Electronic Supplementary Information (ESI)

A novel probe for selective colorimetric sensing of Fe(II) and Fe(III) and specific fluorometric sensing of Fe(III): DFT calculation and logic gate application

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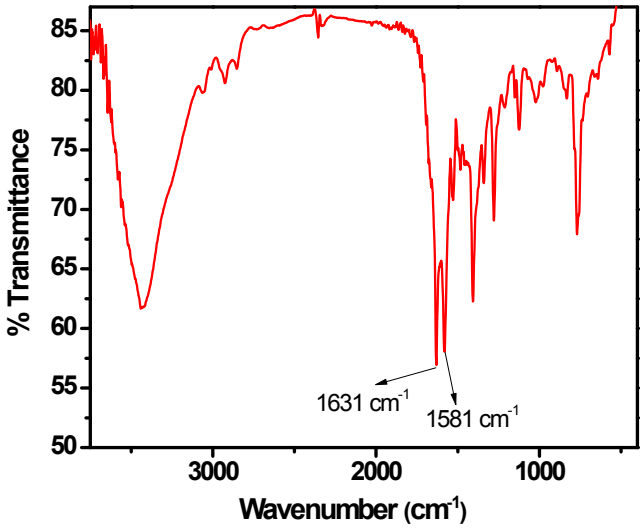

Fig. S1 IR spectra of probe **1**.

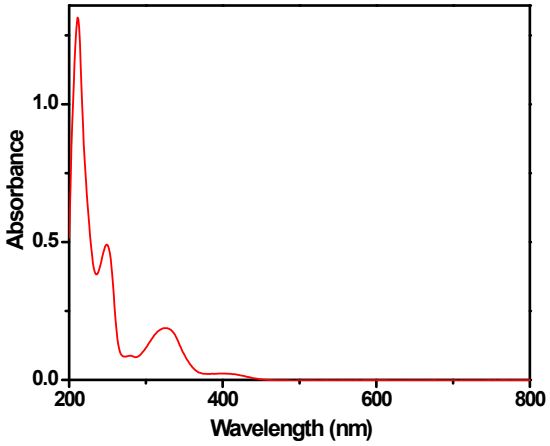

Fig. S2 UV-vis absorption spectra of probe **1** (20 μM) in methanol.

