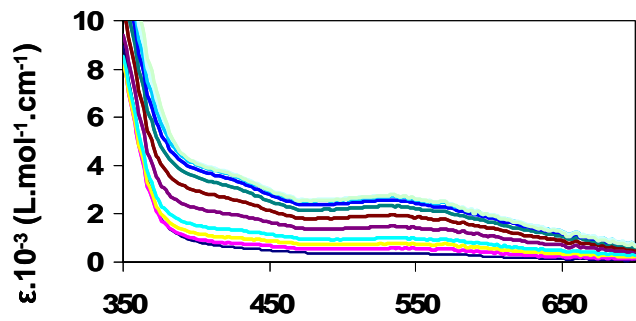
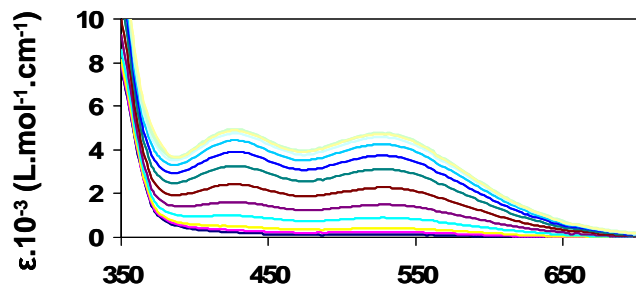
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## Supporting Information

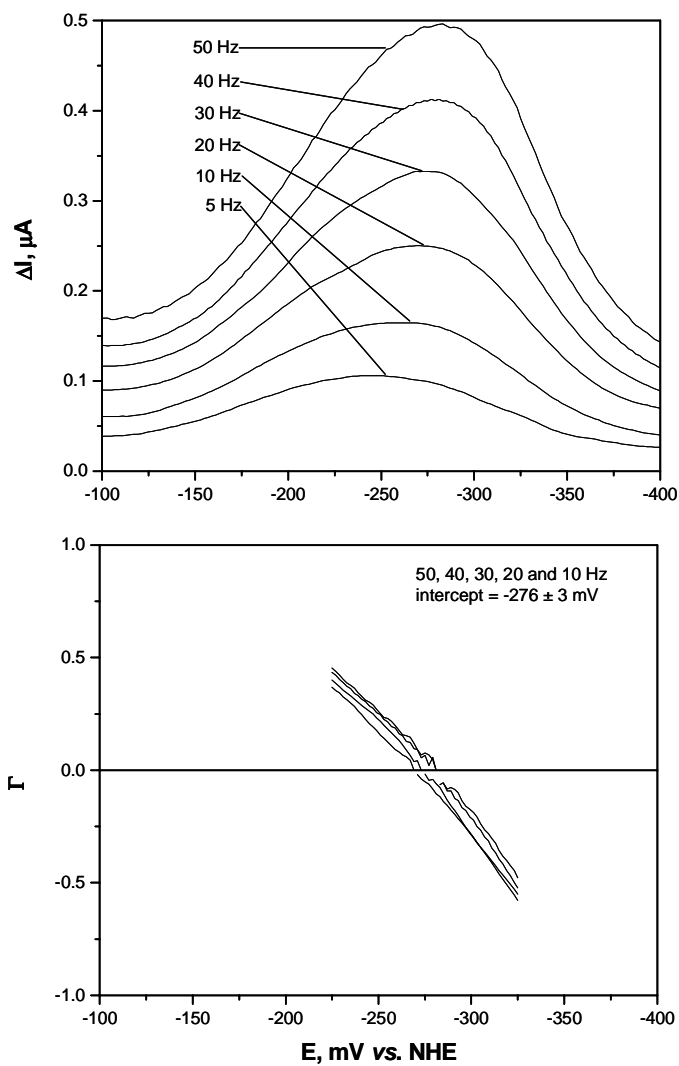


**Figure S-1.** Spectral data (left) and speciation diagrams (right) for spectrophotometric titrations of 3,4-LI(Me-3,2-HOPO)(TAMmeg)<sub>2</sub> (top), 3,4-LI(TAMmeg) (center) and 5-LIO(TAMmeg)<sub>2</sub>(TAM) (bottom).

