

## Supporting Information

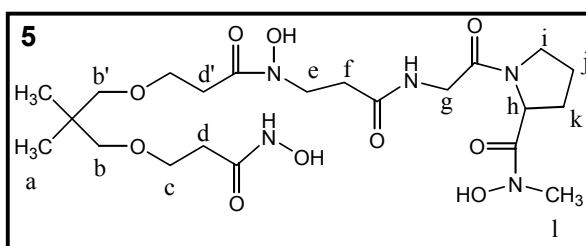
### General

$^1\text{H}$  NMR spectra were measured on an Avance DPX-250 MHz spectrometer (Bruker) using the solvent deuterium signal as an internal reference. All J values are given in Hertz. IR spectra were recorded on a Protégé 460 FTIR spectrometer. MS-ES was measured in the Chemical Service Unit (Dr. Ariyeh Tishbi) in WIS (Rehovot). Flash chromatography was performed using Merck 230-400 mesh silica gel.

### Selected Spectroscopic Data for final compounds 5-7:

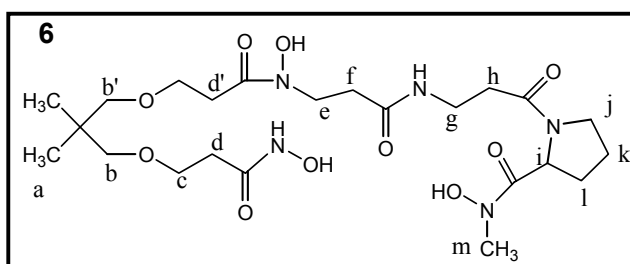
#### Compound 5:

$^1\text{H}$  NMR (400 MHz, d-MeOH)  $\delta$  5.05 (m, 1H, **h**), 4.22 (m, 2H, **e**), 3.92 (m, 2H, **g**), 3.55-3.69 (ov, 6H, **c** and **i**), 3.21 (s, 3H, **l**), 3.18 and 3.16 (s, 4H, **b'** and **b**), 2.73 (m, 2H, **d'**), 2.60 (t, J = 6.4 Hz, 2H, **d**), 2.33 (t, J = 6 Hz, 2H, **f**), 1.96-2.01 (m, 4H, **j** and **k**), 0.84 (s, 6H, **a**). **MS-ES**:  $m/z = 556.63$   $[\text{M}+\text{Na}]^+$ . **MS-ES** of **5-Fe(III)** = 609.44  $(\text{M}+\text{Na})^+$



#### Compound 6:

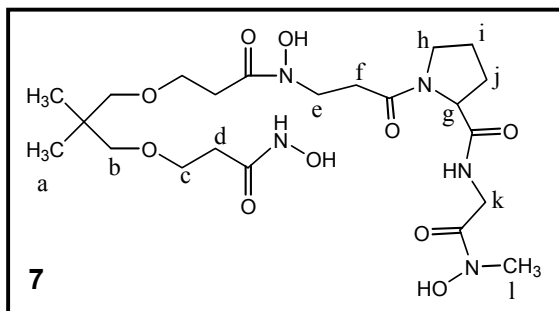
$^1\text{H}$  NMR (400 MHz, d-MeOH)  $\delta$  5.05 (m, 1H, **i**), 3.86 (m, 2H, **e**), 3.59-3.68 (ov, 6H, **c** and **j**), 3.40-3.45 (m, 2H, **g**), 3.23 (s, 3H, **m**), 3.19 and 3.17 (s, 4H, **b'** and **b**), 2.72 (t, J = 4 Hz, 2H, **d'**), 2.58-2.63 (m, 2H, **h**), 2.48 (m, 2H, **f**), 2.32 (t, J = 3.8 Hz, 2H, **d**), 2.20-2.27 and 1.88-1.95 (m, 2H, **k**), 1.96-2.02 (m, 2H, **l**), 0.84 (s, 6H, **a**). **MS-ES**:  $m/z = 570.65$   $[\text{M}+\text{Na}]^+$ . **MS-ES** of **6-Fe(III)** = 623.39  $(\text{M}+\text{Na})^+$