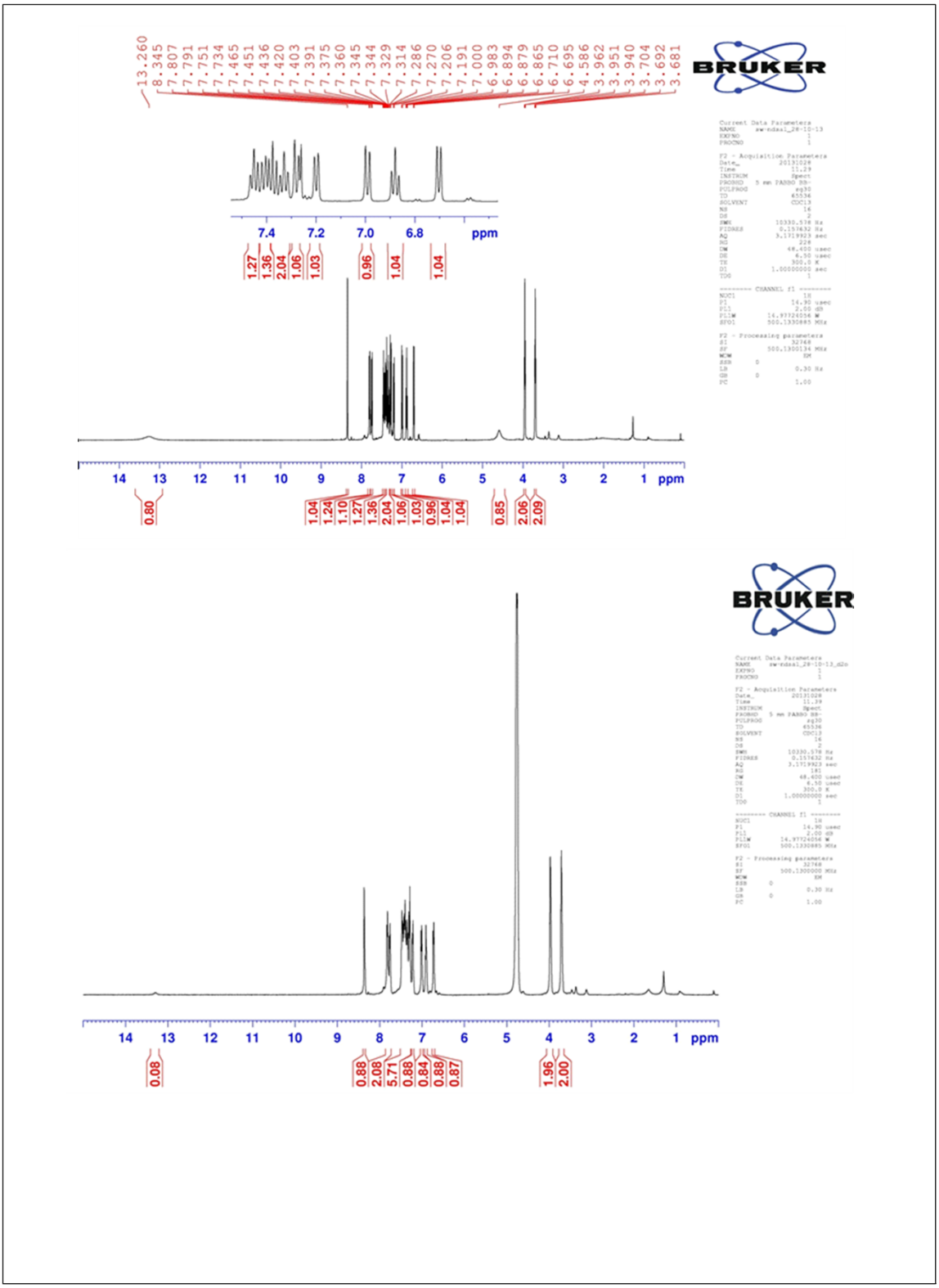

Fig. S3 (A) ^{1}H-NMR spectrum of probe **1** in $CDCl_3$. (B) ^{1}H-NMR D_2O exchange spectrum of

probe **1** in $CDCl_3$ at room temperature.

