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 [M+Na]$^+$. MS-ES of 5-Fe(III) = 609.44 (M+Na)$^+$

![Compound 5](image)

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 [M+Na]$^+$. MS-ES of 6-Fe(III) = 623.39 (M+Na)$^+$

![Compound 6](image)
Compound 7:

$^1$H NMR (400 MHz, d-MeOH) δ, 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 [M-H]$^+$. **MS-ES** of 7-Fe(III) = 609.38 (M+Na)$^+$

Mass spectrum (electrospray) of analog 5 with Fe(III):
UV-VIS Titrations with $\text{Fe}^{\text{III}}$: Figures S1, S2 and S3.

**Figure S1**

Iron(III)-titration with compound 5

Incremental Addition of $\text{Fe}^{\text{III}}$ (0.1 eq)

**Figure S2**

Iron(III)-titration with compound 6

Incremental Addition of $\text{Fe}^{\text{III}}$ (0.1 eq)
All titrations were carried out by adding 50 µl aliquots of FeCl₃ (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 Fe³⁺, indicating the formation of a 1:1 Fe³⁺:Ligand complex.