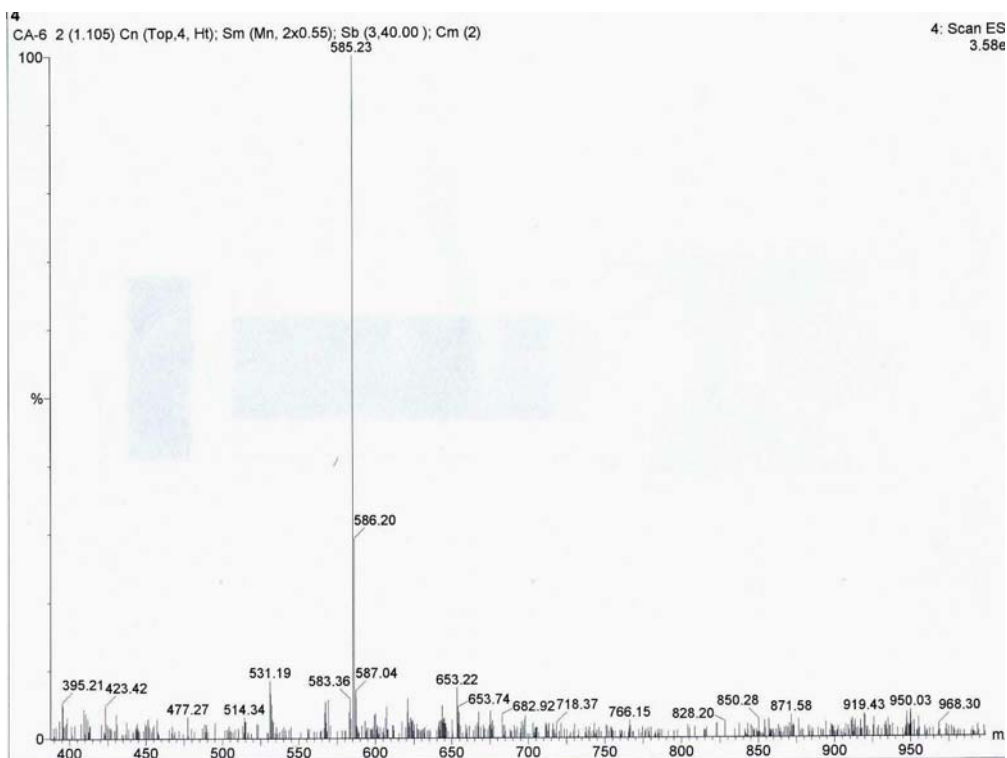
**Compound 7:**

$^1\text{H NMR}$  (400 MHz, d-MeOH)  $\delta$ , 4.52 (m, 1H, **g**), 4.19 (m, 2H, **e**), 3.95 (m, 2H, **h**), 3.69-3.76 (m, 4H, **c**), 3.53-3.61 and 3.37 (m, 2H, **k**), 3.24 (m, 1H, **l**), 3.21-3.24 (m, 4H, **b**), 2.70-2.81 (m, 4H, **d**), 2.37 (m, 2H, **f**), 1.96-2.42 (m, 4H, **i** and **j**), 0.88 (s, 6H, **a**).

**MS-ES:**  $m/z = 532.35$   $[\text{M}-\text{H}]^+$ . **MS-ES of 7-Fe(III)** = 609.38  $(\text{M}+\text{Na})^+$



**Mass spectrum (electrospray) of analog 5 with Fe(III):**



UV-VIS Titrations with Fe<sup>III</sup>: Figures S1, S2 and S3.