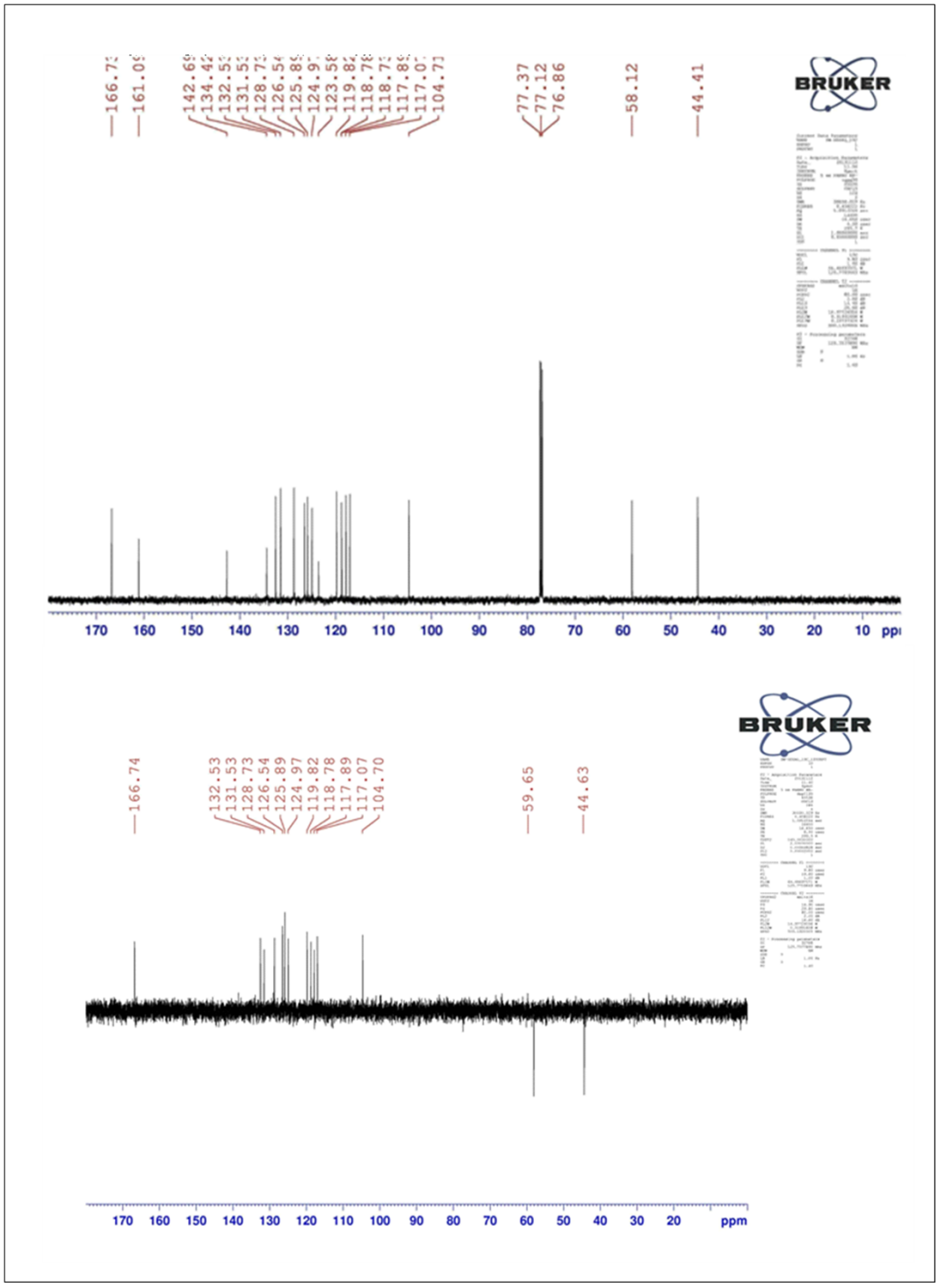

Fig. S4 (A) ^{13}C-NMR spectrum (B) ^{13}C-NMR 135 dept of probe **1** in $CDCl_3$ at room

temperature.

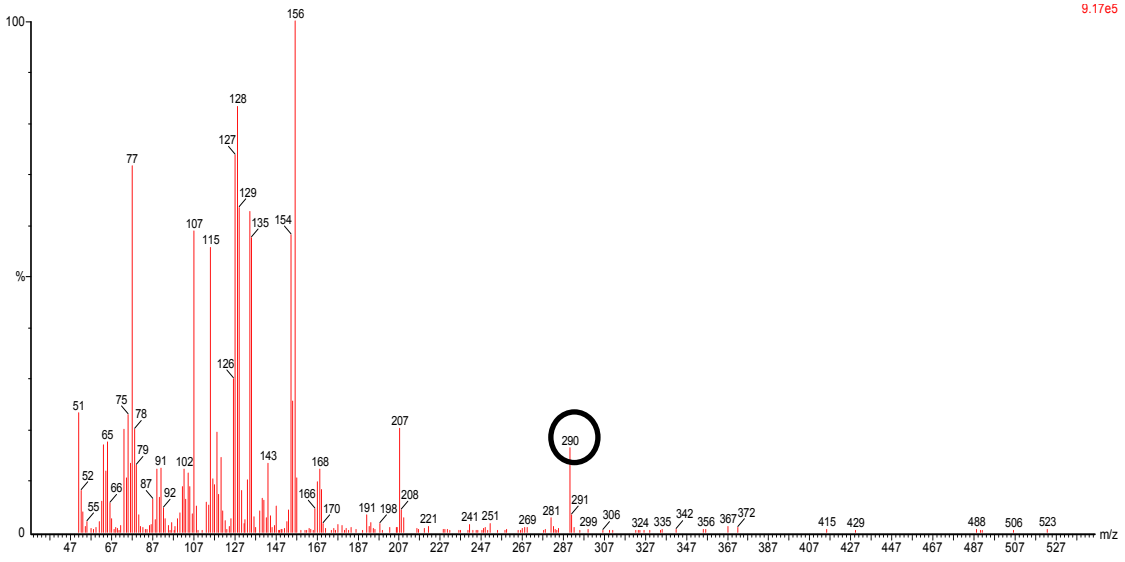

Fig. S5 GC-MS spectrum of probe **1**.