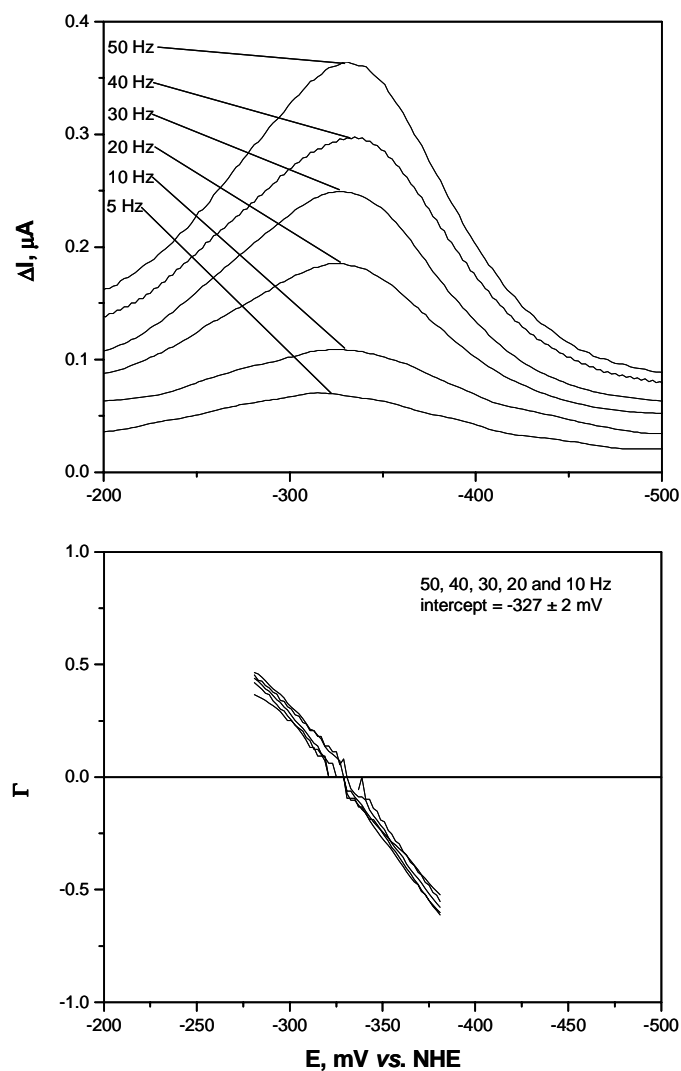


$\lambda \text{ (nm)}$

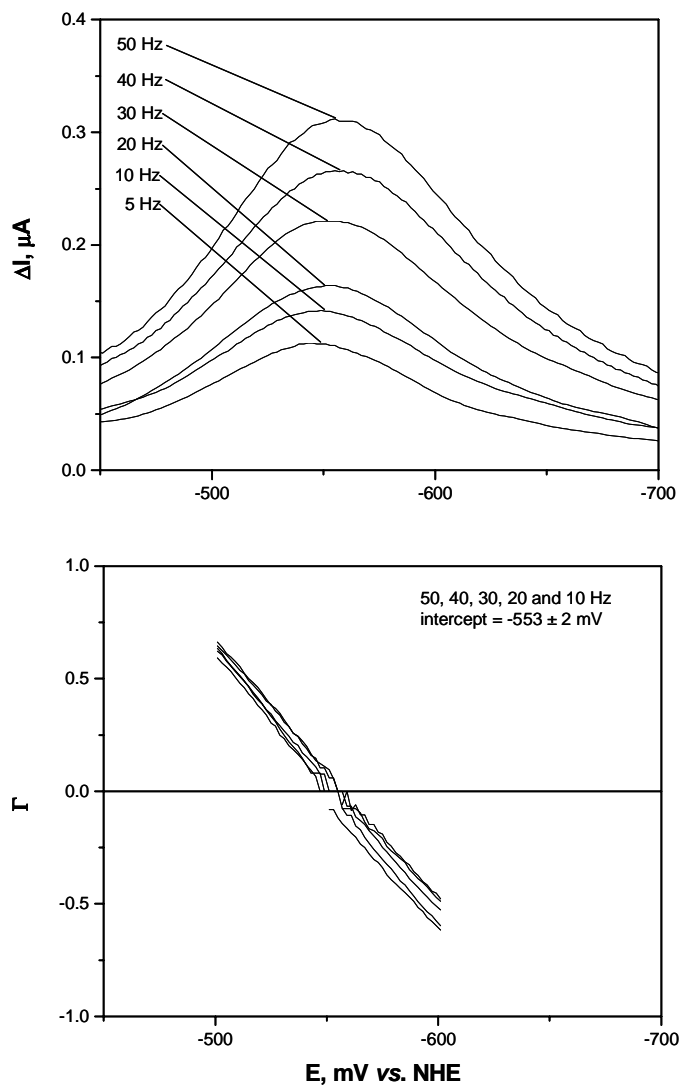
**Figure S-2.** Spectral data for EDTA-competition spectrophotometric titrations of 3,4-LI(Me-3,2-HOPO), 3,4-LI(Me-3,2-HOPO)<sub>2</sub>(TAMmeg), 3,4-LI(Me-3,2-HOPO)(TAMmeg)<sub>2</sub>, 3,4-LI(TAMmeg) and 5-LIO(TAMmeg)<sub>2</sub>(TAM) in order from top to bottom.



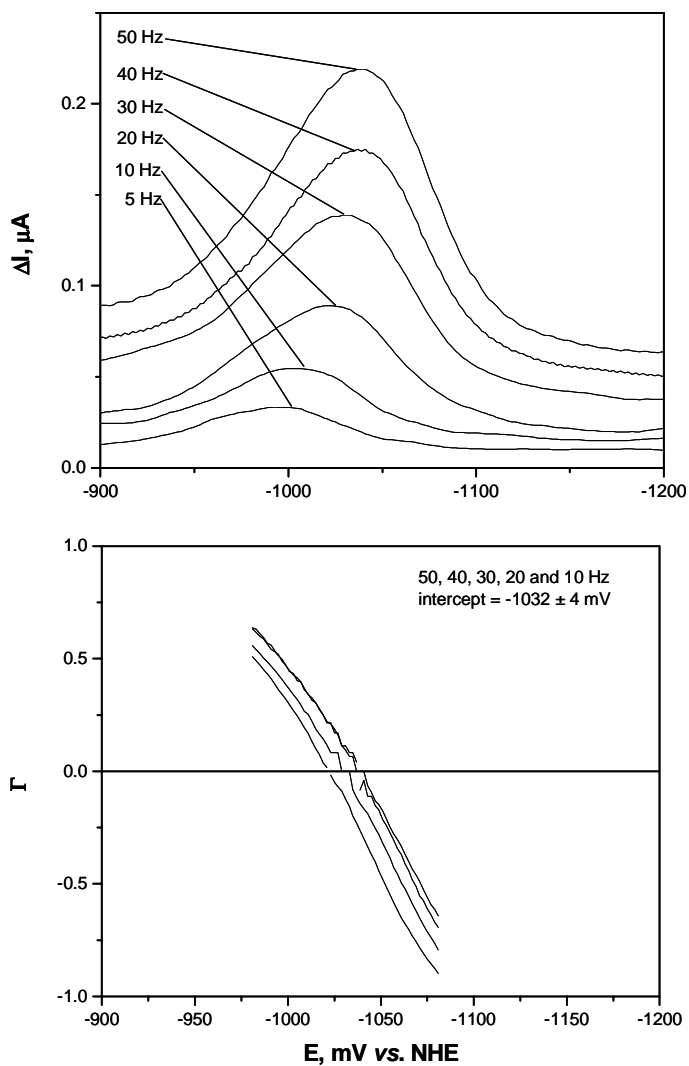
**Figure S-3.** Upper panel: Square wave voltammograms at the HMDE of  $5 \times 10^{-5}$  M Fe[3,4-LI(Me-3,2-HOPO)] in 0.01 M ammonium acetate buffer, pH 7.5, ionic strength 0.1 M (KCl),  $E_{sw} = 25$  mV,  $E_{step} = 2$  mV, frequencies given in hertz. Lower panel: Conversion of the voltammograms to the  $\Gamma$  function, according to eq. 1.



