Supporting Information

Synthesis and Bioimaging of a BODIPY-based Fluorescence Quenching Probe for Fe³⁺

Junqiang Leng, Xinyu Lan, Shuang Liu, Wenxuan Jia, Wenshuai Cheng, Jianbo Cheng, Zhenbo Liu*

School of Chemistry and Chemical Engineering, Yantai University, Yantai 264005, P.R. China *Corresponding author. Email: zhenboliu@foxmail.com

Contents

Fig. S1. ¹H NMR spectrum of BODIPY-CL

Fig. S2. ¹³C NMR spectrum of BODIPY-CL

Fig. S3. ESI-MS spectrum of BODIPY-CL

Fig. S4. Effects of pH on the recognition of **BODIPY-CL** (10 μ M) for Fe³⁺ (50 μ M) under PBS/acetonitrile (8:2, v/v, pH = 7.4) buffer solution. $\lambda_{ex} = 371$ nm The data indicate the fluorescence intensities at 512 nm. Each datum was acquired 10 min after Fe³⁺ addition

Fig. S5. ESI mass spectrum of BODIPY-CL (10 μ M) with Fe³⁺ (10 equiv) with positive ion mode in acetonitrile solution

Fig. S6. Energy optimized structure for the Probe BODIPY-CL

Fig. S7. Theoretically obtained UV-visible spectra of the Probe BODIPY-CL

Fig. S8. Theoretically obtained fluorescence emission spectra of the Probe BODIPY-CL

Table S1. Energies of the molecular orbitals in eV for the probe BODIPY-CL



Fig. S1. ¹H NMR spectrum of BODIPY-CL.



Fig. S2. ¹³C NMR spectrum of BODIPY-CL.



Fig. S3. ESI-MS spectrum of BODIPY-CL.



Fig. S4. Effects of pH on the recognition of **BODIPY-CL** (10 μ M) for Fe³⁺ (50 μ M) under PBS/acetonitrile (8:2, v/v, pH = 7.4) buffer solution. $\lambda_{ex} = 371$ nm The data indicate the fluorescence intensities at 512 nm. Each datum was acquired 10 min after Fe³⁺ addition.



Fig. S5. ESI mass spectrum of BODIPY-CL (10 μ M) with Fe³⁺ (10 equiv) with positive ion mode in acetonitrile solution.



Fig. S6. Energy optimized structure for the Probe BODIPY-CL.



Fig. S7. Theoretically obtained UV-visible spectra of the Probe BODIPY-CL.



Fig. S8. Theoretically obtained fluorescence emission spectra of the Probe BODIPY-CL.

Orbitals	BODIPY-CL
НОМО	-0.19939
HOMO 1	-0.23974
HOMO 2	-0.24698
НОМО 3	-0.26370
LUMO	-0.08941
LUMO 1	-0.04418
LUMO 2	-0.02531
LUMO 3	0.03095
E _{LUMO} - E _{HOMO}	0.10998

Table S1. Energies of the molecular orbitals in eV for the probe BODIPY-CL.