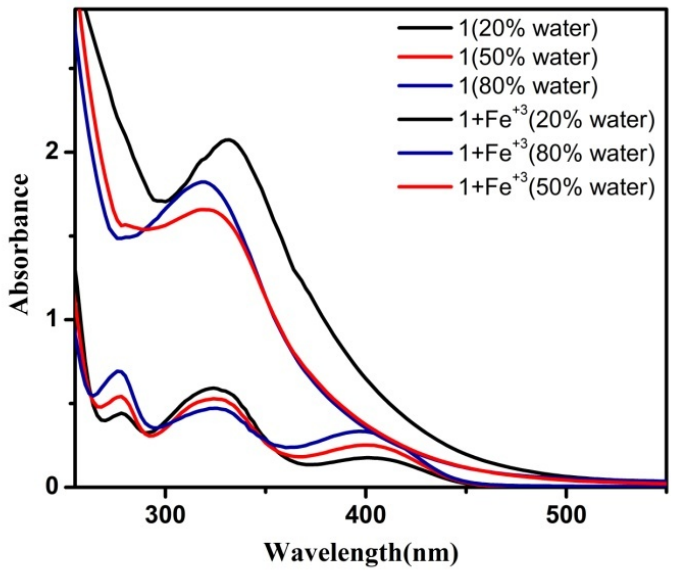

Fig. S6 Changes observed during absorption spectral studies of **1** (20 μM) and **1**+ Fe(III)

upon addition of different amounts of water in methanol.

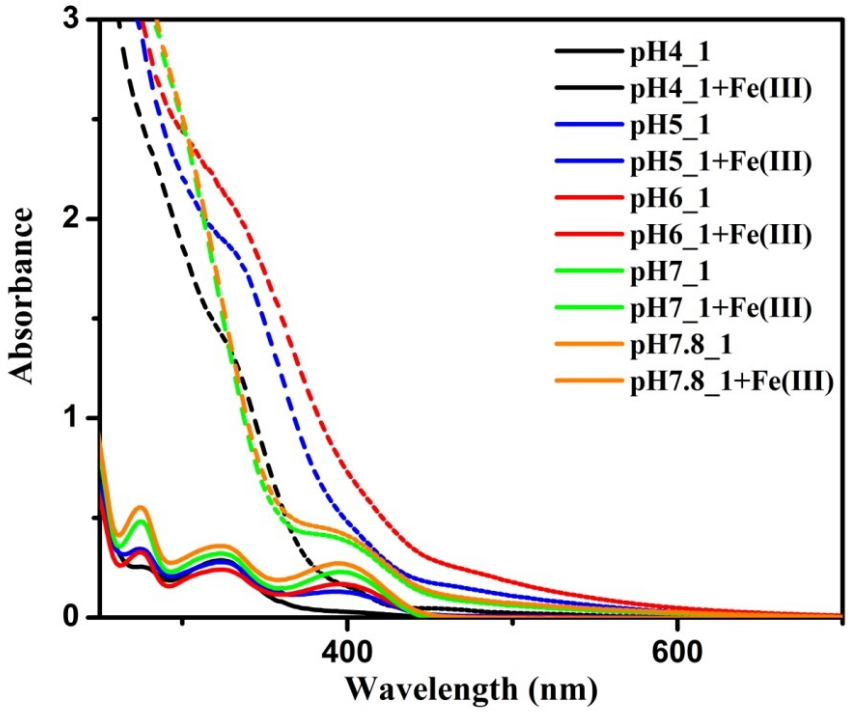

Fig. S7 Effect of pH during absorption spectral studies of 1(20 μM) and 1+ Fe(III) in water –methanol(4:1).

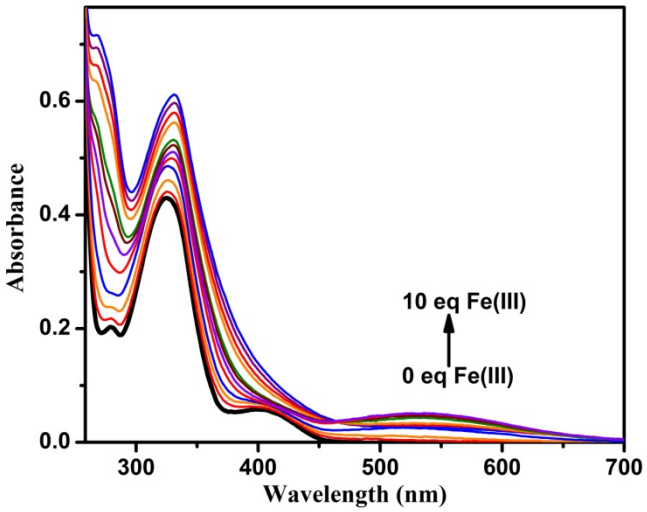

Fig. S8 Absorption spectra of **1** (5μM) upon addition of different amounts of Fe(III) in methanol.