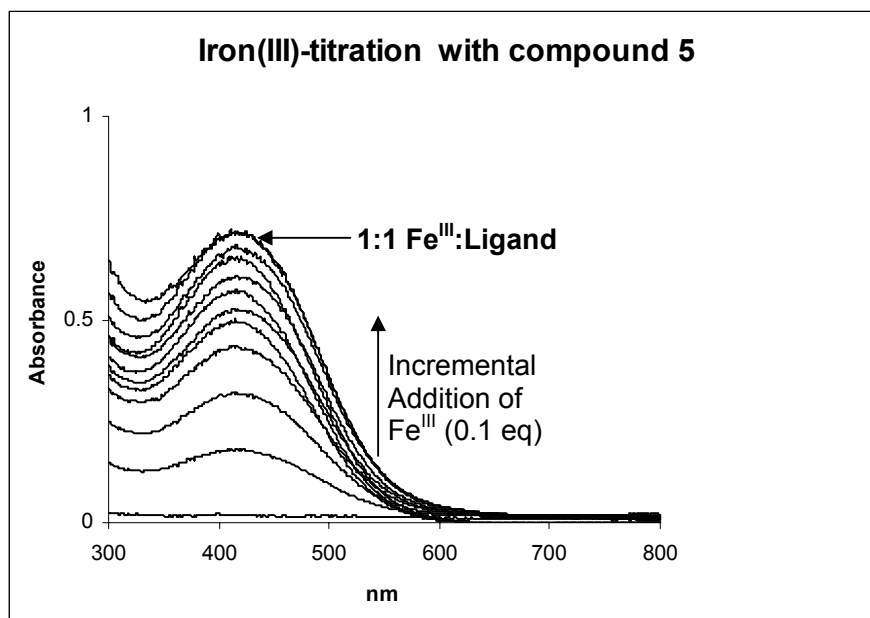


Figure S1

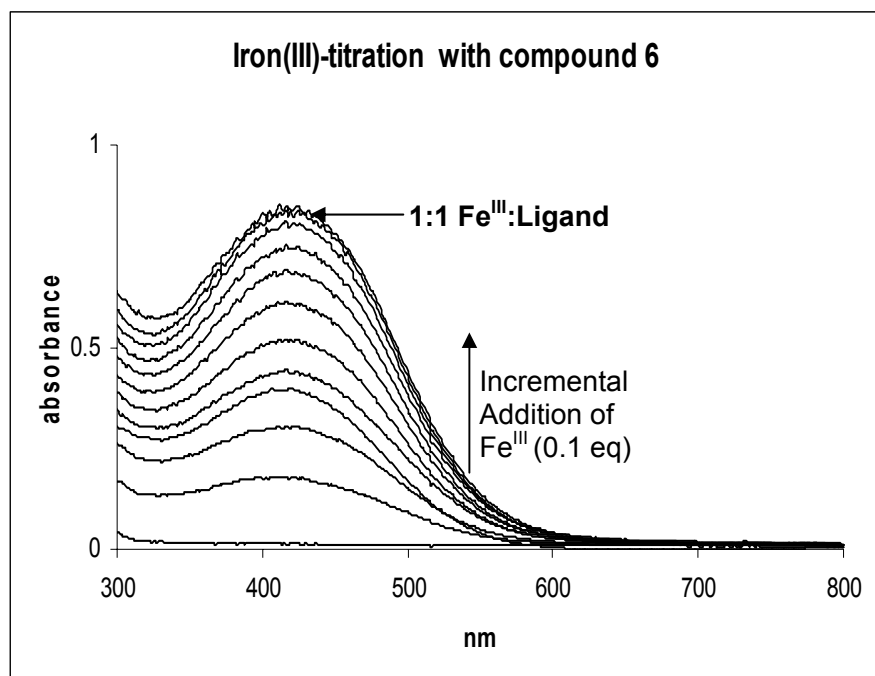
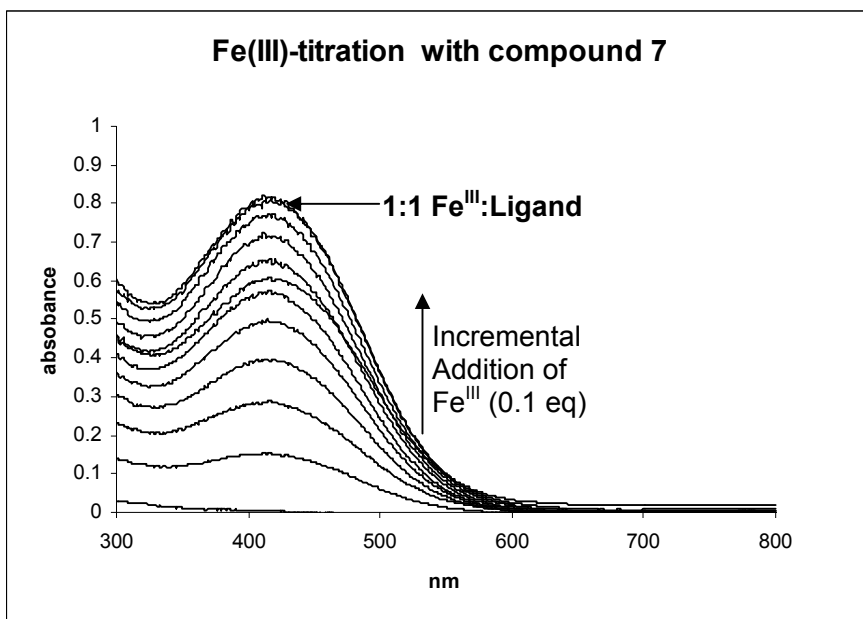


Figure S2



**Figure S3**

All titrations were carried out by adding 50  $\mu$ l aliquots of FeCl<sub>3</sub> (1 mM) to the 1mM solutions of the free ligand dissolved in MeOH (0.5 ml) and adjusting each sample to a final volume of 2 ml by adding a 0.1M NaOAc : MeOH solution (1:4). Spectrum saturates after addition of 1 equivalent Fe<sup>III</sup>, indicating the formation of a 1:1 Fe<sup>III</sup>:Ligand complex.