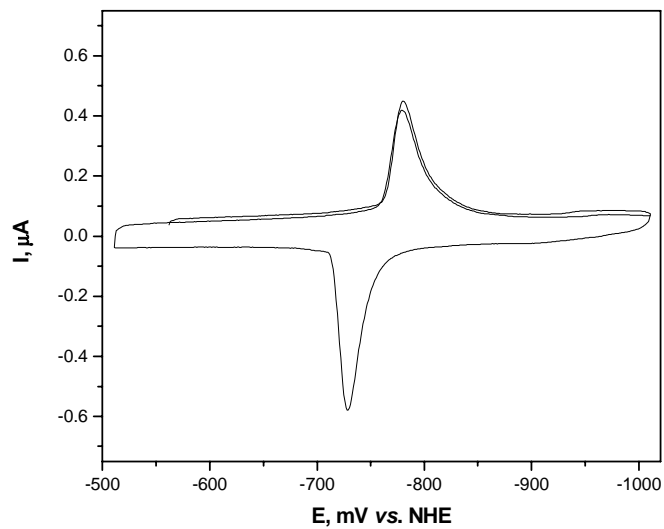
**Figure S-4.** Upper panel: Square wave voltammograms at the HMDE of  $5 \times 10^{-5}$  M Fe[3,4-LI(Me-3,2-HOPO)<sub>2</sub>(TAMmeg)] in 0.01 M ammonium acetate buffer, pH 8, ionic strength 0.1 M (KCl),  $E_{sw} = 25$  mV,  $E_{step} = 2$  mV, frequencies given in hertz. Lower panel: Conversion of the voltammograms to the  $\Gamma$  function, according to eq. 1.



**Figure S-5.** Upper panel: Square wave voltammograms at the HMDE of  $5 \times 10^{-5}$  M Fe[3,4-LI(Me-3,2-HOPO)(TAMmeg)<sub>2</sub>] in 0.01 M ammonium acetate buffer, pH 8.5, ionic strength 0.1 M (KCl),  $E_{sw} = 25$  mV,  $E_{step} = 2$  mV, frequencies given in hertz. Lower panel: Conversion of the voltammograms to the  $\Gamma$  function, according to eq. 1.



**Figure S-6.** Upper panel: Square wave voltammograms at the HMDE of  $5 \times 10^{-5}$  M Fe[3,4-LI(TAMmeg)] in 0.01 M ammonium acetate buffer, pH 9.0, ionic strength 0.1 M (KCl),  $E_{sw} = 25$  mV,  $E_{step} = 2$  mV, frequencies given in hertz. Lower panel: Conversion of the voltammograms to the  $\Gamma$  function, according to eq. 1.



**Figure S-7.** Cyclic voltammogram at the HMDE of  $5 \times 10^{-5}$  M  $\text{Fe}[5\text{-LIO}(\text{TAMmeg})_2(\text{TAM})]$  in 0.01 M ammonium acetate buffer, pH 9.0, ionic strength 0.1 M (KCl), scan rate 200 mV/s, negative direction, initial potential  $E = -561$  mV.