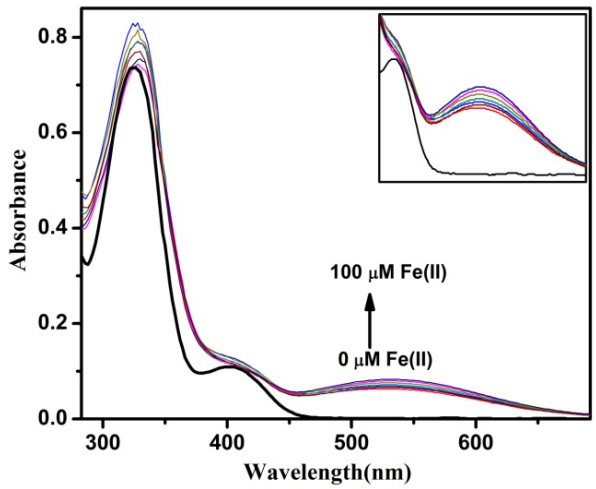

Fig. S9 Absorption spectra of **1** (5μM) upon addition of different amounts of Fe(II) in methanol.

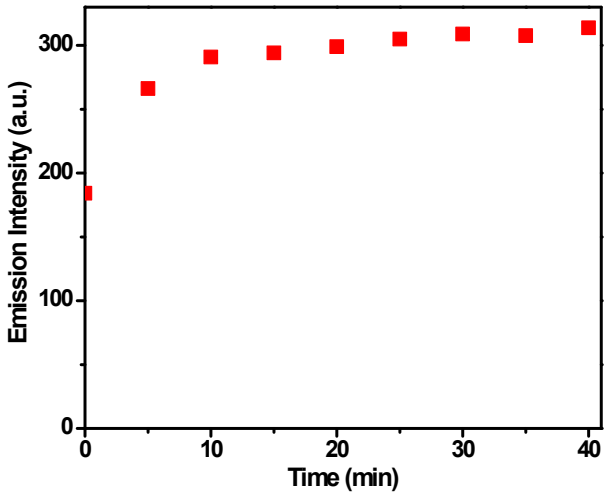

Fig. S10 Plot of emission intensity **1** (5×10^{-5}M) from 0 min to 40 min at λ_{ex} 320 nm.

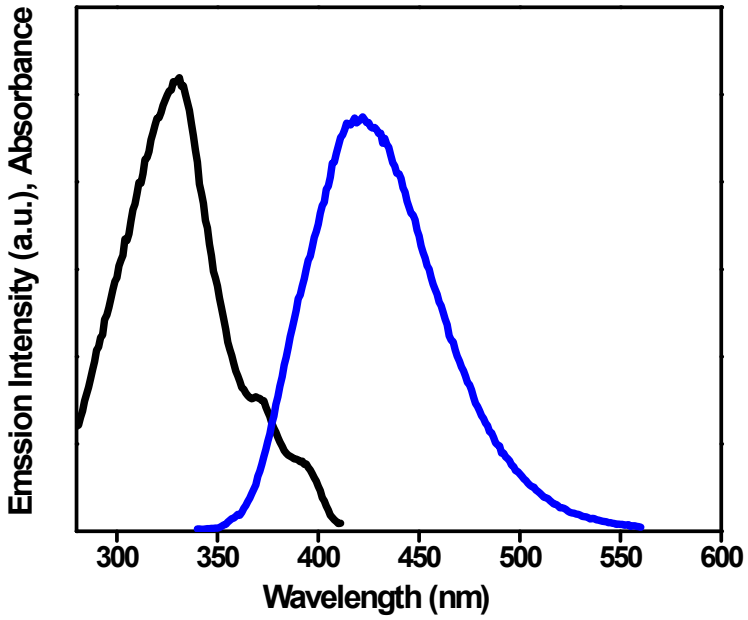

Fig. S11 Excitation spectra and emission spectra of probe 1 (50 μM) in methanol solution. Black line is the excitation spectra, and the blue line is the emission spectra. The maximum excitation and emission are at 330 nm and 420 nm, respectively.

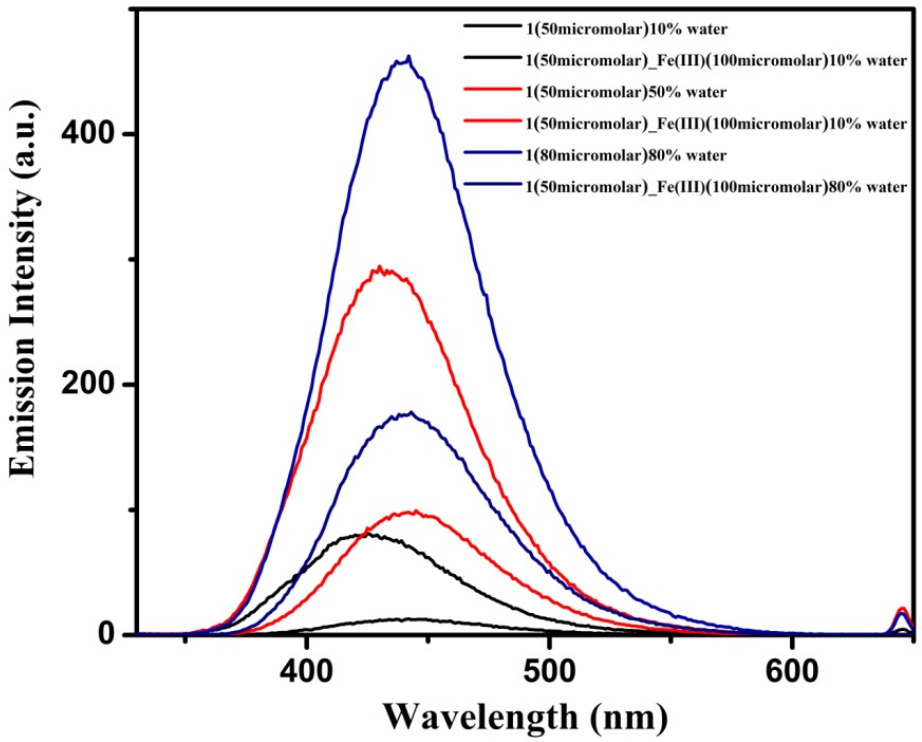

Fig. S12 Effect of pH during absorption spectral studies of **1** (20 μM) and **1** + Fe(III) in water –methanol(4:1).

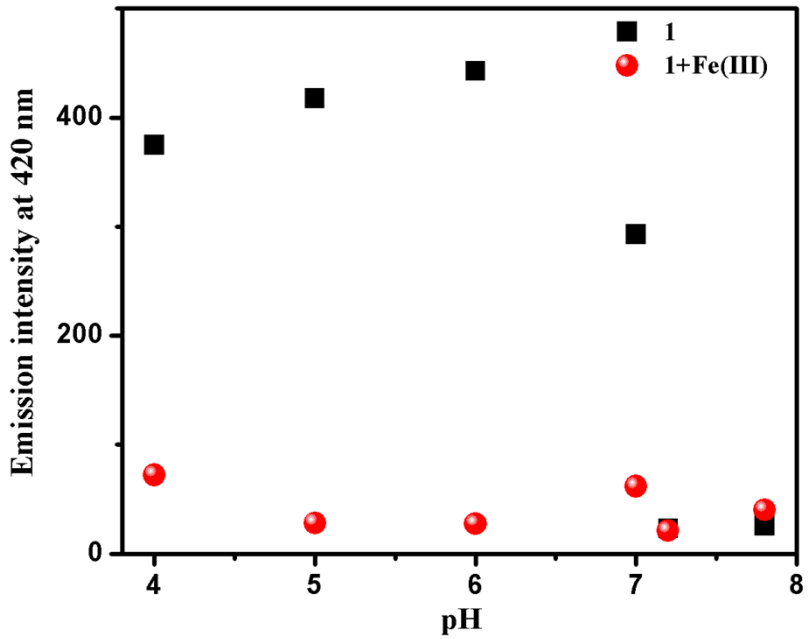

Fig. S13 Effect of pH during emission spectral studies of **1** (20 μM) and **1** + Fe(III) in water – methanol (4:1).

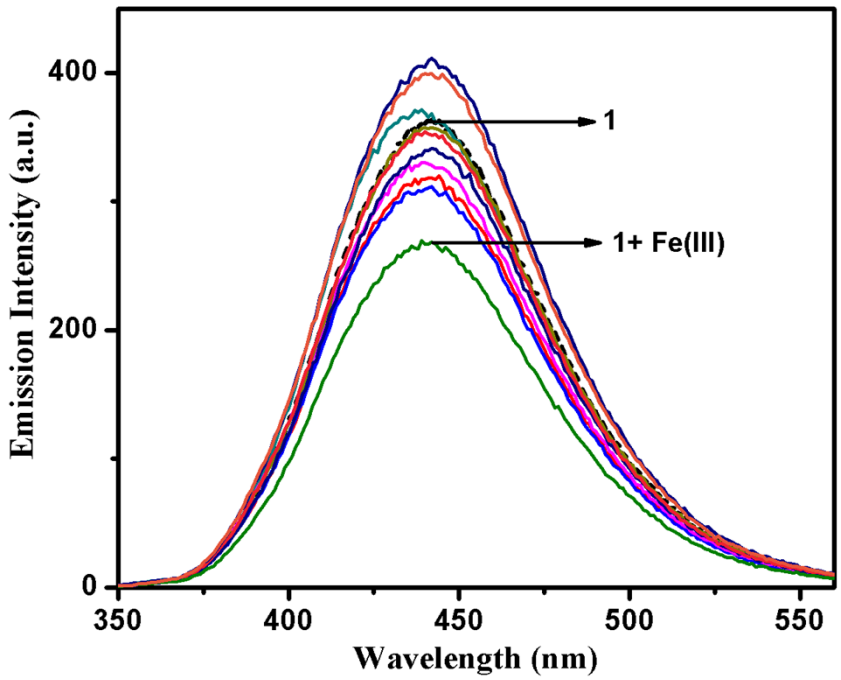

Fig. S14 Emission spectral studies of **1** (20 μM) and other representative metals in water – methanol (4:1).

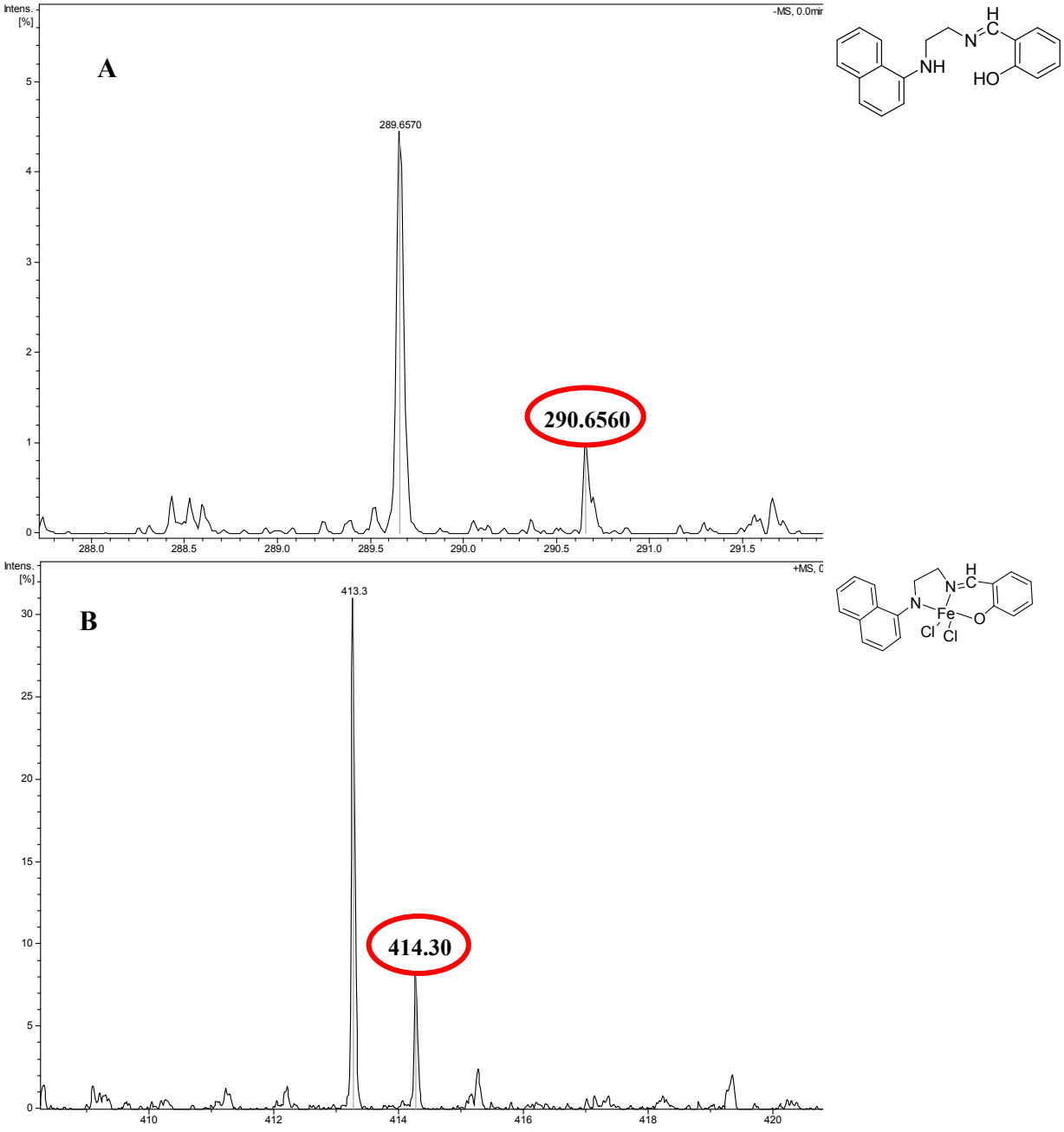

Fig. S15 ESI mass spectra of (A) **1** and (B) **1**+Fe (III) 10 eq in methanol-acetonitrile mixture.

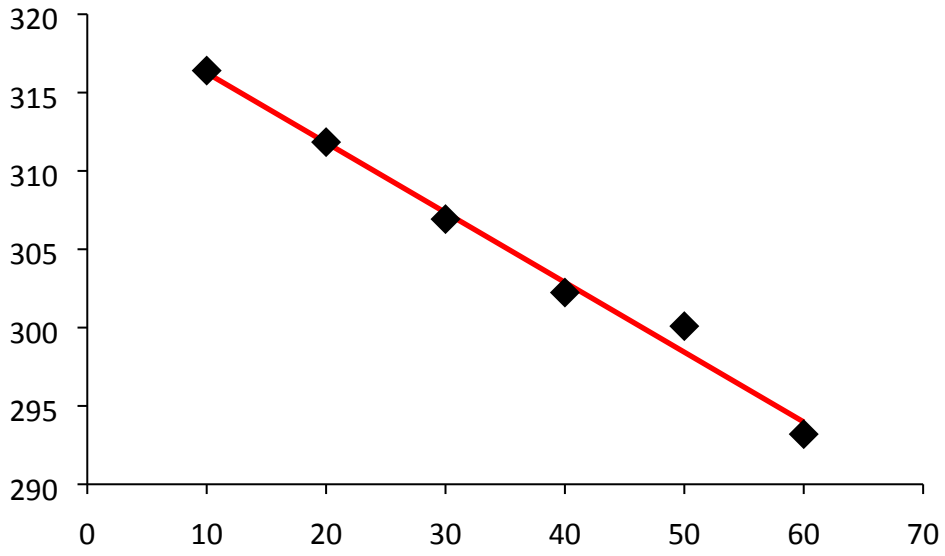

Fig. S16 Limit of detection calculated for a linear range of 10-60 μM at wavelength 426 nm.

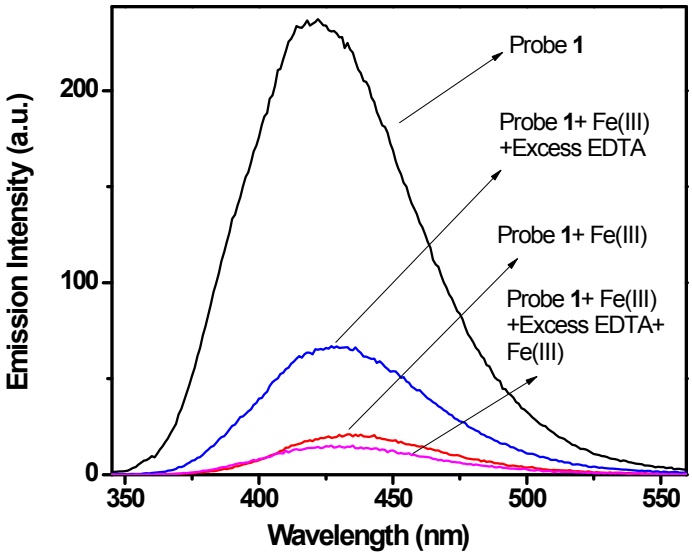

Fig. S17 Reversibility experiment from fluorescence spectra of probe **1** in the presence of Fe(III) with excess of EDTA methanol.